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HYDROGEN ASSISTED DIESEL COMBUSTION

A Thesis in
Energy and Geo-Environmental Engineering

by

Gregory K. Lilik

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The thesis of Gregory K. Lilik was reviewed and approved* by the following:

André L. Boehman  
Professor of Fuel Science and Materials Science and Engineering  
Thesis Advisor

Harold Schobert  
Professor of Fuel Science

Angela Lueking  
Assistant Professor of Energy and Geo-Environmental Engineering

Daniel C. Haworth  
Professor of Mechanical Engineering

Yaw D. Yeboah  
Professor of Energy and Mineral Engineering  
Head of the Department of Energy and Mineral Engineering

*Signatures are on file in the Graduate School
ABSTRACT

In this study, the effect of hydrogen assisted diesel combustion on conventional and advanced combustion modes was investigated on a DDC/VM Motori 2.5L, 4-cylinder, turbocharged, common rail, direct injection light-duty diesel engine, with exhaust emission being the main focus. Hydrogen was substituted for diesel fuel on a percent energy basis of 0%, 2.5%, 5%, 7.5%, 10% and 15%. The conventional combustion modes studied consisted of four engine combinations of speed and load (1800 rpm at 25% of maximum output, 1800 rpm at 75% of maximum output, 3600 rpm at 25% of maximum output, and 3600 rpm at 75% of maximum output). A significant retarding of injection timing by the diesel fuel injection timing map in the engine’s electronic control unit (ECU) was observed during the increased aspiration of hydrogen. The retarding of injection timing resulted in significant emission reductions, however, the same emission reductions were achieved without aspirated hydrogen by manually retarding the injection timing. Subsequently, hydrogen assisted diesel combustion was conducted, with the pilot and main injection timings locked, to study the effects caused directly by hydrogen addition.

Hydrogen assisted diesel combustion resulted in a modest increase of NOX emissions and a NO / NO2 trade-off in which NO emissions decreased and NO2 emissions increased, with NO2 becoming the dominate NOX component in some circumstances. Increased aspiration of hydrogen resulted in PM, and HC emissions which fluctuated with speed and load. Predominantly, CO and CO2 decreased with the increase of
hydrogen. The aspiration of hydrogen into the engine modestly decreased fuel economy
due to the reduction of oxygen in the cylinder charge.

In the advanced combustion portion of the study, the engine was operated under a
partially-premixed charge compression ignition PCCI mode known as high efficiency
clean combustion (HECC), in which NO\textsubscript{X} and PM emissions dramatically decreased
while fuel economy was maintained. Hydrogen assisted diesel combustion was
performed while the engine operated in the HECC mode, which resulted in emissions and
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<tr>
<td>BSU</td>
<td>Bosch smoke unit</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
</tr>
<tr>
<td>CI</td>
<td>Compression ignition</td>
</tr>
<tr>
<td>COV</td>
<td>Coefficient of variance</td>
</tr>
<tr>
<td>CPC</td>
<td>Condensation particle counter</td>
</tr>
<tr>
<td>CRT</td>
<td>Continuously regenerating trap</td>
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<td>Differential mobility analyzer</td>
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<tr>
<td>ECU</td>
<td>Electronic control unit</td>
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<td>Engine gas recirculation</td>
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<td>Modulated kinetics</td>
</tr>
<tr>
<td>NMHC</td>
<td>Non-methane hydrocarbons</td>
</tr>
<tr>
<td>PAH</td>
<td>Polycyclic aromatic hydrocarbons</td>
</tr>
<tr>
<td>PCCI</td>
<td>Premixed charge compression ignition</td>
</tr>
<tr>
<td>PM</td>
<td>Particulate matter</td>
</tr>
<tr>
<td>PPM</td>
<td>Part-per-million</td>
</tr>
<tr>
<td>RCM</td>
<td>Rapid compression machine</td>
</tr>
<tr>
<td>RPM</td>
<td>Rotation per minute</td>
</tr>
<tr>
<td>RSS</td>
<td>Root-sum-square</td>
</tr>
<tr>
<td>SI</td>
<td>Spark ignited</td>
</tr>
<tr>
<td>SMPS</td>
<td>Scanning mobility particle sizer</td>
</tr>
<tr>
<td>SOF</td>
<td>Soluble organic fraction</td>
</tr>
<tr>
<td>SOI</td>
<td>Start of injection</td>
</tr>
<tr>
<td>SRDC</td>
<td>Smokeless locally rich diesel combustion</td>
</tr>
<tr>
<td>TCD</td>
<td>Thermal conductivity detector</td>
</tr>
<tr>
<td>TDC</td>
<td>Top-dead-center</td>
</tr>
</tbody>
</table>
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Chapter 1

Introduction

1.1 Motivation

Fears of dwindling oil reserves and new regulations on diesel engine emissions have driven research to focus on the use of alternative fuels. The utilization of alternative fuel diminishes the reliance on petroleum based fuel which is a step towards energy security. In this thesis, hydrogen was used as a supplemental fuel in a production diesel engine and thus replaced a portion of the diesel fuel demanded to produce engine output. The engine exhaust emissions, produced when hydrogen fuel was substituted for diesel, were of primary interest. By changing the fuel used to power an engine, the resulting engine-out emissions will change. However, as in the case of NO\textsubscript{X} emissions from biodiesel, the emissions resulting from alternative fuels may not be beneficial [1].

The literature review, presented in Chapter 2, on diesel pilot hydrogen ignition, indicates that hydrogen substitution is a promising method of reducing undesired exhaust emissions, especially at high rates of hydrogen substitution. The literature reports studies exclusively performed on small or single cylinder diesel engines. The hydrogen assisted diesel combustion studies in this thesis were performed on a DDC/VM Motori 2.5L, 4-cylinder, turbocharged, common rail, direct injection light-duty diesel engine. This engine was available in the European version of the Jeep Cherokee and Chrysler Voyager.
Advanced combustion modes, such as homogeneous charge compression ignition (HCCI) and premixed charge compression ignition (PCCI), are currently of interest to further reduce diesel emissions, specifically NO\textsubscript{X} and particulate matter (PM). As presented in the literature review of Chapter 2, HCCI and PCCI modes induce the engine to combust the fuel in the pre-mixed phase, resulting in a fuel lean charge and lowered combustion temperature, and thus, resulting in an engine operation away from zones of NO\textsubscript{X} and PM formation. In this thesis, the DDC 2.5L engine was operated on a particular PCCI mode, high efficiency clean combustion (HECC), developed by Wagner, Sluder and coworkers at Oak Ridge National Laboratory. This study represents the first published operation of the HECC mode outside of Oak Ridge National Laboratory. In novel experimentation, the DDC 2.5L engine was operated in the HECC mode while hydrogen assisted diesel combustion was performed, in hopes to further reduce NO\textsubscript{X} and PM emissions and reduce cycle-to-cycle variations, common to advanced combustion modes which rely on high percentages of exhaust gas recirculation EGR.

1.2 Objective and Hypothesis

The objectives of this work are to test the following hypotheses.

- A production diesel engine can utilize gaseous hydrogen fuel, via aspiration, in combination with diesel fuel with minimal modifications to the engine.
- The aspiration of hydrogen into a diesel engine will increase the pre-mixed combustion phase of a diesel engine, reducing NO\textsubscript{X} and PM emissions.
• Small quantities of aspirated hydrogen will have little effect on engine performance and emission.

• The HECC mode can be achieved using a production DDC/VM Motori 2.5L, 4-cylinder, turbocharged, common rail, direct injection light-duty diesel engine. While operating in the HECC mode, the addition of hydrogen to the combustion chamber will smooth-out the combustion process, quantified by the coefficient of variance (COV) of the indicated mean effective pressure (IMEP) and further reduce NOX and PM emissions.

Chapter 2

Literature Review

2.1 Diesel Combustion

Diesel engines are of interest due their higher efficiency in comparison to spark ignited (SI) engines. The diesel engine is named after Rudolph Diesel who first invented the engine in 1897. The diesel engine, also known as the compression ignition (CI) engine, operates under the basis of the diesel cycle. The idealized diesel cycle is a constant pressure heat addition cycle, which differs from the idealized Otto cycle of the SI engine in which heat addition occurs at a constant volume. Figure 2.1 displays the ideal diesel cycle.
The four processes of the diesel cycle shown in Figure 2.1 are [3]:

1 to 2 isentropic compression
2 to 3 constant pressure heat addition
3 to 4 isentropic expansion
4 to 1 constant volume heat rejection

The four processes of the diesel cycle are related to the four strokes (or stages) of the diesel engine given in Figure 2.2. However, for every four strokes of a diesel engine, there are two complete revolutions of the engine. During the intake stroke the piston moves down at which time, the intake values are open, drawing air into the cylinder. During the compression stroke, the intake valves close and the position travels to its apex known as top-dead-center (TDC), where the air undergoes isentropic compression. According to the ideal gas law, increased pressure causes an increase in temperature. The cylinder now contains compressed hot air. Diesel fuel is then injected into the cylinder. As the diesel fuel enters the cylinder it autoignites due to the high temperature and pressurized air. The combustion of the diesel fuel increases the in-cylinder temperature.

Figure 2.1: Pressure–volume diagram of an ideal Diesel cycle. [2]
and pressure which pushes the piston down during the expansion (or power) stroke. The piston then moves to the bottom of the cylinder. At this point the exhaust valves open as the cylinder moves back up to TDC forcing the exhaust gases out of the cylinder, for the exhaust stroke.

A key thermodynamic concept of the internal combustion (IC) engine is that air is the working fluid. An IC engine is an air pump. Thus, the torque and power rating of an IC engine are governed by the amount of air which can be forced into the cylinders. Therefore, turbochargers are used to increase the mass of the air charge in a diesel engine. In comparison to the SI engine, a CI engine operates at low RPM (rotation per minute). Thus, a CI engine at a given cylinder displacement will have a lower power rating than an SI engine of similar displacement.

Figure 2.2: Four-stroke engine cycle [4].
Typically, hydrocarbon fuels have been used to fuel IC engines. Complete combustion of hydrocarbon fuel occurs under stoichiometric conditions. The stoichiometric air-fuel ratio is the ratio of air to fuel where there is just of enough of both for complete oxidation of the fuel. The value of the stoichiometric air-fuel ratio is unique to every hydrocarbon fuel. In the generic formula for diesel fuel, \( C_{10.8}H_{18.7} \), the stoichiometric air fuel ratio is 14.33 g-air/g-fuel. Under stoichiometric combustion the maximum heat release for a given fuel is achieved [5]. Equation 2.1 and 2.2 display the generic formula for hydrocarbon combustion [6]. In this equation, complete combustion is assumed. The only products are CO\(_2\) and H\(_2\)O. To a first approximation, N\(_2\) in the air does not react but merely acts as an inert diluent.

\[
C_x H_y + a(O_2 + 3.76N_2) \rightarrow xCO_2 + (y/2)H_2O + 3.76aN_2 \quad 2.1
\]

\[
a = x + y/4 \quad 2.2
\]

Complete combustion, shown in Eq. 2.1, in which only CO\(_2\), H\(_2\)O and N\(_2\) are the products, never occurs in reality. Intermediate products are formed and incomplete combustion occurs due to the air-fuel mixture not being stoichiometric. Globally the air-fuel ratio of a CI engine is lean, but in local regions where combustion principally occurs, the ratio is rich. There will also be pockets of lean and stoichiometric combustion occurring. The equivalence ratio (\(\phi\)), defined in Eq. 2.3 [6], is used to express whether a mixture is rich or lean. Equivalence ratio is the ratio of the calculated stoichiometric air-fuel ratio over the actual air-fuel ratio.
Different products of incomplete combustion are created as the equivalence ratio locally shifts from lean to rich [6]. Equation 2.1 can be expanded to include products of incomplete combustion by adding the water-gas shift reaction, Eq. 2.4, to the equation. The result is Eq. 2.5, in which no dissociation to minor species is assumed.

\[
\phi = \frac{\left(\frac{A_F}{F}\right)_{\text{stoichiometric}}}{\left(\frac{A_F}{F}\right)_{\text{actual}}} = \frac{\left(\frac{E_A}{A}\right)_{\text{actual}}}{\left(\frac{E_A}{A}\right)_{\text{stoichiometric}}} \tag{2.3}
\]

Equation 2.5 is only a simple model, since an abundance of minor species are actually formed from the combustion of a hydrocarbon fuel. However, a more complex model requires computer software to account for the conditions such as pressure, temperature, and localized equivalence ratio along with the reactions that occur between all the intermediate species.

Equation 2.7 and Eq. 2.8 are derived from the simple model of Eq. 2.5. The equations display the different products of the reaction, which occur when the equivalence ratio is fuel lean and when the equivalence ratio is fuel rich (i.e., \(\phi>1\)). For \(\phi\) lean or stoichiometric:
For $\phi$ rich or stoichiometric:

\[
C_xH_y + a(O_2 + 3.76N_2) \rightarrow \quad \text{2.7}
\]

\[
bCO_2 + dH_2O + fO_2 + 3.76aN_2
\]

The conventional CI combustion process can be further explained by Figure 2.3, in which the rate of heat release from a directly injected diesel fuel is examined vs. crank angle. The diesel combustion process can be broken up into four different phases: ignition delay period, premixed combustion phase, mixing-controlled combustion phase, and the late combustion phase. The ignition delay period begins at the start of injection (SOI). During the ignition delay period, the rate of heat release drops below zero due to the fuel absorbing heat while vaporizing [1]. Next is the premixed combustion phase where a rapid rate of heat release occurs. The portion of the fuel which has mixed with air forms a combustible mixture and ignites. After all of the premixed air-fuel charge is consumed, the mixing controlled combustion phase begins. Here the combustion transitions from a premixed flame to diffusion flame. The rate of combustion is controlled by the fuel vaporization and mixing, in contrast to the fast burn of the kinetics-driven premixed flame. During the mixing-controlled combustion phase, the end of injection (EOI) occurs. In the late combustion phase, unburned fuel seeks oxygen as it is turbulently mixing throughout the cylinder [5].
Figure 2.3 indicates that, in conventional diesel operation, the majority of the heat release occurs during the mixing-controlled combustion phase and thus most emissions will be created in the mixing controlled phase. Dec furthered the understanding of the mixing-control combustion phase, in a sequence of laser diagnostic studies [7]. Dec developed a generalized explanation for the behavior of the combusting diesel jet. He described the structure of the diffusion flame, indicating the layers by equivalence ratio and concentration of soot which varies throughout the combusting diesel jet.

Westbrook later added detail to the generalized depiction of the diesel spray flame, Figure 2.4, to include approximate temperatures and indicated the regions in which NOX, CO2, H2O CO and UHC are produced [8]. This generalized description of
the diesel spray flames provides an excellent framework to explain the experimental observation of the diesel combustion process. The cold fuel enters the cylinder where it is vaporized by the hot compressed air. The fuel and air mix reach a combustible equivalence ratio at ~4 and reach autoignition at ~650K [9]. Temperature builds as equivalence ratio drops and oxidation increases. The inner region of the jet indicates incomplete combustion due to lack of oxygen, and the formation of soot precursors. The outer layers of the jet have near-stoichiometric equivalence ratios and generate high combustion temperatures as a consequence. The emissions generated in the diffusion flame, seen in Figure 2.4 are undesired products of incomplete combustion, and other pollutant formation pathways.
2.2 Nitrogen Oxide Emissions

Oxides of nitrogen, known as NO\textsubscript{x}, are of concern due to their health and environmental effects. NO\textsubscript{x} is a blanket term which refers to nitric oxide (NO) and nitrogen dioxide (NO\textsubscript{2}). 95% of engine emitted NO\textsubscript{x} is NO [5]. In the atmosphere, NO oxidizes into NO\textsubscript{2}. Unburned hydrocarbons and sunlight increase the rate of oxidation of
NO into NO₂. NO₂ is poisonous to the respiratory system causing both lung infection and respiratory allergies. NO₂ is toxic in levels greater than 0.05 ppm. [10]

NO₂ is also harmful to the environment. NO₂ affects the photochemistry of both the troposphere and stratosphere. Photochemical smog is formed in high traffic areas. NOₓ mixes with OH* and HO₂ radicals to form HNO₂ which forms acid rain [10].

NO usually accounts for the majority of the NOₓ produced from IC engines. NO can be formed by three different mechanisms which are the thermal or Zeldovich mechanism, the Fenimore or prompt mechanism, and the N₂O intermediate mechanism. [3] The Zeldovich mechanism produces the majority of NO in diesel engines. It occurs due to high combustion temperatures. The extended Zeldovich mechanism is given as:

\[ O + N₂ \rightarrow NO + N \]  \hspace{1cm}  \text{Equation 2.9}

\[ N + O₂ \rightarrow NO + O \]  \hspace{1cm}  \text{Equation 2.10}

\[ N + OH \rightarrow NO + H \]  \hspace{1cm}  \text{Equation 2.11}

Equation 2.9 is endothermic and has activation energy of +75.0 kcal. Equation 2.10 is exothermic and has an activation energy of +31.8 kcal. Equation 2.11 is exothermic and has an activation energy of +49.4 kcal.

NOₓ is formed in regions of the flame where there is enough energy for nitrogen to oxidize. NOₓ formation is thus governed by temperature and the availability of oxygen. Unfortunately, diesel engines operate under fuel lean conditions and produce high temperatures from diffusion flame combustion.
2.3 Particulate Matter Emissions

PM along with NOX are the most problematic diesel emissions. Particulate matter (PM) is of concern due to its effects on health. PM that has a diameter of 0.10μm can permeate through the lungs and cause numerous health problems. PM causes cancer, autoimmune disorders, alteration in blood coagulability and increased cardiovascular disorders [11].

PM is made of two main components: a solid carbon fraction, or soot, and a soluble organic fraction (SOF). Lubrication oils and water bound sulfates compose minor contributions to the total PM [12]. Figure 2.5 depicts the general layout of the components of PM.

Figure 2.5: Schematic of Diesel Particles and Vapor Phase Compounds, redrawn by Hess [12].
The organic fraction is made of unburned hydrocarbons that are absorbed by the soot or condense onto the soot along with lube oil and sulfates. Sulfates, however, are less of a concern with the recent mandate towards low sulfur fuels. Soot is produced in the locally fuel rich zones of a flame. The production of soot is a competition between formation and oxidation. Total particulate matter is a product of an incomplete combustion path. The PM formation path is a complex process in which the following steps are generally accepted: first aromatic ring (soot growth), polycyclic aromatic hydrocarbons growth (growth due to SOF), particle nucleation, and particle growth (growth due to SOF, lube oils and sulfates) [12].

In a recent review paper, Tree and Svensson discussed the current understanding of the soot formation process, which can be broken up into 6 steps: pyrolysis, nucleation, coalescence, surface growth, agglomeration and oxidation. In this process, liquid or vapor phase hydro-carbons form solid soot particles [13].

Oxidation of carbon can occur during any of the 5 formation steps, in that, once a carbon atom is partially oxidized, it will no longer be able to form soot. The pyrolysis step forms soot precursors known as polycyclic aromatic hydrocarbons (PAH), via a competition between fuel pyrolysis and oxidation of fuel, which both occur at high temperatures. Because of this competition, a diffusion flame will produce more soot than a premixed flame in which oxygen is readily available to mix with the fuel.

In the nucleation step, particles form from gas phase reactants. In this process, the precursor aromatic rings grow in the presence of acetylene to develop into particle nuclei. Surface growth is the process in which the nuclei soot particles gain mass by absorbing gaseous hydrocarbons. The size to which the soot particles grow is dependent on the
residence time of the particles. The final step of soot formation involves the agglomeration of the spherical soot particle. In this process the primary particles formed during surface growth combine together for form chains of particles [13].

Figure 2.6: Soot formation process from gas phase to solid agglomerated particles [13].

New regulations for diesel engine emissions have driven a shift in focus to advanced combustion modes and use of alternative fuels. The emission restrictions on NOX and PM have exponentially increased since the 1970’s. Figure 2.7 show the EPA heavy duty highway engine emissions standard from the 1970’s to present.
2.4 Carbon Monoxide Emissions

Carbon monoxide (CO) is of concern because it is poisonous to humans. CO enters the blood stream via the lungs through respiration. In the blood stream CO forms carboxyhemoglobin with the hemoglobin in the blood. The presence of
carboxyhemoglobin reduces the amount of oxygen available in the blood resulting in hypoxia and at high levels can cause death [15].

CO is directly linked to the air-fuel ratio. It is usually generated when there is a lack of oxygen. Diesel engines operate under a globally lean stoichiometry; however, there are still locally rich regions in the diffusion flame. The principal formation path of CO is given by Eq. 2.12, where R is the hydrocarbon radical [5].

\[ RH \rightarrow R \rightarrow RO_2 \rightarrow RCHO \rightarrow RCO \rightarrow CO \]  

2.12

CO emissions, like PM, are a result of a competition between formation and oxidation. However, the oxidation of CO has a slower reaction; the formation will win out under rich charge conditions. The oxidation of CO is given in Eq. 2.13.

\[ CO + OH \rightarrow CO_2 + H \]  

2.13

In addition, Dec and Sjoberg have shown that CO emissions at low loads increase as the equivalence ratio is lowered to between 0.1 to 0.12 [16]. This is logical since incomplete combustion occurs when the air-fuel charge is overly lean as well as overly rich.

2.5 Carbon Dioxide Emissions

Carbon dioxide (CO₂) is of concern because it is a greenhouse gas. However, it is also a direct product of hydrocarbon fuel combustion [5]. Rather than a pollutant emission due to incomplete combustion, CO₂ is a representation of fuel conversion
efficiency when viewed on a brake specific basis (per unit of net energy output) and represent the most desired final products, along with $\text{H}_2\text{O}$, from hydrocarbon combustion.

2.6 Unburned Hydrocarbon Emissions

Unburned hydrocarbon (HC) emissions are of concern because of their effect on health and the environment. Recall that some HC emissions contributed to the organic fraction of PM and are carcinogenic when absorbed by the body. HC emissions are broken into two categories, methane (CH$_4$) and non-methane hydrocarbons (NMHC). CH$_4$ has 21 times the greenhouse gas potential of CO$_2$ [17]. The NMHC are very reactive in the atmosphere and produce photochemical smog, which is an irritant to the respiratory system. Table 2.1 lists the reactivity of specific HCs [5].

<table>
<thead>
<tr>
<th>Hydrocarbon</th>
<th>Relative reactivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1-C4 paraffins</td>
<td>0</td>
</tr>
<tr>
<td>Acetylene</td>
<td></td>
</tr>
<tr>
<td>Benzene</td>
<td></td>
</tr>
<tr>
<td>C4 and higher molecular weight paraffins</td>
<td>2</td>
</tr>
<tr>
<td>Monoalkyl benzenes</td>
<td></td>
</tr>
<tr>
<td>Ortho- and para-dialkyl benzenes</td>
<td></td>
</tr>
<tr>
<td>Cyclic paraffins</td>
<td></td>
</tr>
<tr>
<td>Ethylene</td>
<td>5</td>
</tr>
<tr>
<td>Meta-dialkyl benzenes</td>
<td></td>
</tr>
<tr>
<td>Aldehydes</td>
<td></td>
</tr>
<tr>
<td>1-Olefins (except ethylene)</td>
<td>10</td>
</tr>
<tr>
<td>Diolefins</td>
<td></td>
</tr>
<tr>
<td>Tri- and tetraalkyl benzenes</td>
<td></td>
</tr>
<tr>
<td>Internally bonded olefins</td>
<td>30</td>
</tr>
<tr>
<td>Internally bonded olefins with substitution at the double bond</td>
<td>100</td>
</tr>
<tr>
<td>Cycloolefins</td>
<td></td>
</tr>
</tbody>
</table>
HC emissions are due to incomplete combustion and occur from four main sources. Fuel can disperse into regions of the cylinder where it is so locally fuel lean and/or cool that combustion cannot occur. A charge can be overly fuel rich and thus will not combust. Fuel can be trapped in the fuel injector and come out when it is too late to combust. Finally the fuel spray can penetrate to the cylinder wall where it penetrates crevices and mixes with the lubricating oil. On the cylinder wall, combustion of the fuel can be quenched by the cool temperature of the cylinder wall [3, 5].

2.7 Hydrogen

Hydrogen is of interest as a transportation fuel because it is a promising replacement to fossil hydrocarbons. The burning of hydrogen does not produce any carbon emissions, depending upon the source of the hydrogen. The zero emission combustion potential of hydrogen is displayed in, for stoichiometric combustion of hydrogen [5].

\[ H_2 + \frac{1}{2}(O_2 + 3.773N_2) \rightarrow H_2O + 1.88N_2 \] \hspace{1cm} 2.14

Unfortunately, pure diatomic hydrogen (H\(_2\)) is not found in nature. Rather energy much be consumed to generate diatomic hydrogen out of hydrogen containing molecules. For this reason hydrogen is often referred to as an energy carrier rather than a fuel [19].

Hydrogen can be produced by either reforming a hydrocarbon-based fuel or electrolysis. Methane, CH\(_4\), is the primary hydrocarbon fuel for reforming due to its high hydrogen content. Steam reforming of CH\(_4\) accomplished by the reaction in Eq. 2.15.
The water gas shift reaction, Eq. 2.16, is then used to produce CO₂ and hydrogen from the product CO [20].

\[ CH_4 + H_2O \leftrightarrow CO + 3H_2 \]  

\[ CO + H_2O \leftrightarrow CO_2 + H_2 \]  

Electrolysis, Eq. 2.17, produces hydrogen from electricity and water [21].

\[ H_2O_{(l)} + electricity \rightarrow H_2_{(g)} + \frac{1}{2}O_2_{(g)} \]  

Hydrogen production from steam methane reforming and electrolysis are not emission free. CO₂ is produced during methane reforming. The electricity used in electrolysis must be generated, which produces emissions depending on the fuel source.

Chui and coworkers conducted a life cycle analysis study to compare the possible pathways to produce hydrogen, based on steam methane reforming and electrolysis [21]. The 11 pathways to hydrogen production are given in Figure 2.8 and Figure 2.9. The life cycle analysis showed electrolysis with hydroelectric power to be the preferred path to hydrogen production.
Figure 2.8: Fuel stages for energy and technology types for hydrogen production [21].
2.8 Diesel Pilot Ignited Hydrogen Combustion

Hydrogen has an autoignition temperature of 858K requiring an ignition source to combust in an IC engine [22]. Diesel fuel which has an autoignition temperature of 525K can be used as a pilot to ignite hydrogen. The literature contains a body of work in which hydrogen was used in conjunction with diesel fuel to power CI engines. This dual-fuel combustion is often called diesel pilot-ignited hydrogen combustion. Diesel pilot-ignited hydrogen combustion at low quantities of hydrogen is beneficial since the diesel fuel is being replaced by hydrogen, which may stretch the supply of hydrocarbon fuels.
There is a range of emissions results reported on diesel pilot hydrogen combustion. This literature must be examined critically. The size, power output and rotational speed of the engine used in the studies skew these emission results. Lower emissions are achievable at the cost of de-rating an engine, to the point of unusable road performance.

Varde and Varde conducted some of the earliest work on hydrogen substitution [23]. The work was conducted on a 4.75 kW, single cylinder direct injection, naturally aspirated diesel engine. A pilot injection of diesel fuel was fixed at 22° BTDC and engine speed was fixed at 2400 RPM. The hydrogen was fumigated into the air intake. In this work, propane, natural gas and hydrogen were compared in “dual-fuel” combustion. The flows of the gases were reported by an H/C ratio, which included the diesel fuel. In the case of hydrogen, 15% of the total fuel energy was used as the maximum flow rate. A reduction of smoke was reported when hydrogen was introduced at a full rated load. A 50% reduction of smoke was reported at part load when 15% of the total fuel energy was hydrogen. Increasing the hydrogen at part load past 15% of total fuel energy was shown to increase soot levels, due to insufficient oxygen. NOX was seen to increase with hydrogen substitution at both part and full load. An increase of 30% NOX was reported at full rated load with 15% of the total fuel energy being hydrogen. HC levels were also seen to increase with increased flow rates of hydrogen at part and full load.

Lambe and Watson conducted a study in which they optimized a CI engine for hydrogen combustion with a diesel pilot [22]. A Petter PH1W, 6kW open chamber, naturally aspirated, direct injection, diesel engine was used in the study. A delayed port admission system was used to supply hydrogen. The system administered hydrogen via a secondary valve that allowed the flow of hydrogen into the cylinder when the intake
valve opened. Under high loads, an atomized water jet was administered to prevent curve knock. Hydrogen comprised 65% to 95% of the fuel energy. To accomplish such high fuel substitution levels, a minimum pilot diesel fuel quantity was first found. At low loads, lower efficiency was achieved running in a dual-fuel mode compared to running with diesel alone. At higher loads of 75% of maximum output the dual-fuel operation was more efficient than the diesel-only operation. Exhaust emissions were taken at 1000 RPM and 1500 RPM at unclear quantities of hydrogen (somewhere between 65% and 95%) and were compared to diesel-only combustion. At 1000 RPM and full load, smoke was reported to be reduced by 82% with dual-fuel combustion. At 1500 RPM and full load, smoke was reported to be reduced by 20%. NOX tended to increase at 1000 RPM under light loads, with dual-fuel combustion. At 1500 RPM NOX increased under dual-fuel combustion. CO2 emissions decreased for all loads under dual-fuel combustion. At 1000 RPM, CO2 decreased by 20%. At 1500 RPM, CO2 decreased by 85%. For both speeds, CO emissions decreased overall. HC emissions increased for both speeds. Nitrogen oxides were reduced by up to 70% in some cases. It was observed that combustion under dual-fuel operation is controlled by flame propagation rather than autoignition.

Tomita and coworkers investigated diesel and hydrogen dual-fuel combustion using a four-stroke, single cylinder, diesel engine with a single cylinder [24]. Injection timing was altered over a wide range of crank angles from 67.7 BTDC to 3.2 ATDC. Testing was conducted at 1000 RPM. The hydrogen as aspirated into the air intake. A pilot injection of diesel was used to ignite the hydrogen. Hydrogen flow rate was quantified in two ways, the total equivalence ratio and as the ratio of the hydrogen equivalence ratio over the total equivalence ratio. The equivalence ratio of diesel-only
and dual-fuel were made equal for comparison. Smoke was seen to decrease to near zero levels at all injection timings and at all equivalence ratios of hydrogen. NO\textsubscript{X} emissions dropped to zero at injection timings of 40\textdegree\ BTDC and earlier for all equivalence ratios of hydrogen. However, at timings later then 40\textdegree\ BTDC, NO\textsubscript{X} emissions increased over diesel-only combustion. HC emissions made only modest decrease with increasing hydrogen. CO\textsubscript{2} emissions decreased with increasing levels of hydrogen. Thermal efficiency was found to increase significantly at injection timings of 30\textdegree\ BTDC and earlier.

Kumar and Nagalingam investigated the performance increase of hydrogen on vegetable oil in a CI engine [25]. In this work, hydrogen-diesel combustion was also studied for comparison. The study was conducted on a Kirloscar AV1, single cylinder, four-stroke CI engine with a power rating of 3.7kW at 1500 RPM. The tests were conducted at 1500 RPM at 80\% and 100\% of maximum output. The diesel fuel was injected at 27 BTDC. The hydrogen was inducted into the air intake. Hydrogen flow rate was reported as “hydrogen mass share” given in equation Eq. 2.18.

$$\text{Hydrogen mass share} = \frac{m_{H2}}{m_{H2} + m_f} \quad 2.18$$

The hydrogen mass share used in their testing ranged between 0\% and 30\%, with 5\% reported to be the optimum hydrogen mass share. Justification for this was unclear. Brake thermal efficiency increased by 1.7\% at 100\% of maximum output. At 40\% maximum output, 5\% hydrogen mass share caused a 1.5\% reduction of brake thermal efficiency. The lower efficiency at 40\% of maximum output was reported to be due to insufficient diesel fuel to ignite the hydrogen. The smoke reduced from 3.9 BSU (Bosch...
smoke unit) to 2.7 BSU at 5% mass share and at 100% of maximum output. At 40% of maximum output, smoke dropped from 1.5 BSU to 1 BSU at 5% of hydrogen mass share. HC emissions reduced from 100 ppm to 70 ppm at 100% of maximum output at 5% hydrogen mass share. At 40% of maximum output, HC emissions decreased from 30 ppm to ~25 ppm, at 5% hydrogen mass share. CO emissions reduced from 20% to 0.14% at 100% of maximum output and 5% hydrogen mass share. At 40% of maximum output, CO emissions decreased from 0.9% to 0.6 %, at 5% hydrogen mass share. NO emissions increased from ~775 ppm to ~895% at 100% of maximum output and 5% hydrogen mass share. At 40% of maximum output, NO showed no significant variation at 5% hydrogen mass share.

In a fundamental study, Lu and coworkers conducted spectral analysis and chemiluminescence imaging hydrogen addition to a HSDI engine under conventional and low-temperature combustion [26]. The work was conducted on a rapid compression machine (RCM) with optical access, which operated at ~1000 RPM. Hydrogen was supplied to the cylinder along with the air. Hydrogen was added at a rate of 0%, 5%, 10% and 15% of the energy released. The LTC mode was based on 25% and 50% EGR and late injection timing. They reported that under mixing-controlled diesel combustion, small amounts of hydrogen had no significant effects on soot temperature, soot concentration or peak pressure. Under LTC, 15% hydrogen fuel energy led to increased soot concentration and soot temperature. The study also examined the OH radical to determine if it would burn part of the soot formed during early combustion. At 10% energy release from hydrogen, in LTC condition, the OH radical was found to further reduce soot concentration due to long residence timings.
The diesel pilot ignited hydrogen combustion literature varies in emissions results from study to study. Given the literature, diesel pilot ignited hydrogen combustion appears to be a promising method to reduce petroleum fuel consumption while achieving emissions reduction. However, these results must be qualified on a full size automotive diesel engine to validate the benefits associated with diesel pilot-ignited hydrogen combustion.

The findings in the published literature on hydrogen assisted diesel combustion are qualitatively presented in Table 2.2. The table indicates inconsistent results from the aspiration of hydrogen into a diesel engine, though it should be noted that the published studies consisted of a broad variation in testing conditions and parameters. A definitive study is thus necessary to clarify these inconsistent results.

Table 2.2: Qualitative results given in the literature on hydrogen assisted diesel combustion. Where + indicates an increase and - indicates a decrease in the given emission species or parameter.

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<tbody>
<tr>
<td>No&lt;sub&gt;x&lt;/sub&gt;</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>+</td>
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<td>Soot</td>
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<td>HC</td>
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<td>CO</td>
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<td>CO&lt;sub&gt;2&lt;/sub&gt;</td>
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<td>Brake thermal</td>
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<td>efficiency</td>
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<td>Ignition delay</td>
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<td>+</td>
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<td>Peak cylinder</td>
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<tr>
<td>pressure</td>
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2.9 Engine Gas Recirculation

Engine gas recirculation (EGR) is a technique used to reduce NO\textsubscript{X} emissions in compression ignition engines. EGR is accomplished by looping exhaust gas back into the intake manifold. The EGR level is controlled by a valve in the loop before the exhaust gas enters the turbocharger. The pressure differential between the exhaust and intake will limit the percent of EGR possible [28].

Engine gas recirculation reduces NO\textsubscript{X} emissions in two ways. CO\textsubscript{2} a major product of combustion and has a high specific heat. The high CO\textsubscript{2} content of EGR gas acts as a heat sink to reduce adiabatic flame temperature and thus reduce NO\textsubscript{X}. Secondly, circulation of EGR into the air intake dilutes the O\textsubscript{2} content of air. This reduces combustion temperatures and provides less O\textsubscript{2} to combine with N\textsubscript{2} to form NO\textsubscript{X}.

However, the reduction in O\textsubscript{2} content, moreover, the shift of air-fuel charge to a fuel rich ratio, increases PM production [5, 28, 29].

Exhaust gas recirculation percentage (EGR\%) can be quantified based on the volume percent of CO\textsubscript{2} in the ambient air intake air, and exhaust, as given in Eq. 2.19[29].

\[
EGR\% = \frac{CO_{2\text{Intake}}(vol\%) - CO_{2\text{Ambient}}(vol\%)}{CO_{2\text{Exhaust}}(vol\%) - CO_{2\text{Ambient}}(vol\%)}
\]

EGR decreases engine efficiency. Pump losses increase as EGR rates increase. The indicated work decreases as incomplete combustion increases, in the form of increased CO and HC emissions. Also, indicated work suffers from the reduced cylinder
temperatures. EGR is cooled using engine coolant to recover and prevent the loss of volumetric efficiency caused by fumigating the intake charge with excessively hot gases. However, cooling the EGR increases the losses from heat rejection [30].

Simulated EGR is also used in laboratory settings when large quantities of EGR rates are required. Bottled CO₂ typically is used to simulate EGR. However, results achieved from simulated EGR are somewhat skewed due to the lack of water vapor and combustible species present in actual EGR gas. Studies have been conducted to compare actual EGR to simulated EGR [28].

Large rates of EGR increase cylinder to cylinder variation [31]. Under high EGR conditions, individual cylinders do not receive uniform charges of EGR. This is due to the short mixing length between the point where the EGR meets the intake and a given cylinder. This will result in varying emissions from cylinder to cylinder [32].

2.10 Homogeneous Charge Compression Ignition

Homogeneous charge compression ignition (HCCI) combustion is an advanced combustion mode of interest due to its potential for low NOₓ and PM emissions while achieving high efficiency. HCCI utilizes advantages associated with spark ignition engines and compression ignition engines [33]

HCCI combines a homogeneous charge with a compression ignition combustion process. The homogenous mixture of HCCI is fuel lean and/or dilute. Combustion of the charge occurs globally without a propagating flame, resulting in combustion with local hotspots [34]. Fuel lean mixtures produce less PM due to the high rate of oxidization
occurring in the locally lean charges. The locally lower temperatures of HCCI produce less NOX. In contrast, the stratified diffusion flame, conventionally used in compression ignition engines, has layers of fuel rich zones where PM is created. Also, at the periphery of these fuel rich zones pockets of high temperature are present, which generate thermal NOX.

The stated efficiency of HCCI is higher than that of SI engines but equivalent to CI engines. The high efficiency derives from the reduction of pumping losses which are present when the intake air is throttled, such as in the case of stoichiometric SI engines [33].

Some obstacles still remain before HCCI will be realized in production applications. The largest problem facing HCCI is the requirement for an ignition control system with varying speeds and loads. The ignition timing is based on fueling rate and in-cylinder temperature. This is difficult to control in a transient state with varying power demands. Another challenge for HCCI is its lack of ability to operate in high load. At high loads HCCI combustion occurs rapidly causing increased levels of NOX, noise and possibly damage to the mechanical components of the engine. HCCI also does not work properly under cold start operation. The cold cylinder walls absorb the heat of compression preventing an HCCI engine from firing. HCCI produces excess amounts of CO and HC, which is an issue because catalyst technology does not work properly at low exhaust temperatures [35].
2.11 Partially-premixed Charge Compression Ignition

HCCI can be approximated in a CI engine by early fuel injection combined with high EGR. The acronym PCCI has been used in the literature on advanced combustion with multiple meanings. Neely and coworkers used PCCI to refer to premixed controlled compression ignition combustion, having an increased, advanced pilot injection, and a retarded main injection [36]. Kanda [37] and Araki[38] refer to PCCI as premixed charge compression ignition, in which diesel fuel is injected early. Sluder and coworkers refer to PCCI as partially-premixed charge compression ignition [39]. No matter what the PCCI acronym stands for, PCCI commonly refers to an advanced combustion process that allows for a large premixed burn. In PCCI, fuel is injected early into the cylinder, during which an ignition delay occurs until cylinder conditions are right for autoignition. During the ignition delay atomized diesel fuel mixes with air, creating a locally fuel lean charge. If injection of diesel fuel continues past the point of autoignition, the burn will transition from a premixed burn to a diffusion burn.

The contrast between HCCI and PCCI should be noted. The air-fuel charge in HCCI is homogeneous when it enters the cylinder. In PCCI, advanced injection of fuel leads to an extended premix-combustion phase. PCCI can be seen as an intermediate step between conventional diesel combustion and HCCI. The charge in PCCI is not mixed as well, thus there will be more hot spots. Also, since PCCI injects fuel via the diesel fuel injector, the long ignition delay may result in diesel fuel penetration to the cylinder walls, resulting in incomplete combustion. Like HCCI, PCCI suffers from increased HC and CO emissions related to the overly lean combustion conditions. However, PCCI permits
a practical route to approximate HCCI, because injection timing and EGR level can be used in concert to control ignition timing.

### 2.12 Low Temperature Combustion

Low temperature combustion (LTC) is a generic term that refers to an engine condition which operates below that required for the formation of NOX ($\phi<2.5, 2000K < T$) and/or PM ($\phi>~2.5, 1700K < T < 2400K$) [40]. Combustion temperature can be lowered by introducing EGR or by altering the combustion process to be locally fuel lean. These techniques can be used in tandem. EGR is used as a thermodynamic “dead weight” to reduce the rate of heat release in the cylinder. EGR is introduced into the cylinder by displacing the intake air. Thus, O$_2$ is reduced, which successfully reduces NOX. However, PM emissions increase due to the reduction in oxygen and the resulting inhibition of soot oxidation. HCCI-like conditions are coupled with EGR to reduce PM emissions. A well mixed air-fuel charge is locally fuel lean. A fuel lean charge will produce less heat and have more O$_2$ locally available to oxidize PM or prevent formation of PM.

The concept of LTC is best presented by a 3D-CFD model originally developed by Akihama and coworkers [40]. This map plots local equivalence ratio verses local flame temperature. The map provides insight into the NOX-PM trade off which is at the heart of diesel engine emissions. Figure 2.10 displays an updated version of Akihama and coworkers’ model.
LTC has been heavily explored with the recent onset of strict diesel emissions regulation. Here the most pertinent variations of LTC are discussed.

### 2.13 Smokeless Locally Rich Diesel Combustion

Smokeless locally rich diesel combustion (SRDC) was developed by Toyota [41]. The mode is entered by introducing extremely large amounts of cooled EGR (~60%). This lowers the air-fuel ratio to stoichiometric levels (~20 A/F ratio). However, the EGR decreases the local combustion temperature below the PM formation temperature. [40] [42] The concept of SRDC emissions reduction is summarized in Figure 2.11.

Figure 2.10: 3D-CFD model of local equivalence ratio vs. local temperature [36].
2.14 Modulated Kinetics

Modulated kinetics (MK) was developed by Nissan [27]. The MK condition is achieved by using single pulse fuel injection, retarding fuel injection after TDC, utilizing moderate levels of EGR (~30%) and increasing swirl [43]. The results of these modifications are increased ignition delay causing increased mixing of fuel and air. The concept of MK’s emissions reductions is summarized in Figure 2.12.
Modulated kinetics is stated to reduce NO\textsubscript{X} by the formerly mentioned methods [42]. EGR reduces the O\textsubscript{2} content and slows the heat release rate. Smoke or PM will increase with decreased levels of O\textsubscript{2}. PM is reduced via the premixed charge coupled with retarded injection timing and low temperatures to inhibit PM formation. MK is reported to produce increased levels of HC emission, SOF emissions and increased fuel consumption which are associated with HCCI-like modes. To combat these increases in some emissions, MK utilizes swirl which is augmented by piston configuration and fuel injection pressure [42].

Singh and coworkers conducted a study in which SRDC and MK were compared on a single cylinder high speed direct injection (HSDI) turbocharged engine. The study found that both SRDC and MK did reduce NO\textsubscript{X} and PM. However significant disadvantages offset the emission reductions. The MK mode neared the misfiring limit of the engine. HC emission and fuel consumption were found to be high due to late
combustion. The main disadvantage of SRDC is the high EGR requirement, which resulted in a fuel economy penalty. The study also found that increases in swirl and injection pressure could be used to further reduce NOX and PM. However these decreases would be offset by a penalty in fuel consumption [42].

2.15 High Efficiency Clean Combustion

High efficiency clean combustion (HECC) was developed at Oak Ridge National Laboratory. HECC, formally known as Efficient-LTC, is accomplished by a combination of single pulse injection, EGR (50%), early injection timing, and increased injection pressure. The EGR reduces NOX emissions and increases PM emissions. The early injection allows time for the diesel fuel to mix with air before combustion. Thus, an extended premixed combustion phase occurs, accompanied by a shorted mixing-controlled combustion phase. The premixed air and fuel are locally fuel lean, thus decreasing PM. As the premixed air-fuel charge is consumed, the combustion transitions to a diffusion burn. Increasing the injection pressure decreases the injection duration, which causes more fuel to be premixed and burned during the premixed combustion phase. The HECC mode provides a decrease in NOX emissions and PM emissions while maintaining or even increasing fuel efficiency. However, the HECC mode results in increased HC and CO emissions, which is common with HCCI-like modes [39, 44-49].

In a recent study Wagner, Sluder and coworkers, who developed the HECC mode at Oak Ridge National Laboratory, have shown the HECC mode to be operable at 1500 RPM at 1.0 bar IMEP, 1500 RPM at 2.6 bar IMEP, 2000 RPM at 2.0 bar IMEP and 2300
RPM and 4.2 bar IMEP. The tests were conducted on a modified Mercedes 1.7-liter, direct-inject diesel engine with cooled EGR. In all four of the engine conditions, NOX was reduced by more than 80% compared to the baseline. PM decreased between 30% - 50% and was even further decreased from 85% - 100% when the fuel injector nozzles were replaced to further increase atomization. HC levels doubled at the lowest speed and only slightly increased at the highest speed. The CO emissions double in three of the four conditions. The fuel consumption remained the same as the baseline for all four conditions. Figure 2.13 is a concept map that summarizes the techniques used to achieve the SRDC, MK and HECC LTC modes.

Figure 2.13: Concept map of various LTC modes.
2.16 Research Objective Identified via the Literature Review

The literature to date on the topics of hydrogen assisted diesel combustion and HECC contains gaps which require further experimental research. The gaps in the literature aimed to be filled by the work in thesis are as follows:

- To perform hydrogen assisted diesel combustion on a light-duty production diesel engine under laboratory conditions.
- To verify that the aspiration of hydrogen into a diesel engine will increase the pre-mixed combustion phase, decreasing NO\textsubscript{X} and PM emissions.
- To verify that small quantities of aspirated hydrogen will have little effect on engine performance and emissions.
- To demonstrate that the HECC mode can be achieved using a production DDC/VM Motori 2.5L, 4-cylinder, turbocharged, common rail, direct injection light-duty diesel engine.
- To demonstrate that while operating in the HECC mode, the addition of hydrogen to the combustion chamber will smooth-out the combustion process, quantified by the coefficient of variance (COV) of the indicated mean effective pressure (IMEP) and further reduce NO\textsubscript{X} and PM emissions.
Chapter 3

Experimental Setup

3.1 Engine Test Stand

A heavily instrumented DDC/VM Motori 2.5L, 4-cylinder, turbocharged, common rail, direct injection light-duty diesel engine was used for steady-state testing. Engine specifications are given in Table 3.1 and the general engine layout is given in Figure 3.1.

Table 3.1: DDC 2.5L Engine Specification.

<table>
<thead>
<tr>
<th>Engine</th>
<th>DDC 2.5L TD DI-4V Automotive Diesel Engine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement</td>
<td>2.5L</td>
</tr>
<tr>
<td>Bore</td>
<td>92 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>94 mm</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>17.5</td>
</tr>
<tr>
<td>Connecting Rod Length</td>
<td>159 mm</td>
</tr>
<tr>
<td>Rated Power</td>
<td>103KW@4000 RPM</td>
</tr>
<tr>
<td>Peak Torque</td>
<td>340Nm@1800 RPM</td>
</tr>
<tr>
<td>Injection System</td>
<td>Bosch electronically controlled common-rail injection system</td>
</tr>
<tr>
<td>Valve Train</td>
<td>4 valves/cylinder</td>
</tr>
</tbody>
</table>
A 250HP Eaton eddy current water-cooled dynamometer was coupled to the 2.5L DDC engine to generate load. The engine and dynamometer were controlled by a Digalog Testmate control unit.

### 3.2 Data Acquisition

Time-based data acquisition was managed using a custom programmed National Instruments LabView VI. Analog signals from pressure transducers, thermocouples, mass flow meters, and emissions data were read by a series of National Instruments FieldPoint modules, including a FP-2015, a FP-AO-210, a FP-DO-403, a FP-AI-102, a FP-AI-112 and three FP-TC-120 modules. The data collected by the FieldPoint modules were saved every 10 seconds during 15 minutes of sampling per test.
3.3 Electronic Control Unit Modification

The electronic control unit (ECU) is the computer that controls engine operation. An unlocked ECU was used to modify and control main injection and pilot injection timings, as well as, EGR valve position, and fuel rail pressure. The unlocked ECU was connected to an ETAS MAC 2 unit via an ETK connection. The MAC 2 unit was connected to a PC running ETAS INCA v5.0 software. INCA managed the ECU modifications in real-time.

3.4 EGR Operation

The DDC 2.5L engine regulates EGR rates using an ECU map based on engine speed and injection volume. The ECU map dictates the flow rate by varying the amplitude of the signal sent to a proportional pneumatic valve. The stock DDC 2.5L engine then introduces EGR to the intake manifold via a Y-pipe. The Y-pipe was modified to include a stainless steel tube which extended into the engine’s intake manifold, as given in Figure 3.2. CO₂ emissions were sampled from this tube, thus providing an accurate indication of CO₂ levels in the intake manifold charge.
It was necessary to aspirate simulated EGR into the engine’s air intake to achieve a well-mixed and high concentration of EGR charge (~50%). Bone-dry CO₂ with a purity of 99.8% was used as simulated EGR. The flow rate of the simulated EGR was monitored and regulated using an array of Matheson model 605 rotameters. The simulated EGR was aspirated after the charge air cooler, as seen in Figure 3.3.
The simulated EGR was dispersed and mixed with the boosted air using a custom built mixing manifold. The manifold consisted of four porous metal (Hastelloy) filters, customarily used as spargers, placed on the radial of the manifold. Two of the porous metal filters were used to inject simulated EGR. The other two porous metal filters were used to inject hydrogen gas. The manifold is seen in Figure 3.4.
3.5 Hydrogen Flow Rate Monitoring and Control

Hydrogen was supplied to the engine from a Structural Composites Industries 5000 psi 87.99L tank, which was located outdoors, adjacent to the testing facility. A diagram of the hydrogen delivery system is given in Figure 3.5. While the system was designed to withstand 2000 psi of hydrogen, only a 150 psi flow was necessary to achieve the required flow demands. The hydrogen delivery system was designed with redundant safety features, such as two pressure relief valves, and indoor and outdoor iTrans Fixed Point Monitors for hydrogen leak detection. This system also included a pneumatic tank...
shut-off valve, which would automatically close in the case of engine failure. Stainless steel (304) tubing and fittings were used to construct the hydrogen delivery system, which featured Swagelok fittings and valves. To prevent indoor leaks, weld connections were implemented when possible. Indoors, a fume hood was placed above the mechanical connections of the system to collect any leaking hydrogen.

A regulator and a needle valve were used to control the flow rate of hydrogen to the engine. Since the test plan called for a wide range of hydrogen flow rates, two mass flow meters of different ranges, were used to monitor the hydrogen. While a Sierra

Figure 3.5: Diagram of the hydrogen delivery system.
Instruments Toptrak model 820 mass flow meter monitored flows between 0-50slpm, a Teledyne Hastings Nall-P mass flow meter monitored flows between 50-200 slpm. The hydrogen was aspirated into the engine using the same method described for simulated EGR aspiration in Figure 3.3 and Figure 3.4.

3.6 Diesel Fuel Flow Rate

Diesel fuel consumption was measured using a Sartorius electronic microbalance. The custom LabView VI calculated diesel fuel consumption rates based on 100 measurements of fuel tank mass, tracking the small change in mass over 60 seconds.

3.7 Gaseous Emissions: AVL Combustion Emissions Bench II

An AVL Combustion Emissions Bench II was used to measure gaseous emissions. The bench was composed of six gas specific analyzers. Hot exhaust gases were sampled from the engine’s exhaust pipe by head-line filters, and then fed through heated lines kept at a constant temperature of 190 °C. NOX and NO were measured using an EcoPhysics chemiluminescence analyzer. NO2 was assumed to be the value of NO subtracted from NOX. Total hydrocarbons and methane were measured by using two separate ABB Flame Ionization detectors. CO and CO2 were measured by two separate Rosemount infrared analyzers, and O2 was measured by using a Rosemount paramagnetic analyzer. The hot exhaust sample going to the CO, CO2 and O2 analyzers was first chilled to reduce moisture.
3.8 Gaseous Emissions: GC

The hydrogen content of the exhaust gas was measured using a HP 6890 gas chromatograph (GC). The GC included a thermal conductivity detector (TCD) and a flame ionization detector (FID). Exhaust gas was supplied to the GC via a headline filter and heated sample line, kept at a constant 190°C. A 10ft (for TCD) and a 36ft (for FID) HayeSep D packed stainless steel, 100/125 mesh, 1/8” diameter column were used to concurrently analyze on-line permanent gases, water, and hydrocarbons. A factory set analysis method was used to examine exhaust samples. Argon was used as the carrier gas to pass the exhaust gas through the system, and flowed at 30 mL per minute for 16 minutes. The argon flow then ramped up to a rate of 60 mL per minute for 19 minutes. The GC initiated analysis at an oven temperature of -15°C for 17 minutes, and increased at a rate of 30°C per minute for 8 minutes. The GC then held to 255°C for 10 minutes, with a total sampling time of 35 minutes.

3.9 Particulate Matter Emissions: BG-1

Particulate matter was measured using a Sierra Instruments BG-1 Micro-Dilution test stand. The samples were taken at a dilution ratio of 10, a total flow rate of 110 slpm and a sample flow rate of 10 slpm over 5 minutes. The particulate matter samples were collected on Pallflex 90mm Filters, Type EMFAB TX40HI20-WW. The filters were weighed on a Sartorius M5P electronic microbalance, before and after sampling. The scale was located in an environmental chamber set at 25°C, with 45% relative humidity. The filters were placed in the environmental chamber 48 hours prior to mass analysis.
Five sample filters were taken per mode and the four sample fitters having the lowest standard deviation were averaged to represent the mass produced at a given mode.

3.10 Particulate Matter Emissions: SMPS

A TSI 3936 Scanning Mobility Particle Sizer (SMPS) was used to analyze the size distribution of the particulate matter. The SMPS instrument included a TSI series 3080 Electrostatic Classifier with a Differential Mobility Analyzer (DMA), a series 3776 Condensation Particle Counter (CPC), and a series 3065 Thermal Denuder. A PC running Aerosol Instrument Manager Software collected and managed the sampled data.

The BG-1 was used to draw and dilute samples from the exhaust. The BG-1 drew samples at a dilution ratio of 10, a total flow rate of 108.6 slpm and a sample flow rate of 100 slpm. The SMPS drew samples from the BG-1 at a rate of 1.4 slpm. The SMPS measurements were conducted using three different sample methods: passing the samples through the Thermal Denuder, passing the samples through the Thermal Denuder at 300°C and having the samples by-passing the Thermal Denuder. The sampling methods affected the content of the volatile hydrocarbon present on the particulate matter. A large number of samples (~6) should have been taken on the SMPS to correct for and average out the inconsistent residence timing of the exhaust samples in the dilation chamber of the BG-1. Unfortunately, due to the limited test time possible before the hydrogen tank emptied, only three SMPS data samples were taken during this study at each operating condition.
3.11 Cylinder Pressure Trace Analysis

Pressure traces were measured using AVL GU12P pressure transducers, which replaced the glow plug in each of the four cylinders. The pressure trace voltages from the pressure transducers were amplified by a set of Kistler type 5010 dual mode amplifiers. The amplified voltages were read by an AVL Indimodul 621 data acquisition system. Needle lift data were collected from a Wolff Controls Inc. Hall-effect needle lift sensor, which was placed on the injector of Cylinder 1. The needle lift signal was also collected by the Indimodul, which was triggered by a crank angle signal from an AVL 365C angle encoder placed on the crankshaft. The pressure traces and needle lift data were recorded at a resolution of 0.1 crank angle degrees, and were averaged over 200 cycles. The real-time Indimodual data were transferred to a PC, which ran AVL Indicom 1.3 and Concerto 3.90 to calculate the apparent heat release rate.

The apparent rate of heat release for each of the four cylinders was calculated from the volume and pressure trace data. The calculation is a built-in feature of Indicom/Concerto and is based on cylinder pressure. The algorithm neglects losses and assumes a polytropic coefficient of 1.37 for diesel fuel. The apparent rate of heat release algorithm is given in Eq. 3.1 [50].

\[
Q_i = \frac{K}{\kappa - 1} \left[ \kappa \cdot P_i \cdot (V_{i+n} - V_{i-n}) + V_i \cdot (P_{i+n} - P_{i-n}) \right]
\]

Where:

\( n \) is the interval (0.1 degree)
κ is the polytropic coefficient \( \kappa = \frac{c_p}{c_v} \) where \( c_p \) is the temperature at a constant pressure and \( c_v \) is the temperature at a constant volume of the fuel.

P is the cylinder pressure.

V is the volume.

### 3.12 Test Plan

This thesis contains two different studies, which both utilized hydrogen assisted diesel combustion. In the first study, hydrogen assisted diesel combustion was explored under four conventional steady-state operation modes, which are given in Table 3.2.

<table>
<thead>
<tr>
<th>3600 rpm (75% load)</th>
<th>3600 rpm (25% load)</th>
<th>1800 rpm (75% load)</th>
<th>1800 rpm (25% load)</th>
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<tr>
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<td></td>
<td></td>
</tr>
<tr>
<td>0% H₂</td>
<td>2.5% H₂</td>
<td>7.5% H₂</td>
<td>15% H₂</td>
</tr>
</tbody>
</table>

These four modes were chosen to provide a range of high and low loads at high and low speeds to examine the effect of hydrogen substitution on emissions and combustion behavior. In this study, the maximum rate of aspirated hydrogen substitution at a given mode was discovered, as seen in Table 3.3.
The second study examined the effect of hydrogen assisted diesel combustion on advanced combustion modes, given in the test matrix of Table 3.4. In this study, it was necessary to first locate an engine specific “HECC” mode, which was defined as providing simultaneous a reduction of NOX and PM while maintaining or increasing fuel efficiency. The criteria for the HECC mode were based on work by Wagner, Sluder and coworkers. A HECC operation mode is entered at a single pulse injection by advancing injection timing, increasing rail pressure, and increasing EGR to ~50%. The definition of “LTC” operation mode was also based on Wagner, Sluder and coworkers’ work, i.e. a ~50% EGR without any other modification from the Baseline mode at the same speed and load as the HECC mode. The Baseline mode was defined as the same speed and load as the HECC mode without any modifications.

<table>
<thead>
<tr>
<th>1800 rpm (75% load)</th>
<th>0% H₂</th>
<th>2.5% H₂</th>
<th>7.5% H₂</th>
<th>15% H₂</th>
<th>25% H₂</th>
<th>30% H₂</th>
<th>35% H₂</th>
<th>...% H₂</th>
</tr>
</thead>
</table>

Table 3.3: Test matrix for conventional combustion modes with hydrogen substitution on the basis of fuel energy percent, in which the maximum % hydrogen limit was found.

| ~50% EGR "HECC" |       |       |       |       |
| ~50% EGR "LTC"  |       |       |       |       |
| Baseline         |       |       |       |       |
| 0% H₂            | 2.5% H₂ | 7.5% H₂ | 15% H₂ |

Table 3.4: Test matrix for advanced combustion modes with hydrogen assisted diesel combustion on the basis of fuel energy percent.
Chapter 4

Discussion and Results of Conventional Combustion Modes with Hydrogen Substitution

4.1 Introduction

In this section the results of experimentation on hydrogen substitution of conventional diesel combustion modes are discussed. The hydrogen for diesel substitution rate was defined on the percentage energy basis. In an exploratory search, the maximum possible rate of hydrogen substitution was found for a given mode. For the 1800 rpm at 75% maximum output mode, 30% hydrogen substitution was found to be the operable limit. At 35% the engine simply shut down from being choked. There were no significant reductions in emission trends past the 15% substitution point, thus 15% hydrogen substitution was marked as the limit for rigorous testing.

Hydrogen was substituted for diesel in a span up to 15% on a fuel energy basis, in four unique modes. A level of 15% hydrogen substitution was also chosen because it is below the lower explosion limit of hydrogen in air, 4.1% volume, for all modes tested. Furthermore, increasing the hydrogen substitution past 15% would have required an excessive flow rate of hydrogen, rates nearing 200 slpm in high load modes.

Results of each of the four baseline test modes are compared on the basis of parameter change. The effect of hydrogen substitution is then reported and explained. Hydrogen substitution caused only modest changes in emissions. Many of the effects on
emissions were mode dependent. Though hydrogen caused a modest reduction in emissions, hydrogen can be substituted for diesel without penalty.

### 4.2 Mode Parameters

Table 4.1 lists the parameters of the modes explored in this study. These parameters are for the baseline mode (0% hydrogen on the fuel energy basis). Hydrogen substitution caused small changes to the EGR %, intake manifold gas temperature and the exhaust gas temperature parameters. The injection timing was electronically held constant by reprogramming the engine’s ECU. Speed and load were held constant by using a combination of dynamometer and engine controllers.

<table>
<thead>
<tr>
<th>Mode</th>
<th>Load (kW)</th>
<th>EGR (%)</th>
<th>Boost (bar)</th>
<th>Intake Manifold Gas (°C)</th>
<th>Exhaust Gas (°C)</th>
<th>Pilot Inj. (°ATDC)</th>
<th>Main Inj. (°ATDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1800 rpm @ 25% Max. Ouput</td>
<td>15.7</td>
<td>10.5</td>
<td>0.2</td>
<td>56.3</td>
<td>332.5</td>
<td>-17.4</td>
<td>2.9</td>
</tr>
<tr>
<td>1800 rpm @ 75% Max. Ouput</td>
<td>46.5</td>
<td>0.7</td>
<td>0.7</td>
<td>42.0</td>
<td>476.9</td>
<td>-38.3</td>
<td>-6.2</td>
</tr>
<tr>
<td>3600 rpm @ 25% Max. Ouput</td>
<td>26.1</td>
<td>1.4</td>
<td>0.9</td>
<td>70.3</td>
<td>247.9</td>
<td>-56.8</td>
<td>-12.3</td>
</tr>
<tr>
<td>3600 rpm @ 75% Max. Ouput</td>
<td>78.2</td>
<td>1.0</td>
<td>1.1</td>
<td>76.5</td>
<td>476.4</td>
<td>-58.1</td>
<td>-13.6</td>
</tr>
</tbody>
</table>

### 4.3 Hydrogen Substitution

Figure 4.1 displays the actual values of hydrogen substitution. The flow rate of hydrogen to be used for substitution was calculated from the diesel flow rate, which varies and shifts with the operation of the engine, even at steady state. There is slight variation of hydrogen percentage at the given points between modes. However, this
variation is small and the step changes in hydrogen percentage are large enough to ignore this discrepancy.

Figure 4.1: Actual hydrogen percentage energy substitution for the four modes tested, with [ ] 0%, [ ] 2.5%, [ ] 5%, [ ] 7.5%, [ ] 10% and [ ] 15% hydrogen substitution on an energy basis.

4.4 Needle Lift

The needle lift provides an indication of the injection timing and duration. The needle lift also indicated whether the injection timing had shifted. Three needle lift traces were taken at 1800 rpm at 25% maximum output without the addition of hydrogen. These three repeated needle lift traces are given in Figure 4.2.
Figure 4.2 indicates that the injection timing is indeed locked down. Though, the needle lift trials share a common profile, they vary in starting height. Figure 4.3 and Figure 4.4 are needle lift profiles with hydrogen substitution. Hydrogen substitution causes the absolute height of the needle lift to reduce. This indicates smaller volume of diesel fuel passes through the fuel injectors as hydrogen substitution increases. It is important to note that hydrogen substitution did not cause a shift in injection timing or injection duration.
Figure 4.3: Needle lift at 1800 rpm at 25% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.

Figure 4.4: Needle lift at 1800 rpm at 75% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.
4.5 Pressure Trace

Pressure traces were measured on all four cylinders. Apparent heat release rates for each cylinder were calculated from the pressure traces. Historically, there has been variation in pressure traces between the four cylinders of Penn State’s Detroit Diesel 2.5L TD DI-4V Automotive Diesel Engine. Mainly, the difference is due to the condition of individual piston rings of each cylinder. Piston rings prevent combustion gases from blowing by the pistons into the crank case. If the high pressure combustion gases pass by the piston rings, the pressure traces and the calculated apparent heat release rate will be affected.

As a result of the difference in cylinder pressure held by the piston rings, the completeness of combustion will vary from cylinder to cylinder. Incomplete combustion from a cylinder will increase emissions such as hydrocarbons, carbon monoxide and particulate matter. This incomplete combustion is further exacerbated when large amounts of EGR are introduced. The EGR will absorb energy released from the combustion process, reducing the rate of oxidation.

A variation in cylinder to cylinder pressure is to be expected. Figure 4.5 is the plot of the pressure trace for all four cylinders. Cylinder 3 is seen in this plot and others to be the representative average of pressure trace and thus of the heat release. Cylinder 3 will be used in plots when mode to mode comparisons are made.
Pressure traces indicate the in-cylinder pressure caused by combustion and volume change. Figure 4.6 to Figure 4.9 display the pressure traces from the four test modes, with hydrogen substitution. In general an increase of speed, and even more so, an increase in load will increase the combustion pressure. The maximum in cylinder pressure is desired to occur after top dead center so that energy from combustion will be released during the power stroke.

Optimum power release does not occur in the low speed modes, but does in the two high speed modes. The 1800 rpm at 25% maximum output mode has its maximum pressure peak occurring at top dead center. This means that a large pressure increase occurring before top dead center, which is fighting the piston’s travel during the compression stroke. The 1800 rpm at 75% maximum output condition has a delay in
pressure release. This too will cause a drop in efficiency. The pressure is being delayed from creating power during the power stroke.

Hydrogen causes the maximum in-cylinder pressure to increase in all four modes. The effect is greater in the high load modes, where more complete combustion of the fuel occurred. Also, in the high load modes, hydrogen causes the maximum pressure peak to occur earlier. The substitution of hydrogen for diesel fuel decreases the amount of diesel fuel injected in both the pilot and main injections. Hydrogen combusts as the premixed fuel is ignited by the diesel pilot injection. A large amount of fuel and thus pressure is released during the pilot injection. This pressure accumulates with the pressure from the main injection and leads to a higher maximum pressure.

Figure 4.6: Pressure trace at 1800 rpm at 25% maximum output, with 0%, 2.5%, 7.5% and 15%. Hydrogen substitution on an energy basis.
Figure 4.7: Pressure trace at 1800 rpm at 75% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.

Figure 4.8: Pressure trace at 3600 rpm at 25% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.
Figure 4.10 through Figure 4.13 display the apparent heat release rates of the four test modes with hydrogen substitution. The baseline apparent heat release rate of each of the four modes is different due to the load, speed and injection timing of the modes. In the case of the low speed modes a well defined apparent heat release rate from the pilot injection was seen. The combustion of the pilot injection fuel is known as the premixed combustion phase [5]. Here heat release is caused by the combustion of a premixed flame. Since the hydrogen is introduced into the cylinder during the intake stroke, no further hydrogen is available for combustion after the intake valve shuts. The bulk of the hydrogen is burned in the premixed combustion phase of the pilot injection. GC exhaust

Figure 4.9: Pressure trace at 3600 rpm at 75% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.
data indicated an increase of hydrogen in the exhaust as fumigated levels of hydrogen increase. This however is a small amount of unburned hydrogen which is analogous to unburned hydrocarbons seen in exhaust.

Figure 4.10 and Figure 4.11 show slight ignition delay in the premixed combustion phase, with increased levels of hydrogen. The diesel fuel acts as a pilot to ignite the hydrogen, since hydrogen as a lower cetane number then diesel fuel. Increasing levels of hydrogen slightly increase the apparent heat release rate of the premixed combustion phase. With the increase in hydrogen, less diesel fuel is injected. Thus, less heat is absorbed during the fuel vaporization phase between the premixed combustion phase and the mixing-control combustion phase of the main injection [5]. The heat release during the mixing-controlled combustion phase is decreased with the increase of hydrogen substitution. This is because less diesel fuel is injected during the main injection phase when hydrogen substitution occurs. Overall, the introduction of hydrogen has modest effects on the apparent heat release rates.
Figure 4.10: Apparent heat release rate at 1800 rpm at 25% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.

Figure 4.11: Apparent heat release rate at 1800 rpm at 75% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.
Figure 4.12: Apparent heat release rate at 3600 rpm at 25% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on a energy basis.

Figure 4.13: Apparent heat release rate at 3600 rpm at 75% maximum output, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.
4.7 Bulk Cylinder Gas Temperature

The temperature of the bulk cylinder gas was calculated from the pressure traces using the ideal gas law. Figure 4.14 displays the maximum in cylinder gas temperature for all four modes with 0%, 2.5%, 7.5% and 15% hydrogen substitution.

![Graph showing bulk cylinder gas temperature](image)

Figure 4.14: Maximum bulk cylinder gas temperature of the four modes tested, with 0%, 2.5%, 7.5%, and 15% hydrogen substitution on an energy basis.

The 1800 rpm at 25% maximum output mode has a bulk cylinder gas temperature nearing that of the other three modes even though it utilizes ~10% EGR, where the other modes utilize less than 2% EGR. The 1800 rpm at 25% maximum output mode would be expected to have a lower temperature since EGR lowers combustion temperatures [6]. Jacobs et al. explain that in the presence of EGR the bulk gas temperature will increase due to the increase in temperature of the intake charge and the decreasing of trapped mass.
[30]. Furthermore, Jacobs, et al. go on to say that flame temperature would therefore be a more accurate predictor of NO\textsubscript{X} formation than that of bulk gas temperature.

According to Figure 4.14, hydrogen makes less than a 0.5% difference in bulk cylinder temperature even at 15% energy input. According to the calculation of the cylinder bulk gas temperature, hydrogen makes relatively little change. To further understand what is occurring in the cylinder, adiabatic flame temperature must be considered. A complex model, outside the scope of this work, is necessary to calculate the adiabatic flame temperature, due to the consumption of the hydrogen fuel during the combustion of the pilot injected diesel fuel.

### 4.8 Exhaust Temperature

The exhaust temperature is examined in Figure 4.15. The exhaust temperature provides an indirect representation of the global combustion temperature. Enthalpy is removed from the exhaust gases by the turbocharger and EGR loop resulting in a reduced exhaust gas temperature. However, exhaust temperature will provide an indication of major alteration in combustion conditions and the engine’s mode of operation, which is useful to ensure repeatability of engine operation.
4.9 Equivalence Ratio

The equivalence ratio is defined as:

\[ \phi = \frac{(\frac{F}{A})_{\text{actual}}}{(\frac{F}{A})_{\text{stoichiometric}}} \]  \hspace{1cm} 4.1

Where \((\frac{F}{A})_{\text{actual}}\) is the actual fuel-air ratio and \((\frac{F}{A})_{\text{stoichiometric}}\) is the stochiometric fuel-air ratio. The actual fuel-air ratio was calculated in real-time based on flow rates of hydrogen, diesel and air.

The high load modes utilize a larger amount of fuel, which leads to a higher equivalence ratio. Also, the high speed modes have increased levels of air density, via the turbo charger. These reasons explain why each of the four modes have the baseline

![Figure 4.15: Exhaust temperature of the four modes tested, with hydrogen substitution on an energy basis.](image)
equivalence ratio given in Figure 4.16. For example, the low amount of fuel and high level of boost air in 3600 rpm at 25% maximum output mode, produces a noticeably lower equivalence ratio compared to the other modes.

The equivalence ratio is used to provide insight into the gaseous exhaust emissions. Increased levels of hydrogen cause an increasing trend in equivalence ratio. The increase in equivalence ratio is because the hydrogen is introduced into the engine via the air intake. By doing so, some portion of intake air must be displaced to give way to the hydrogen. In the 3600 rpm at 75% maximum output mode hydrogen is seen to decrease the equivalence ratio. This is due to the large level of boosted air, that has a greater effect on lowering the equivalence ratio than hydrogen does on increasing the equivalence ratio when hydrogen substitution occurs.

Figure 4.16: Equivalence ratio of the four modes tested, with □ 0%, ▲ 2.5%, ▼ 5%, ■ 7.5%, ▼▼ 10% and ■■ 15% hydrogen substitution on an energy basis.
4.10 Gaseous Emissions

Gaseous emissions are presented in brake specific units (g/kW\text{Output-hr}). They were also calculated in fuel energy specific units (g/kW\text{Fuel energy in-hr}). The fuel energy specific unit values yield plots with similar trends as those of the brake specific emission plots. Thus, the brake specific emission plots are presented.

4.11 Erroneous NO\textsubscript{X} Emissions Measurements

Injection timing was locked down during fuel substitution to prevent the engine’s ECU from shifting injection strategies. Locking down the injection timing is important because of the engine’s response to fuel substitution. During testing, the speed and load were held at constant values. As hydrogen levels increased, the engine throttled back diesel fuel to maintain a constant speed. The ECU’s injection strategy is based on engine speed and diesel fuel injection volume. The injection timing was manually held constant to prevent the injection strategy from moving to a later injection, when injected diesel fuel volume decreased. A shift in injection strategies will cause erroneous emissions and de-rate the engine.

Erroneous NO\textsubscript{X} emissions measurements due to a shift in injection timing are displayed in Figure 4.17. These erroneous emissions, with timing drift, are compared to the emissions with the injection timing locked. Brake specific NO\textsubscript{X} emissions are greatly reduced as hydrogen substitution increases and injection timing is allowed to drift to a late injection strategy. These large NO\textsubscript{X} emission reductions are not caused by the combustion of hydrogen. The emission reductions caused by the shift in injection timing
were recreated, without hydrogen substitution, by varying the injection timing to the
same shifted injection timing observed with hydrogen substitution. Figure 4.18 displays
the needle lift caused by the hydrogen substitution, when injection timing is not locked.

![Graph showing brake specific NOx emissions at 1800 rpm at 75% maximum output with injection timing allowed to drift and when locked down, with 0%, 2.5%, 5%, 15%, 25%, and 30% hydrogen substitution.](image)

**Figure 4.17:** Brake specific NOx emissions at 1800 rpm at 75% maximum output when injection timing is allowed to drift and when injection timing is locked down, with 0%, 2.5%, 5%, 15%, 25%, and 30% hydrogen substitution on an energy basis.

**Table 4.2:** Percent difference of brake specific NOx emissions from the baseline at 1800 rpm at 75% maximum output with 0%, 2.5%, 5%, 15%, 25%, and 30% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>1800 @ 75% with Timing Drift</th>
<th>1800 @ 75% with Timing Locked</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 % Diff.</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5 % Diff.</td>
<td>-6.6</td>
<td>0.4</td>
</tr>
<tr>
<td>5 % Diff.</td>
<td>-5.7</td>
<td>0.8</td>
</tr>
<tr>
<td>15 % Diff.</td>
<td>-17.2</td>
<td>1.1</td>
</tr>
<tr>
<td>25 % Diff.</td>
<td>-55.7</td>
<td>-0.9</td>
</tr>
<tr>
<td>30 % Diff.</td>
<td>-54.8</td>
<td>-2.7</td>
</tr>
</tbody>
</table>
Large reductions in NO\textsubscript{X} emission, reported in the literature to be caused by hydrogen substitution, are not due to hydrogen. The emissions reductions are from a shift in injection timing along the engine’s injection timing map. Thus, it would be necessary to reprogram a vehicle’s ECU to properly utilize hydrogen substitution with de-rating the engine when retrofitting a vehicle.

![Graph showing needle lift at 1800 rpm at 75% maximum output, with injection timing not locked, and with 0%, 15%, and 30% hydrogen substitution on an energy basis.](image)

Figure 4.18: Needle lift at 1800 rpm at 75% maximum output, when injection timing is not locked, with 0%, 15%, and 30% hydrogen substitution on an energy basis.

### 4.12 Gaseous Emissions: NO\textsubscript{X}

The 1800 rpm at 25% maximum torque mode has lower base levels of brake specific NO\textsubscript{X} due to the mode’s use of ~10% EGR. The other modes utilize less than 2% EGR, which accounts for the difference in base NO\textsubscript{X} levels. NO\textsubscript{X} emission increased slightly in all four modes with the introduction of hydrogen. Hydrogen substitution has its
greatest effect on the low load modes. In the high load modes, the increase caused by hydrogen is small and falls within the error bars. The largest increase of NO\textsubscript{X} occurs in the 3600 rpm at 25\% maximum output mode. This mode sees an increase of 9\% from the baseline with the substitution of 15\% hydrogen. NO and NO\textsubscript{2} must be examined to further explain and understand the NO\textsubscript{X} emissions.

Figure 4.19: Brake specific NO\textsubscript{X} emissions of the four modes tested, with □ 0\%, ■ 2.5\%, ■ 5\%, ■ 7.5\%, ■ 10\% and ■ 15\% hydrogen substitution on an energy basis.
Table 4.3: Percent difference of brake specific NO\textsubscript{X} emissions from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>1800 @ 25%</th>
<th>1800 @ 75%</th>
<th>3600 @ 25%</th>
<th>3600 @ 75%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 % Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5 % Diff.</td>
<td>3.0</td>
<td>0.9</td>
<td>4.3</td>
<td>-0.6</td>
</tr>
<tr>
<td>5 % Diff.</td>
<td>4.6</td>
<td>0.8</td>
<td>6.6</td>
<td>-0.3</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>3.4</td>
<td>1.0</td>
<td>7.8</td>
<td>1.3</td>
</tr>
<tr>
<td>10 % Diff.</td>
<td>2.5</td>
<td>1.0</td>
<td>7.7</td>
<td>2.0</td>
</tr>
<tr>
<td>15 % Diff.</td>
<td>1.8</td>
<td>1.6</td>
<td>9.0</td>
<td>3.1</td>
</tr>
</tbody>
</table>

4.13 Gaseous Emissions: NO

NO classically accounts for the largest contribution of NO\textsubscript{X}. Figure 4.20 displays the brake specific NO emissions from the modes tested. In comparison between the two high load modes and the two low load modes, the high load modes produce higher levels of NO. The increased levels of NO are thermal NO, produced from the increased heat release that occurs at high load conditions.

The two high load modes and two low load modes have similar magnitudes and trends, respectively. However, there is a slight discrepancy between the two low load modes. The 1800 rpm at 25% maximum output mode has a lower magnitude of NO compared to that of the 3600 at 25% maximum outputs. This again can be explained by the ~10% EGR used in the 1800 rpm at 25% maximum output mode.
Figure 4.20: Brake specific NO emissions of the four modes tested, with □ 0%, ▄ 2.5%, ▇ 5%, ▅ 7.5%, ▌ 10% and ▀ 15% hydrogen substitution on an energy basis.

Figure 4.20 shows a general trend of decreasing levels of NO with the increase of hydrogen. The decrease is more pronounced and even outside of the error bars in the case of the two low load modes. The higher load modes show a less significant decreasing trend that falls within the error bars after 2.5% hydrogen substitution.

Table 4.4 show that in the low loads modes, 2.5% of hydrogen substitution can reduce brake specific NO by 17%. Table 4.4 also points out that higher speeds are affected more by hydrogen substitution, than lower speeds.
4.14 Gaseous Emissions: NO₂

As with the case of brake specific NO emissions, the high speed modes produce similar magnitudes of brake specific NO₂ emissions. However, the low speed modes again produce a dissimilar amount NO₂. To explain this discrepancy the production of NO₂ must be examined.
The major path in the production of NO$_2$ is from NO [51]. This path is given in Eq. 4.2.

$$NO + HO_2 \leftrightarrow NO_2 + OH \quad 4.2$$

The HO$_2$ is produced from the increased levels of hydrogen. Glassman states that the most probable initial step in the combustion of oxygen and hydrogen is [52]:

$$H_2 + O_2 \leftrightarrow HO_2 + H \quad 4.3$$

With the path from NO to NO$_2$ in mind, the difference in magnitude between the low load conditions can again be explained by the $\sim$10% of EGR used in the 1800 rpm at 25% maximum output mode. There is more NO available in the 3600 rpm at 25% maximum output mode to be converted to NO$_2$.

Figure 4.21: Brake specific NO$_2$ emissions of the four modes tested, with $\square$ 0%, ■ 2.5%, □ 5%, ■ 7.5%, □ 10% and ■ 15% hydrogen substitution on the energy basis.
Table 4.5: Percent difference of brake specific NO$_2$ emissions from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>1800 @ 25%</th>
<th>1800 @ 75%</th>
<th>3600 @ 25%</th>
<th>3600 @ 75%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 % Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5 % Diff.</td>
<td>53.3</td>
<td>72.1</td>
<td>28.6</td>
<td>105.1</td>
</tr>
<tr>
<td>5 % Diff.</td>
<td>68.0</td>
<td>87.1</td>
<td>41.5</td>
<td>124.9</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>70.8</td>
<td>85.8</td>
<td>47.9</td>
<td>135.4</td>
</tr>
<tr>
<td>10 % Diff.</td>
<td>70.2</td>
<td>94.8</td>
<td>51.5</td>
<td>139.6</td>
</tr>
<tr>
<td>15 % Diff.</td>
<td>74.8</td>
<td>90.2</td>
<td>56.6</td>
<td>139.1</td>
</tr>
</tbody>
</table>

Table 4.5 displays the percent difference of the increase of NO$_2$ caused by the hydrogen substitution. Since the baseline values of NO$_2$ are initially very low, the effect caused by hydrogen is quite dramatic. Figure 4.22 shows the transition from NO being the dominant contributor to NO$_X$, to NO$_2$ being the dominant contributor to NO$_X$, due to hydrogen substitution, in the case of 3600 rpm at 25% of maximum output. A shift in NO$_X$ species also occurs in the 1800 rpm at 25% of maximum output mode; however the NO$_2$ does not overcome the NO, as in the case presented in Figure 4.22. This is due to the EGR in the 1800 rpm at 25% of maximum output mode. A slight shift in NO$_X$ species occurs in the high load modes as well, but this shift is small compared to that of the low load modes.
The conversion from NO to NO\(_2\), due to hydrogen substitution, is beneficial even though NO\(_X\) levels increase. NO\(_2\) is used as the oxidizer in Continuously Regenerating Trap (CRT) systems, which are used to reduce particulate matter emissions [53]. If NO\(_2\) is not present in large enough quantities, it is necessary to oxidize NO into NO\(_2\), to enable passive regeneration in the CRT [54]. The oxidation of NO to NO\(_2\) would require an oxidation catalyst to be placed upstream of the CRT. The increased production of NO\(_2\) from hydrogen substitution would reduce the need for NO oxidation catalysts in the CRT system.

![Graph showing Brake specific NO\(_X\), NO and NO\(_2\) emissions vs. energy percent from hydrogen fuel for 3600rpm at 25% of maximum output.](image)

Figure 4.22: Brake specific NO\(_X\), NO and NO\(_2\) emissions vs. energy percent from hydrogen fuel for 3600rpm at 25% of maximum output.
4.15 Gaseous Emissions: HC

HC emissions are difficult to sample. They tend to drop out of the heated exhaust sample and condense if they encounter cold spots in the sampling apparatus. This is reflected in the 1800 rpm at 25% maximum output mode seen in Figure 4.23.

![Brake Specific HC Emissions Graph](image)

**Figure 4.23:** Brake specific HC emissions of the four modes tested, with □ 0%, ■ 2.5%, □ 7.5% and ■ 15% hydrogen substitution on an energy basis.

HC emissions are products of incomplete combustion. Incomplete combustion can occur when the in cylinder temperature and pressure are not high enough to completely combust the injected fuel. HC emissions will also occur, if injected diesel fuel penetrates past the flame front and reaches the cylinder walls. Also, atomized fuel may also seep into the crevices of the cylinder, excluding it from combustion.

The low load modes have increased levels of brake specific HC emissions. This is due to the incomplete combustion that occurs at low load. The 3600 rpm at 25%
maximum output mode has a larger degree of incomplete combustion. This is due to this mode’s overly lean equivalence ratio.

Both of the high load modes have low levels of HC emission. The 3600 rpm at 25% maximum output mode has higher levels of HC emission, due to the cycle speed of the mode, which reduces the time for the fuel to completely combust.

At high loads, hydrogen substitution reduces brake specific HC emissions. This is because there is less diesel fuel in the main injection that can be lost to incomplete combustion by either hiding in a crevice or gathering on the cylinder walls. However, in the low load modes, brake specific HC emissions increase due to hydrogen substitution. In the low load modes the heat release is much lower than that of the high load modes. When hydrogen substitution occurs there is less diesel fuel injected during the main injection, which further reduces the heat release. This reduction in heat release acts to further increase the amount of HC released from incomplete combustion.

Table 4.6: Percent difference of brake specific HC emissions from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>1800 @ 25%</th>
<th>1800 @ 75%</th>
<th>3600 @ 25%</th>
<th>3600 @ 75%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 % Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5 % Diff.</td>
<td>11.4</td>
<td>-1.7</td>
<td>5.3</td>
<td>-4.2</td>
</tr>
<tr>
<td>5 % Diff.</td>
<td>32.6</td>
<td>36.7</td>
<td>13.6</td>
<td>4.5</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>4.4</td>
<td>-9.7</td>
<td>7.0</td>
<td>-10.7</td>
</tr>
<tr>
<td>10 % Diff.</td>
<td>-4.0</td>
<td>-25.5</td>
<td>17.6</td>
<td>-11.4</td>
</tr>
<tr>
<td>15 % Diff.</td>
<td>-8.2</td>
<td>-30.4</td>
<td>12.1</td>
<td>-8.8</td>
</tr>
</tbody>
</table>
4.16 Gaseous Emissions: Unburned Hydrogen

Unburned HC emissions can be correlated directly to the unburned hydrogen seen in Figure 4.24. There is very little unburned hydrogen. Levels of unburned hydrogen increase with low load modes that suffer from incomplete combustion. Unburned hydrogen also increases as the substitution percent increases.

Figure 4.24: Brake specific H₂ emissions of the four modes tested, with 0%, 2.5%, 7.5%, and 15% hydrogen substitution on an energy basis.

4.17 Gaseous Emissions: CO

CO emissions correlate with and are primarily controlled by air fuel ratio. Heywood states that a diesel engine operates in fuel lean conditions and thus CO emissions are unimportant and do not need to be discussed [5]. Nonetheless, the
formation of CO is directly linked to the availability of HC. The principal CO formation is based on the hydrocarbon combustion mechanism[51].

The mechanism is summarized by:

\[ RH \rightarrow R \rightarrow RO_2 \rightarrow RCHO \rightarrow RCO \rightarrow CO \]

The R stands for a hydrocarbon radical.

In the case of 3600 rpm at 25% of maximum output mode, the brake specific CO levels are higher than those of the other modes. At this mode, the turbo-charger is active, increasing the density of the charged air, while the low load is demanding little fuel.

Hence the equivalence ratio is lean as seen in Figure 4.16. Even though this mode is lean, there is a large amount of CO. The large CO content is due to incomplete combustion which is redetected in the increased levels of brake specific hydrocarbon at this mode.

---

**Figure 4.25:** Brake specific CO emissions of the four modes tested, with □ 0%, □ 2.5%, □ 5%, □ 7.5%, □ 10% and □ 15% hydrogen substitution on an energy basis.
4.18 Gaseous Emissions: CO₂

Carbon dioxide is one of the main products of combustion when burning hydrocarbon fuels. Reducing hydrocarbon fuel will reduce the amount of carbon dioxide formed during combustion. This is accomplished during hydrogen substitution.
There is an increased level of brake specific CO$_2$ in the 3600 rpm at 25% maximum output mode. The excess CO$_2$ is coming from the high levels of CO in this mode. CO converts to CO$_2$ in the path given in Eq. 4.5 [52].

\[
CO + HO_2 \rightarrow CO_2 + OH
\]  
4.5
In general, the introduction of hydrogen causes an almost 1 to 1 reduction of CO₂. As the fraction of hydrogen increases, the quantity of diesel fuel decreases. Hence there are less HC radicals available to form CO.

4.19 Gaseous Emissions: Particulate Matter

The majority of particulate will be created in the diffusion flame during the mixing control burn phase, where fuel pyrolysis occurs. The creation of particulate is a competition between formation and oxidation [5]. In conditions where higher temperatures occur, particulate will be oxidized and emitted levels will decrease.

A correlation between levels of brake specific particulate emissions and apparent heat release rate can be made. In the apparent heat release rate plots above, the high load modes had higher rates of heat release. Below in Figure 4.26 the high load modes have lower levels of brake specific particulate emissions, than those of the low load modes. The higher apparent heat release rates signify a higher rate of oxidation occurred in the high load modes.

Hydrogen substitution appears to reduce brake specific particulate emissions at high speeds and increase brake specific particulate emissions at slow speeds. These trends can be explained by again looking at the apparent heat release rates of the modes. In the case of the low speed modes hydrogen decreases the apparent heat release rates of the low speed modes, reducing oxidation. In the high speed modes there is a slight decrease in apparent heat release rates, but the decrease of hydrocarbon fuel levels during hydrogen substitution reduces the amount of carbon available to form particulate.
Figure 4.27: Brake specific PM emissions of the four modes tested, with □ 0%, ▪ 2.5%, ■ 7.5% and ■ 15% hydrogen substitution on an energy basis.

Table 4.9: Percent difference of brake specific HC emissions from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>1800 @ 25%</th>
<th>1800 @ 75%</th>
<th>3600 @ 25%</th>
<th>3600 @ 75%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 % Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5 % Diff.</td>
<td>4.5</td>
<td>35.4</td>
<td>-16.5</td>
<td>-0.8</td>
</tr>
<tr>
<td>7.5 % Diff.</td>
<td>25.2</td>
<td>56.1</td>
<td>-1.3</td>
<td>-8.5</td>
</tr>
<tr>
<td>15 % Diff.</td>
<td>31.4</td>
<td>77.7</td>
<td>-9.8</td>
<td>-16.0</td>
</tr>
</tbody>
</table>
4.20 Brake Specific Fuel Consumption

The brake specific fuel consumption was calculated based on the consumption of both diesel and hydrogen fuel. Internal combustion engines are most efficient at high loads. This is reflected in Figure 4.27. The 3600 rpm at 25% maximum output mode, has the poorest efficiency of all the modes. This is due to the large amount of incomplete combustion which occurs in this mode.

![Figure 4.28: Brake specific fuel consumption of the four modes tested, with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis.](image)

Hydrogen substitution decreased the brake specific fuel efficiency of the modes due to the reduction of air. Fumigation of hydrogen into the air intake displaces air for fuel in the form of hydrogen. Air is the working fluid of an engine, thus a reduction in air will reduce the output of an engine. Brake specific fuel efficiency loses experienced when hydrogen is fumigated into the air intake, would be recovered by direct injection of hydrogen into the combustion cylinder.
The benefits of hydrogen for diesel fuel substitution are more modest than those reported from anecdotal reports. The cause of the emission reductions seen in anecdotal reports are from injection timing shifts, not hydrogen combustion. However, hydrogen substitution does yield modest emissions reduction with limited penalty. The foremost benefit is the reduction in hydrogen carbon fuel during substitution for hydrogen. Fumigation of hydrogen into the air intake was seen to displace up to 30% of the diesel fuel energy required to run a compression ignition engine at a high load. Also carbon dioxide was reduced by at a nearly a one to one percentage reduction on the basis of fuel energy.

Hydrogen substitution causes a dramatic shift of the NO\textsubscript{X} species, from NO dominance to NO\textsubscript{2} dominance. This NO\textsubscript{X} shift has the potential to be coupled with CRTs to oxide soot.
The benefits of hydrogen substitution are significant, since these results show that substitution of the diesel fuel with hydrogen can be accomplished with little or no detrimental effect. Thus, substantial quantities of diesel fuel can be “displaced” through hydrogen utilization via substitution. The practicality of vehicles utilizing hydrogen substitution is limited by the feasibility of equipment cost versus the cost benefits from the modest emission reductions.
Chapter 5

Discussion and Results of Advanced Combustion Modes with Hydrogen Substitution

5.1 Introduction

In this section, the results of hydrogen assisted combustion under advanced combustion modes are presented. Though an in-depth study of hydrogen assisted combustion under advanced combustion modes is novel, the ability to reproduce the advanced combustion modes on a stock production engine is equally fascinating. The advanced combustion modes used in this study are based on work done by Wagner, Sluder and coworkers at Oak Ridge National Laboratory [39, 44-49].

Wagner, Sluder and coworkers developed an advanced combustion mode known as High Efficiency Clean Combustion (HECC). The HECC mode is an efficient LTC/PCCI mode, which reduces NO\textsubscript{X} and PM while improving brake specific fuel efficiency. An LTC mode is typically classified as a mode in which NO\textsubscript{X} and PM are reduced via high concentrations of EGR. In this study, like the work done at Oak Ridge, an LTC mode is presented as an intermediate step to the HECC mode.

Wagner, Sluder and coworkers preformed their study on a modified Mercedes 1.7L direct-injection diesel engine. This study was conducted on a Detroit Diesel 2.5L TD DI-4V engine. The differences between the two engines made it impossible to repeat the exact conditions preformed at Oak Ridge National Laboratory. However, Wagner, Sluder and coworkers have shown it possible to achieve HECC at a broad range of speeds
and loads [39]. There were also variations in the NO\textsubscript{X} and PM reduction due to the range of speed and load conditions which Wagner, Sluder and coworkers used to achieve the HECC mode.

In this study, a HECC mode was located at 1800 rpm at 25% of maximum output because of its normally high concentrations of EGR. The high EGR concentration is due to the mode’s low speed, which utilizes little boost. High exhaust pressure and low manifold pressure allow EGR to readily overcome the positive pressure of the intake manifold. The HECC mode listed in this study shares trends with Wagner, Sluder and coworkers’ HECC modes. The HECC mode used in this study achieved a 71% brake specific NO\textsubscript{X} reduction, an 80% brake specific PM reduction, a 4% brake specific fuel consumption reduction, a 73% brake specific HC increase, and a 106% CO increase.

The results of hydrogen substitution for diesel fuel on the basis of energy percent are presented below in the baseline mode, LTC mode and HECC mode. Hydrogen substitution was done at 0%, 2.5% 5% 7.5% 10% and 15%, of the fuel energy. Hydrogen substitution in advanced modes caused modest emission reductions, which were similar to emission reductions seen during hydrogen substitution for conventional combustion modes. A 15% hydrogen substitution was achieved in the advanced combustion modes without significant penalty on emissions or performance.
5.2 Exhaust Gas Recirculation

The key parameter used to enter the HECC mode is a high concentration of EGR, ~50%. EGR% was defined as [29]:

\[
EGR\% = \frac{CO_{2_{\text{Intake}}} (\text{vol}\%) - CO_{2_{\text{Ambient}}} (\text{vol}\%)}{CO_{2_{\text{Exhaust}}} (\text{vol}\%) - CO_{2_{\text{Ambient}}} (\text{vol}\%)}
\]  \hspace{1cm} (5.1)

On the Detroit Diesel 2.5L TD DI-4V engine there is an EGR valve that diverts exhaust gas into the intake manifold. This valve is controlled by the engine’s ECU. With the EGR valve fully open, the volumetric flow rate of EGR supplied into the intake manifold from the exhaust manifold was dependent on the gradient between the exhaust manifold pressure and the intake manifold pressure. Engine modes that utilize boost pressure from the turbocharger can not achieve high concentrations of EGR because the boost pressure in the intake manifold is too great for the exhaust gas to overcome.

There are two methods to force large levels of exhaust into the intake manifold via the EGR loop. The first method is to increase the back-pressure on the exhaust. This is accomplished by causing a flow restriction downstream of the EGR loop. A valve on the exhaust pipe can be used as a restriction. In this method, exhaust is forced into the EGR loop due to the downstream restriction. Because an internal combustion engine is an air pump, this method is inherently problematic, ultimately de-rating the engine by preventing the engine from achieving its maximum air throughput.

In the second method, the intake air is choked by a restriction upstream of the intake manifold and EGR loop. A valve can be used to create a restriction, choking the intake air and causing exhaust to be pulled through the EGR loop. Unlike the case of the back pressure method, this intake choking method does not cause the engine to derate
from a pumping restriction. The second method, however, will derate the engine due to the exchange of air (the working fluid of an engine) for EGR.

The choking EGR method was initially used in attempts to enter the HECC mode. Unfortunately, the Detroit Diesel 2.5L TD DI-4V engine was found to produce exorbitant levels of CO emissions and HC emissions at 50% EGR. These high emissions were due to incomplete combustion, with levels varying per cylinder. This incomplete combustion is reflected in the apparent rate of heat release seen in Figure 5.1.

![Figure 5.1](image.png)

**Figure 5.1:** Incomplete combustion seen in Apparent Heat Release Rate in cylinders for 1800 rpm at 20 ft-torque. Pilot injection at -17ATDC and the main injection is at -2.9 ATDC. EGR ~50%. ——dQ1, ——dQ2, ——dQ3 and ——dQ4.

The incomplete combustion was most pronounced in Cylinder 1, which was caused by poor mixing of the EGR and intake air. Since the EGR loop connects to the air intake directly before the air actually enters the intake manifold there is little time for the EGR and air to mix. The phenomenon of high EGR concentrations increasing the cylinder to cylinder variation was noted by Zheng and coworkers [31].
To eliminate the high levels of incomplete combustion, simulated EGR was used to achieve a HECC mode. Bone-dry CO$_2$ with a purity of 99.8% was used as simulated EGR, which was aspirated into the engine air intake downstream of the turbocharger at the same location as hydrogen aspiration. At this point of aspiration the simulated EGR was assumed to be well mixed.

In conjunction with simulated EGR, the Detroit Diesel 2.5L TD DI-4V engine’s EGR valve was set to full open. At 1800 rpm, 25% of maximum output, and with the EGR valve fully open, the engine will produce ~16% EGR. With the engine-produced EGR and simulated EGR added together, the EGR requirement of the HECC mode was met. The method of using simulated EGR reduced the level of incomplete combustion observed during the exploration for the HECC mode.

Wagner, Sluder and coworkers cooled their EGR with a heat exchanger to prevent damaging the plastic intake manifold on their Mercedes 1.7L engine [49]. Cooled EGR is preferable since it will recover the volumetric efficiency of the engine that would otherwise be lost if intake air is hot. The Detroit Diesel 2.5L TD DI-4V engine cools its EGR with a heat exchanger cooled by the circulating engine coolant. The simulated EGR was warmed to room temperature before entering the engine. It should be noted that a small error was introduced by using room temperature simulated EGR (~25°C) compared to using engine exhaust cooled by actual EGR (~50°C).
5.3 Mode Parameters

Table 5.1 lists the parameters of the modes explored in this study. These parameters reflect the operating modes for 0% hydrogen on a fuel energy basis. Hydrogen substitution caused small changes to the EGR %, intake manifold gas temperature, and the exhaust gas temperature parameters. The injection timing was electronically held constant by reprogramming the engine’s ECU. Speed and load were held constant by using a combination of dynamometer and engine controllers.

<table>
<thead>
<tr>
<th>Mode</th>
<th>Speed (rpm)</th>
<th>Load (kW)</th>
<th>EGR (%)</th>
<th>Simulated EGR (%)</th>
<th>Total EGR (%)</th>
<th>Boost (bar)</th>
<th>Rail Pressure (bar)</th>
<th>Intake Manifold Gas (°C)</th>
<th>Exhaust Gas (°C)</th>
<th>Pilot Inj. (°ATDC)</th>
<th>Main Inj. (°ATDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline</td>
<td>1800</td>
<td>15.7</td>
<td>11</td>
<td>0</td>
<td>11</td>
<td>0.17</td>
<td>450</td>
<td>59</td>
<td>342</td>
<td>-17.4</td>
<td>2.9</td>
</tr>
<tr>
<td>LTC</td>
<td>1800</td>
<td>15.7</td>
<td>16</td>
<td>32</td>
<td>48</td>
<td>0.14</td>
<td>450</td>
<td>70</td>
<td>357</td>
<td>-17.4</td>
<td>2.9</td>
</tr>
<tr>
<td>HECC</td>
<td>1800</td>
<td>15.7</td>
<td>16</td>
<td>34</td>
<td>50</td>
<td>0.18</td>
<td>490</td>
<td>75</td>
<td>336</td>
<td>N/A</td>
<td>-4.0</td>
</tr>
</tbody>
</table>

The baseline mode utilized the engine’s default diesel fuel injection strategy for the given speed and load based on the engine’s ECU maps. The LTC mode uses the same locked injection timing as the baseline mode, as well as with the maximum engine produced EGR and aspirated simulated EGR. The HECC mode utilizes a single pulse injection and advanced main injection timing. And in addition to the rail pressure was increased from a default pressure of 450 bar to 490 bar. The HECC mode also uses the maximum engine-generated EGR along with simulated EGR.
5.4 Needle Lift

The needle lift data indicated the crank angle at which fuel is injected, as well as the duration of injection and needle lift height of fuel injected. Figure 5.2 displays the comparison of needle lift for the baseline, LTC, and HECC modes under 0% hydrogen. Predictably, the baseline mode and the LTC mode, had similar start of injection and injection durations. This is due to the injection timing being locked at -17.4 °ATDC for the pilot injection, and 2.9 °ATDC for the main injection timing in both modes. The HECC mode had a single injection that was set at -4 °ATDC. The HECC mode also had higher needle lift since the mode utilized only a single injection and must inject all the required fuel during this single injection. The area under the injection peaks represents the quantity of fuel injected during the actuation of the fuel injector. It is important to note that this HECC mode also utilized increased rail pressure, thus a large quantity of fuel was injected for the given injection duration and needle lift height.
Figures 5.3 through Figure 5.5 are the needle lift of the baseline mode, LTC mode, and HECC mode with hydrogen substitution. The needle lift signal contains noise from external sources. A majority of the noise was filtered out by averaging 200 samples. The needle lift signals’ reluctance to return to zero height after injection was caused by a combination of signal noise and oscillation inherent to a fast-acting spring system. The oscillation observed in the main injection was caused by the preceding pilot injection. As to be expected, the pilot injections in Figure 5.3 and Figure 5.4 overlap. Because of the noise, and the oscillations shifting the height of the injection, the main injection is difficult to analyze. Figure 5.5 reflects the HECC mode, which utilized a single injection. Note that the needle lift signal in Figure 5.5 clearly shows that the increasing rate of hydrogen substitution decreases the height, and thus the quantity of diesel fuel introduced by the injector.
Figure 5.3: Needle lift of baseline mode, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.

Figure 5.4: Needle lift of LTC mode, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.
5.5 Pressure Trace

The pressure traces indicate the pressure due to cylinder volume reduction from the piston’s travel, as well as the pressure created from hot product gases. The baseline mode and the LTC mode have similar pressure traces due to their similar parameters. In Figure 5.6 a 2.7% decrease in maximum pressure occurs in the LTC mode compared to the baseline. The reduction in maximum pressure seen in the pressure traces is due to the LTC mode’s high level of EGR. The EGR absorbs released heat, lowering the adiabatic flame temperature [1]. An increase in EGR levels also leads to a reduction in oxygen, oxidizer need to burn the fuel. Thus, the maximum pressure of the LTC mode is reduced. The maximum pressure produced in the HECC mode with 0% hydrogen substitution was

![Figure 5.5: Needle lift of HECC mode, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.](image-url)
21% lower than that of the baseline mode, due to the large degree of pre-mixed combustion which occurred in the HECC mode. The second pressure peak of the HECC mode is due to the mode’s transition to mixing-controlled combustion, which is further explained by the apparent heat release rate.

Figures 5.7 to 5.9 show the pressure traces of the baseline mode, LTC mode and HECC mode with 0%, 2.5%, 5% and 15% hydrogen substitutions. Increasing levels of hydrogen caused a slight increase in maximum pressure. Table 5.2 compares the increase of peak pressure caused by hydrogen.
Figure 5.7: Pressure trace of baseline mode, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.

Figure 5.8: Pressure trace of LTC mode, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.
Table 5.3 compares the increase of maximum pressure of the baseline mode compared to the LTC mode and the baseline mode compared to the HECC mode. The LTC mode decreases slightly in maximum pressure compared to the LTC mode by 2.7%
at 0% hydrogen substitution. The HECC mode, however, displays a 21.3% decrease in maximum pressure.

Table 5.3: Percent difference of maximum pressure from the baseline mode to the LT mode and HECC mode with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>Baseline to LTC</th>
<th>Baseline to HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0% Diff.</td>
<td>-2.7</td>
<td>-21.3</td>
</tr>
<tr>
<td>2.5% Diff.</td>
<td>-1.7</td>
<td>-21.1</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>-1.7</td>
<td>-20.4</td>
</tr>
<tr>
<td>15% Diff.</td>
<td>-1.1</td>
<td>-20.8</td>
</tr>
</tbody>
</table>

5.6 Coefficient of Variance

The coefficient of variance is a measure used to quantify cycle-to-cycle variation based on the in-cylinder indicated mean effective pressure (IMEP). Heywood defines the coefficient of variance as given in Eq. 5.2 [5].

\[
COV_{\text{imep}} = \frac{\sigma_{\text{imep}}}{\mu} \cdot 100\% = \frac{\sigma}{\mu} \cdot 100\%
\]

5.2

The mean (imep) and the standard deviation (\(\sigma_{\text{imep}}\)) of the coefficient of variance were calculated from 200 cycles of pressure traces. A COV\(_{\text{imep}} > 1\) indicates increased variation between cycles. Table 5.4 displays the coefficient of variance of all four cylinders of the baseline mode, LTC mode, and HECC mode with hydrogen substitution.
When compared to the baseline mode at 0% hydrogen substitution, the LTC mode overall displayed less cycle-to-cycle variation, except in Cylinder 1. The pressure traces show that the 2.5 L DDC engine’s Cylinder 1 performed poorly due to inadequate mixing of the intake charge. The HECC mode also displayed less cycle-to-cycle variation over the baseline mode at 0% hydrogen substitution. The decreased cycle-to-cycle variation of the LTC mode and HECC mode can be attributed to the high EGR content used in these modes. High EGR, however, is reported to increase cycle-to-cycle variation, not decrease it [5, 31]. The hydrogen substitution does not create any appreciable trends in coefficient of variation. A repeatability study with 0% hydrogen has confirmed the lack of a trend in the coefficient of variance seen in table 5.4.

### Table 5.4: Coefficient of variance for all four cylinders baseline mode, LTC mode and HECC mode with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.

<table>
<thead>
<tr>
<th>H2%</th>
<th>Cyl. 1</th>
<th>Cyl. 2</th>
<th>Cyl. 3</th>
<th>Cyl. 4</th>
<th>Cyl. 1</th>
<th>Cyl. 2</th>
<th>Cyl. 3</th>
<th>Cyl. 4</th>
<th>Cyl. 1</th>
<th>Cyl. 2</th>
<th>Cyl. 3</th>
<th>Cyl. 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>5.5</td>
<td>5.2</td>
<td>5.6</td>
<td>4.6</td>
<td>6.4</td>
<td>3.0</td>
<td>3.0</td>
<td>3.3</td>
<td>4.6</td>
<td>3.2</td>
<td>3.2</td>
<td>3.5</td>
</tr>
<tr>
<td>2.5</td>
<td>5.6</td>
<td>5.0</td>
<td>5.2</td>
<td>4.6</td>
<td>7.1</td>
<td>3.3</td>
<td>3.1</td>
<td>3.4</td>
<td>7.1</td>
<td>3.3</td>
<td>3.1</td>
<td>3.4</td>
</tr>
<tr>
<td>7.5</td>
<td>5.6</td>
<td>4.8</td>
<td>5.7</td>
<td>4.5</td>
<td>10.2</td>
<td>3.7</td>
<td>4.3</td>
<td>4.2</td>
<td>10.2</td>
<td>3.7</td>
<td>4.3</td>
<td>4.2</td>
</tr>
<tr>
<td>15</td>
<td>5.4</td>
<td>4.4</td>
<td>5.9</td>
<td>4.4</td>
<td>3.6</td>
<td>3.0</td>
<td>3.6</td>
<td>3.0</td>
<td>3.6</td>
<td>3.0</td>
<td>3.6</td>
<td>3.0</td>
</tr>
</tbody>
</table>

When compared to the baseline mode at 0% hydrogen substitution, the LTC mode overall displayed less cycle-to-cycle variation, except in Cylinder 1. The pressure traces show that the 2.5 L DDC engine’s Cylinder 1 performed poorly due to inadequate mixing of the intake charge. The HECC mode also displayed less cycle-to-cycle variation over the baseline mode at 0% hydrogen substitution. The decreased cycle-to-cycle variation of the LTC mode and HECC mode can be attributed to the high EGR content used in these modes. High EGR, however, is reported to increase cycle-to-cycle variation, not decrease it [5, 31]. The hydrogen substitution does not create any appreciable trends in coefficient of variation. A repeatability study with 0% hydrogen has confirmed the lack of a trend in the coefficient of variance seen in table 5.4.

#### 5.7 Apparent Heat Release Rate

Figure 5.10 displays the apparent heat release rate of the baseline mode, LTC mode, and HECC with 0% hydrogen substitution. The start of combustion of the pilot injection (-7.9TDC) of the LTC mode are delayed compared to the start of combustion of the pilot injection (-8.7 °ATDC) for the baseline mode. The delay in start of combustion observed for the LTC mode is due to the mode’s high concentration of EGR, which
absorbs the heat produced by the in-cylinder compression, requiring further time to achieve ignition. Since its injection timing is different, the HECC mode’s start of combustion (7.1°ATDC) cannot be compared to that of the other modes.

The apparent heat release rate profiles of the baseline mode and LTC mode appear generic, corresponding to the four diesel combustion phases given by Heywood [5]. The HECC mode has a unique apparent heat release rate profile. Diesel fuel is injected into this mode at -4 °ATDC, but combustion does not start until 7.1°ATDC. The HECC mode has an 11.1° ignition delay. This extended start of combustion is due to the large concentration of EGR (~50%) used in the mode, as well as, an advanced injection timing. This mode is unique as it utilizes only three of the four diesel combustion phases given by Heywood, including a longer then usual ignition-delay phase. The single injection of the HECC mode ends at 8.7 °ATDC and the start of combustion begins at HECC (7.1°ATDC). By the time combustion begins almost all of the fuel is injected into the cylinder, thus causing almost all of the fuel to be consumed in a pre-mixed combustion phase. Indicated by the end of injection and start of combustion overlapping, a small quantity of fuel was burned in the mixing-controlled combustion phase. However, the apparent heat release rate plot, given in Figure 5.10, does not indicate the presence of a mixing-controlled combustion phase peak. Rather it indicates the heat release’s transition directly from a pre-mixed combustion phase to a late combustion phase, which is the trailing trace in the HECC mode’s apparent heat release rate plot. The apparent heat release rate plot of the HECC mode provides verification that the mode is a PCCI combustion mode.
Figures 5.11 through 5.13 show the apparent heat release rates of the baseline mode, LTC mode and HECC mode with 0%, 7.5% and 15% hydrogen substitution. Hydrogen substitution caused similar apparent heat release rate plots for both the baseline mode and the LTC mode. Hydrogen substitution caused the premixed combustion phase of the baseline mode and the LTC mode to have a higher peak as hydrogen substitution increased. The peaks of the mixing-controlled combustion phase of both the baseline mode and LTC mode decrease as hydrogen substitution increases. Both the increase of the pre-mixed combustion phase peak and the decrease in the mixing-controlled combustion phase peak are caused by the method in which hydrogen is injected into the engine. The hydrogen is aspirated into the engine along with the intake air. Thus, once the intake valve of a cylinder closes, hydrogen can no longer be added. After the pilot
injection of diesel consumes the hydrogen, there is no more hydrogen available to be burned during the main injection. The engine injected less diesel fuel into the cylinder when hydrogen substitution was increased because the engine was set to a fixed load.

Figure 5.11: Apparent heat release rate of baseline mode, with 0%, 2.5%, 7.5% and 15% hydrogen substitution on an energy basis.
Figure 5.12: Apparent heat release rate of LTC mode, with \(0\%\), \(2.5\%\), \(7.5\%\) and \(15\%\) hydrogen substitution on an energy basis.

Figure 5.13 displays the apparent heat release rate of the HECC mode with hydrogen substitution. The increased substitution of hydrogen did not create appreciable trends in maximum apparent heat release rate. The addition of hydrogen did, however, advance the crank angle of the maximum heat release from \(15.2^\circ\) ATDC at \(0\%\) hydrogen to \(14.9^\circ\) ATDC at \(15\%\) hydrogen substitution. This shift in maximum apparent heat release rate is due to the increased presence of hydrogen, causing greater portions of the fuel to be premixed at an earlier crank angle.
5.8 Equivalence Ratio

Figure 5.14 displays the global equivalence ratio of the three modes tested. The equivalence ratios of the modes are fuel lean. The apparent heat release rate indicated that the baseline mode and LTC mode consist mainly of mixing-controlled combustion phases, thus, combustion takes place as a diffusion flame with an array of locally fuel lean regions and locally fuel rich regions. According to the apparent heat release rate data, the HECC mode is mainly composed of a pre-mixed combustion phase, which indicates that the equivalence ratio is likely locally fuel lean through the air-fuel charge. The difference between the local equivalence ratios of the modes is used to explain exhaust emissions.
The equivalence ratios of the three modes with 0% hydrogen are practically the same when error is taken into consideration. All three modes show a trend of increasing equivalence ratio with increasing hydrogen substitution. This trend is to be expected, since aspirated hydrogen addition will displace intake air, decreasing the air-fuel ratio.

5.9 Exhaust Temperature

Figure 5.15 displays the exhaust temperatures of the three modes tested. Exhaust temperature provides only an indirect indication of the global in-cylinder temperature. A bulk cylinder temperature based on the ideal gas law was not used to calculate temperature because the high levels of EGR used in the modes would result in erroneously high calculated temperatures, due to the increase in temperature of the intake charge and the decreasing of trapped mass [30]. Computational Fluid Dynamics (CFD)
modeling, which is outside the scope of this work, would provide the best indication of the combustion temperatures.

Tables 5.5 and 5.6 compare the three modes with and without hydrogen substitution. Hydrogen substitution clearly increased the exhaust temperature of the baseline mode and the HECC mode. LTC mode however, showed a modest decrease in exhaust temperature, which can be attributed to a shift in laboratory conditions.
5.10 Gaseous Emissions: NO\textsubscript{X}

The high levels of EGR used in the advanced combustion mode lowered the combustion temperature, quenching the production of thermal NO, thus reducing NO\textsubscript{X}. The LTC mode decreased NO\textsubscript{X} emissions by 89.5% compared to the baseline mode with 0% hydrogen substitution. The NO\textsubscript{X} reduction of the HECC mode was less than that of the LTC mode, with a 71.2% NO\textsubscript{X} reduction from the baseline with 0% hydrogen substitution. The HECC mode used on the DDC 2.5L engine was not optimized to

---

Table 5.5: Percent difference of exhaust temperature from 0% hydrogen to 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis for the baseline mode, LTC mode and HECC mode. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th>Diff.</th>
<th>Baseline</th>
<th>LTC</th>
<th>HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5%</td>
<td>0.6</td>
<td>-1.1</td>
<td>0.8</td>
</tr>
<tr>
<td>5%</td>
<td>1.2</td>
<td>-1.3</td>
<td>1.5</td>
</tr>
<tr>
<td>7.5%</td>
<td>1.8</td>
<td>-0.7</td>
<td>0.8</td>
</tr>
<tr>
<td>10%</td>
<td>2.2</td>
<td>-1.1</td>
<td>1.7</td>
</tr>
<tr>
<td>15%</td>
<td>2.9</td>
<td>-0.5</td>
<td>1.5</td>
</tr>
</tbody>
</table>

Table 5.6: Percent difference of exhaust temperature comparing the baseline mode to LTC mode and baseline mode to HECC mode. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th>Diff.</th>
<th>Baseline to LTC % Diff.</th>
<th>Baseline to HECC % Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>4.1</td>
<td>-2.0</td>
</tr>
<tr>
<td>2.5%</td>
<td>2.5</td>
<td>-1.8</td>
</tr>
<tr>
<td>5%</td>
<td>1.7</td>
<td>-1.7</td>
</tr>
<tr>
<td>7.5%</td>
<td>1.6</td>
<td>-3.0</td>
</tr>
<tr>
<td>10%</td>
<td>0.8</td>
<td>-2.6</td>
</tr>
<tr>
<td>15%</td>
<td>0.7</td>
<td>-3.4</td>
</tr>
</tbody>
</table>
produce low NO\textsubscript{X} emissions alone, but was rather optimized for simultaneously low NO\textsubscript{X} emissions, low PM emissions and high thermal efficiency. Rail pressure, injection timing and EGR\% were the variables adjusted in the HECC mode optimization process.

The addition of hydrogen produced modest increases in NO\textsubscript{X} emissions for the baseline mode, although hydrogen caused NO\textsubscript{X} emissions for the LTC mode and HECC mode to more significantly increase on the percent difference basis, as given in Table 5.7. The high levels of EGR used in the LTC mode and the HECC mode dramatically reduced NO\textsubscript{X} emissions from the baseline mode; hydrogen, however, still increased NO\textsubscript{X} emissions independently of the reductions caused by high levels of EGR. The effect of hydrogen on the LTC mode and the HECC mode can be further explained by examining the NO emissions and the NO\textsubscript{2} emissions independently.

Figure 5.16: Brake specific NO\textsubscript{X} emissions of the three modes tested, with ☐ 0\%, ☐ 2.5\%, ☐ 5\%, ☐ 7.5\%, ☐ 10\% and ☐ 15\% hydrogen substitution on an energy basis.
According to Figure 5.17 and Table 5.10, the LTC mode and the HECC mode reduced NO emissions by ~83% compared to the baseline mode at 0% hydrogen substitution. The NO\textsubscript{X} and NO emissions together indicate that the HECC mode did not decrease NO\textsubscript{2} emissions as significantly as the LTC mode. As seen in Table 5.9,
hydrogen substitution did not appreciably effect the advanced combustion modes’ NO emissions.

Figure 5.17: Brake specific NO emissions of the three modes tested, with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis.

Table 5.9: Percent difference of brake specific NO emissions from 0% hydrogen to 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis for the baseline mode, LTC mode and HECC mode. Positive values indicate an increase and negative values indicate a decrease from the baseline.
5.12 Gaseous Emissions: NO₂

Figure 5.18 and Table 5.12 indicate that the LTC mode reduced NO₂ emissions by 119.2%, while the HECC mode only reduced NO₂ emissions 33.8%, in comparison to the baseline mode at 0% hydrogen substitution. The appearance of higher level of NO₂ emissions produced in the HECC mode over the LTC mode is not expected. While the major pathway to NO₂ formation is the oxidation of NO, the LTC and HECC modes both produced similar values of brake specific NO emissions. Upatnieks, Mueller and Martin conducted a study on an optically-accessible, heavy-duty DI diesel engine in which intake oxygen was diluted via nitrogen as simulated EGR, which resulted in an increased NO₂ to NO ratio. The increase of NO₂ and decrease of NO was attributed to an increased quenching of the NO₂-to-NO reaction (Eq. 5.3) due to decreasing flame temperatures [55].

\[
NO₂ + O \rightleftharpoons NO + O₂
\]  

5.3
The observation reported by Upatnieks, Mueller and Martin correspond to the NO and NO₂ emissions of LTC and HECC modes of this study, although CO₂ was used instead of nitrogen. The extended pre-mixed combustion phase of the HECC mode can be assumed to have lower flame temperature than that of the LTC mode, which has majority mixing-controlled combustion phase. This assumed lower flame temperatures of the HECC mode will then further quenching of the NO₂-to-NO reaction, thus HECC mode produced higher NO₂ emissions.

Figure 5.18: Brake specific NO₂ emissions of the three modes tested, with □ 0%, □ 2.5%, □ 5%, □ 7.5%, □ 10% and □ 15% hydrogen substitution on an energy basis.
Hydrogen substitution caused an increase of NO₂ emissions in all three modes. The increased NO₂ in both LTC and HECC modes, however, is counterintuitive since NO₂’s main creation path is from NO and there was no NO increase measured in advanced combustion mode. The most likely explanation is that the hydrogen present caused localized increases in flame temperature, which then created thermal NO. The NO emissions were not measured in the exhaust because the presence of HO₂, created by hydrogen (see Eq. 4.3) reacted with the NO to form NO₂, as given in Eq. 4.2. Kinetic and

<table>
<thead>
<tr>
<th></th>
<th>Baseline</th>
<th>LTC</th>
<th>HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0% Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5% Diff.</td>
<td>53.3</td>
<td>26.3</td>
<td>14.7</td>
</tr>
<tr>
<td>5% Diff.</td>
<td>68.0</td>
<td>43.2</td>
<td>34.8</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>70.8</td>
<td>85.9</td>
<td>45.3</td>
</tr>
<tr>
<td>10% Diff.</td>
<td>70.2</td>
<td>59.5</td>
<td>43.0</td>
</tr>
<tr>
<td>15% Diff.</td>
<td>74.8</td>
<td>83.4</td>
<td>52.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Baseline to LTC % Diff.</th>
<th>Baseline to HECC % Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>-119.2</td>
</tr>
<tr>
<td>2.5%</td>
<td>-135.9</td>
</tr>
<tr>
<td>5%</td>
<td>-135.2</td>
</tr>
<tr>
<td>7.5%</td>
<td>-107.1</td>
</tr>
<tr>
<td>10%</td>
<td>-126.6</td>
</tr>
<tr>
<td>15%</td>
<td>-112.4</td>
</tr>
</tbody>
</table>

Hydrogen substitution caused an increase of NO₂ emissions in all three modes. The increased NO₂ in both LTC and HECC modes, however, is counterintuitive since NO₂’s main creation path is from NO and there was no NO increase measured in advanced combustion mode. The most likely explanation is that the hydrogen present caused localized increases in flame temperature, which then created thermal NO. The NO emissions were not measured in the exhaust because the presence of HO₂, created by hydrogen (see Eq. 4.3) reacted with the NO to form NO₂, as given in Eq. 4.2. Kinetic and
CFD modeling is necessary to further explain the discrepancies between the NO\textsubscript{2} emissions of the advanced combustion modes, with and without hydrogen substitution.

\[ H_2 + O_2 \rightarrow HO_2 + H \] \hspace{1cm} 5.4

\[ NO + HO_2 \rightarrow NO_2 + OH \] \hspace{1cm} 5.5

**5.13 Gaseous Emissions: HC**

The advanced combustion modes increased the HC emissions compared to the baseline mode. The HC emissions of the LTC mode increased by 33\% compared to the baseline mode, while the HECC mode’s HC emissions experienced a significant 73\% increase. HC emissions are reported to increase in PCCI mode, like the HECC mode, caused by overly lean combustion conditions. Wagner, Sluder and coworkers reported increased HC when the HECC mode operated at low engine speed and a decrease in HC emission under high engine speeds. While the cause for the increase in hydrocarbon was not explored by Wagner, Sluder and coworkers the increase was attributed to the mixing timescale of the low speed engine operation [39].
The baseline mode’s HC emissions data appears to contain error in sampling at 5% hydrogen substitution data. HC emission equipment is sensitive to cold spots in the sampling line, which can cause the hydrocarbons to condense and thus result in erroneous emissions. Hydrogen substitution, however, caused an increase of HC emissions at 2.5% and 5% of hydrogen substitution for all three of the modes tested. At 7.5% of hydrogen substitution, the HC emissions decreased. Intuitively, an increase of hydrogen fuel and a decrease in hydrocarbon fuel should reduce HC emissions. Nonetheless, low percentages of hydrogen substitution increased the level of incomplete combustion, thus producing unburned hydrocarbon emissions.

Figure 5.19: Brake specific HC emissions of the three modes tested, with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis.
5.14 Gaseous Emissions: CO

Figure 5.20 shows the HECC mode CO emissions increased by 105% compared to the baseline mode at 0% hydrogen substitution. The LTC mode CO emissions increased by 50% compared to the baseline mode at 0% hydrogen substitution. The dramatic increase in CO emissions, specifically in the HECC mode, can be attributed to incomplete combustion. The HECC mode operates in a locally fuel lean condition. Overly fuel lean combustion will lead to incomplete combustion [16]. High levels of EGR also compound the degree of incomplete combustion [30]. The increased level of

---

Table 5.13: Percent difference of brake specific HC emissions from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>Baseline</th>
<th>LTC</th>
<th>HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0% Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5% Diff.</td>
<td>11.4</td>
<td>15.2</td>
<td>10.9</td>
</tr>
<tr>
<td>5% Diff.</td>
<td>32.6</td>
<td>9.5</td>
<td>11.3</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>4.4</td>
<td>-0.7</td>
<td>3.7</td>
</tr>
<tr>
<td>10% Diff.</td>
<td>-4.0</td>
<td>1.2</td>
<td>4.4</td>
</tr>
<tr>
<td>15% Diff.</td>
<td>-8.2</td>
<td>-9.0</td>
<td>-1.9</td>
</tr>
</tbody>
</table>

Table 5.14: Percent difference of brake specific HC emissions comparing baseline to LTC and baseline to HECC. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>Baseline to LTC % Diff.</th>
<th>Baseline to HECC % Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>33.0</td>
<td>73.9</td>
</tr>
<tr>
<td>2.5%</td>
<td>36.8</td>
<td>73.5</td>
</tr>
<tr>
<td>5%</td>
<td>9.9</td>
<td>54.7</td>
</tr>
<tr>
<td>7.5%</td>
<td>28.0</td>
<td>73.3</td>
</tr>
<tr>
<td>10%</td>
<td>38.0</td>
<td>81.0</td>
</tr>
<tr>
<td>15%</td>
<td>32.2</td>
<td>79.3</td>
</tr>
</tbody>
</table>
CO emissions in the LTC mode was also caused by incomplete combustion due to the high levels of EGR.

Hydrogen substitution caused a significant decrease in CO emissions in all three modes tested, as can be seen in Tables 5.15 and 5.16. The increased levels of hydrogen may have formed HO$_2$ radicals, which in turn attacked the CO. The reduction of air due to hydrogen aspiration decreases the amount of localized air-fuel pockets which are overly fuel lean leading to incomplete combustion and CO formation.
5.15 Gaseous Emissions: CO₂

CO₂ emissions increased in the advanced combustion modes over the baseline modes, due to the increased levels of CO₂ added in the form of EGR. The CO₂ emissions of both LTC and HECC modes nearly overlap, as can be seen in Table 5.18. Even though both of the advanced combustion modes utilized ~50% EGR, the overlap is unexpected because the carbon emissions pathways and the modes’ fuel efficiencies are different.

### Table 5.15: Percent difference of brake specific CO emissions from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th>% Diff.</th>
<th>Baseline</th>
<th>LTC</th>
<th>HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5%</td>
<td>-0.3</td>
<td>-4.9</td>
<td>-3.7</td>
</tr>
<tr>
<td>5%</td>
<td>-8.2</td>
<td>-13.4</td>
<td>-11.3</td>
</tr>
<tr>
<td>7.5%</td>
<td>-16.4</td>
<td>-13.0</td>
<td>-17.0</td>
</tr>
<tr>
<td>10%</td>
<td>-18.8</td>
<td>-21.4</td>
<td>-18.8</td>
</tr>
<tr>
<td>15%</td>
<td>-26.0</td>
<td>-25.9</td>
<td>-29.4</td>
</tr>
</tbody>
</table>

### Table 5.16: Percent difference of brake specific CO emissions comparing baseline to LTC and baseline to HECC. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th>% Diff.</th>
<th>Baseline to LTC % Diff.</th>
<th>Baseline to HECC % Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>50.5</td>
<td>105.7</td>
</tr>
<tr>
<td>2.5%</td>
<td>46.2</td>
<td>103.2</td>
</tr>
<tr>
<td>5%</td>
<td>45.6</td>
<td>103.4</td>
</tr>
<tr>
<td>7.5%</td>
<td>53.7</td>
<td>105.3</td>
</tr>
<tr>
<td>10%</td>
<td>48.1</td>
<td>105.7</td>
</tr>
<tr>
<td>15%</td>
<td>50.6</td>
<td>103.2</td>
</tr>
</tbody>
</table>
Hydrogen substitution reduces brake specific CO\textsubscript{2} emissions in all three modes.

The substitution of hydrogen fuel for hydrocarbon fuel reduces the availability of carbon to produce CO\textsubscript{2}. Table 5.17 shows that CO\textsubscript{2} is reduced more aggressively in the baseline mode as the EGR level was much lower than the advanced combustion modes.

**Figure 5.21:** Brake specific CO\textsubscript{2} emissions of the three modes tested, with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis.

Hydrogen substitution reduces brake specific CO\textsubscript{2} emissions in all three modes.

The substitution of hydrogen fuel for hydrocarbon fuel reduces the availability of carbon to produce CO\textsubscript{2}. Table 5.17 shows that CO\textsubscript{2} is reduced more aggressively in the baseline mode as the EGR level was much lower than the advanced combustion modes.

**Table 5.17:** Percent difference of brake specific CO\textsubscript{2} emissions from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>Baseline</th>
<th>LTC</th>
<th>HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0% Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5% Diff.</td>
<td>-2.1</td>
<td>-3.3</td>
<td>-0.9</td>
</tr>
<tr>
<td>5% Diff.</td>
<td>-3.6</td>
<td>-5.9</td>
<td>-4.0</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>-6.0</td>
<td>-5.1</td>
<td>-3.9</td>
</tr>
<tr>
<td>10% Diff.</td>
<td>-8.0</td>
<td>-7.7</td>
<td>-6.4</td>
</tr>
<tr>
<td>15% Diff.</td>
<td>-12.9</td>
<td>-8.8</td>
<td>-8.5</td>
</tr>
</tbody>
</table>
5.16 Particulate Matter Emissions: BG-1

Particulate matter is mainly created in the diffusion flame of the mixing-controlled combustion phase, as is the case with the baseline mode in Figure 5.22. The PM is formed in fuel-rich zones of the flame, where fuel is pyrolyzed. The LTC mode uses the same injection strategy as the baseline combustion mode, thus the LTC mode’s combustion is also dominated by the mixing-controlled combustion phase. However, the LTC mode utilizes ~50% EGR, which lowers the combustion temperature by absorbing heat. The reduction in combustion temperature lowers the rate at which the PM is oxidized. Furthermore, the reduction of oxygen with the increase of EGR reduced the oxygen available to oxidize soot formed in the diffusion flame. Thus, the PM in the LTC mode is 46% higher then the baseline mode.

The combustion of the HECC mode is dominated by the pre-mixed combustion phase. The pre-mixed air-fuel charge combusts locally fuel-lean at lower temperatures compared to a diffusion flame. The HECC mode also utilizes ~50% EGR, which

<table>
<thead>
<tr>
<th>Baseline to LTC % Diff.</th>
<th>Baseline to HECC % Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>56.5</td>
</tr>
<tr>
<td>2.5%</td>
<td>55.4</td>
</tr>
<tr>
<td>5%</td>
<td>54.4</td>
</tr>
<tr>
<td>7.5%</td>
<td>57.3</td>
</tr>
<tr>
<td>10%</td>
<td>56.8</td>
</tr>
<tr>
<td>15%</td>
<td>60.2</td>
</tr>
</tbody>
</table>
decreases combustion temperatures further. The low combustion temperatures and the low fuel equivalence ratio of the HECC mode shifts the mode outside of the PM formation peninsula of Akihama and coworkers’ local equivalence ratio vs. local temperature model [40]. The rate of oxidation is reduced by lowered combustion temperatures, but so little PM is formed that the HECC mode yields lower PM then the baseline or LTC modes.

Hydrogen caused an increase of PM in the three modes tested. The aspiration of hydrogen reduced the oxygen intake to the engine, thus reducing the oxygen available to oxidize the soot formed in the rich spray flame of the baseline mode and LTC mode. The increase of PM in the HECC mode was less substantial, as seen in Table 5.19. The long ignition delay in the HECC mode allowed the hydrogen more time to mix with the

Figure 5.22: Brake specific PM emissions of the three modes tested, with □ 0%, ■ 2.5%, ■ 7.5%, and ■ 15% hydrogen substitution on an energy basis.
diesel fuel and air. The premixed charge contained lower concentrations of localized hydrogen, thus reducing the spike in local temperatures.

Table 5.19: Percent difference of brake specific PM emissions from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>Baseline</th>
<th>LTC</th>
<th>HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0% Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5% Diff.</td>
<td>4.5</td>
<td>3.9</td>
<td>25.5</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>25.2</td>
<td>5.9</td>
<td>11.6</td>
</tr>
<tr>
<td>15% Diff.</td>
<td>31.4</td>
<td>7.8</td>
<td>14.2</td>
</tr>
</tbody>
</table>

Table 5.20: Percent difference of brake specific PM emissions comparing baseline to LTC and baseline to HECC. Positive values indicate an increase from the baseline, while negative values indicate a decrease.

<table>
<thead>
<tr>
<th></th>
<th>Baseline to LTC</th>
<th>Baseline to HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0% Diff.</td>
<td>46.0</td>
<td>-80.7</td>
</tr>
<tr>
<td>2.5% Diff.</td>
<td>45.4</td>
<td>-62.3</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>27.2</td>
<td>-91.9</td>
</tr>
<tr>
<td>15% Diff.</td>
<td>22.8</td>
<td>-94.7</td>
</tr>
</tbody>
</table>

5.17 Particulate Matter Emissions: SMPS

The SMPS was used to further analyze the PM emissions. The SMPS data compares the concentration in number of PM particles by volume to the diameter of the sampled particles. The SMPS data was taken using three different settings: sampling by
bypassing the thermal denuder, sampling through the thermal denuder at 30°C, and sampling through the thermal denuder at 300°C.

The advanced combustion modes at 0% hydrogen substitution were not limited by hydrogen expenditure and were more thoroughly studied using the SMPS. Figure 5.23, Figure 5.24 and Figure 5.25 compare the baseline mode, LTC mode and HECC mode when sample bypassed the thermal denuder and flowed through the thermal denuder at 30°C and at 300°C. The diluted exhaust sample contained PM made up of a solid carbon fraction (soot) and organic fraction.

The organic fraction is composed of unburned hydrocarbons that conglomerated on the soot particles. The LTC mode and the HECC mode had increased levels of unburned hydrocarbons, which could indicate higher levels of organic fraction on the soot. Figure 5.23 shows that when the sample bypasses the thermal denuder, the LTC mode yields a higher concentration of particles than the baseline mode and the HECC mode’s concentrations are quite reduced. The mass based PM data provides the same trend.
Figure 5.24 shows data for samples flowing through the thermal denuder at 30°C for 0% hydrogen substitution. The concentration of particles is significantly reduced with the sample flowing through the thermal denuder. The baseline mode’s concentration unexpectedly increased over the LTC mode when the sample passed through the 30°C thermal denuder, which is set at that temperature to avoid removing the organic fraction. The thermal denuder is, however, a cylinder full of activated carbon which filters and absorbs the organic fraction from the PM. The LTC mode contained a larger organic fraction of PM than that of baseline mode, which accounts for the shift in concentration seen in Figure 5.24.
Figure 5.24: SMPS thermal denuder at 30°C of the baseline mode, LTC mode and HECC mode with 0% of hydrogen. —— baseline, —— LTC and —— HECC.

Figure 5.25 displays the PM concentrations of the three modes tested, with the sample flowing through the thermal denuder at 300°C for 0% hydrogen substitution. The organic fraction of the PM is completely stripped away and only soot remains, due to the thermal denuder being set to 300°C. Note that the concentrations of all three of the modes are dramatically reduced.
While the HECC mode was being explored on the DDC 2.5L engine, the SMPS was used to generate expedient PM data. In the exploration process, the injection timing was adjusted to locate where the engine operated at simultaneously low NOX emissions and low PM emissions while also maintaining fuel economy. In the exploration process, the engine was found to produce large quantities of nano-particles at 2° BTDC.

Figure 5.26 compares the HECC mode used at 4° BTDC to the mode that produced the nano-particles at 2° BTDC. The PM nano-particles are entirely composed of the organic fraction. As can be seen in Figure 5.26, the thermal denuder removes the nano-particles and an ultra-low soot concentration remains. These findings are intended to be explored in future work.
5.18 Brake Specific Fuel Consumption

Brake specific fuel consumption of the LTC mode compared to the baseline mode increased by an 0.2%. The fuel efficiency of the HECC mode, however, increased by 3.6% over the baseline. Brake specific fuel consumption increased in all three of the tested modes with an increase of hydrogen substitution. It should be noted that the aspiration of hydrogen into the air intake displaced air. Diminution in air, the working fluid of the engine, will reduce volumetric efficiency and fuel economy.

Figure 5.26: HECC mode exploration at 1800 rpm, 4.2 bmeq and 50% EGR with rail pressure at 490 bars. –– TD 30°C at 2 BTDC, —— TD 300°C at 2 BTDC, —— TD 30°C at 4 BTDC and —— TD 300°C at 4 BTDC.
Figure 5.27: Brake specific fuel consumption of the four modes tested, with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis.

Table 5.21: Percent difference of brake fuel consumption from the baseline at the four modes tested with 0%, 2.5%, 5%, 7.5%, 10% and 15% hydrogen substitution on an energy basis. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>Baseline</th>
<th>LTC</th>
<th>HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0% Diff.</td>
<td>n/a</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>2.5% Diff.</td>
<td>0.3</td>
<td>-1.1</td>
<td>0.8</td>
</tr>
<tr>
<td>5% Diff.</td>
<td>0.6</td>
<td>0.8</td>
<td>1.3</td>
</tr>
<tr>
<td>7.5% Diff.</td>
<td>1.1</td>
<td>-0.8</td>
<td>2.1</td>
</tr>
<tr>
<td>10% Diff.</td>
<td>1.4</td>
<td>3.6</td>
<td>2.4</td>
</tr>
<tr>
<td>15% Diff.</td>
<td>2.0</td>
<td>1.6</td>
<td>3.4</td>
</tr>
</tbody>
</table>
Table 5.22: Percent difference of brake specific fuel consumption comparing baseline to LTC and baseline to HECC. Positive values indicate an increase and negative values indicate a decrease from the baseline.

<table>
<thead>
<tr>
<th></th>
<th>Baseline to LTC % Diff.</th>
<th>Baseline to HECC % Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>0.2</td>
<td>-3.6</td>
</tr>
<tr>
<td>2.5%</td>
<td>-1.2</td>
<td>-3.1</td>
</tr>
<tr>
<td>5%</td>
<td>0.5</td>
<td>-2.9</td>
</tr>
<tr>
<td>7.5%</td>
<td>-1.7</td>
<td>-2.6</td>
</tr>
<tr>
<td>10%</td>
<td>2.3</td>
<td>-2.6</td>
</tr>
<tr>
<td>15%</td>
<td>-0.2</td>
<td>-2.2</td>
</tr>
</tbody>
</table>

5.19 Summary

The DDC 2.5L engine operated in a PCCI mode referred to here as HECC. The mode was found at 1800 rpm at 25% of maximum output, with a single injection that was set at -4 °ATDC, ~50% of combined engine produced EGR and simulated EGR and a common rail pressure of 490 bar. Along with the HECC mode, an intermediate mode (LTC mode) utilized ~50% EGR, with all other operation parameters studied held at default. Compared to the default baseline operation at the given speed and load, the HECC mode reduced brake specific NOx emissions by 72.1%, reduced brake specific NO emissions by 83.2%, reduced brake specific NO2 emissions by 33.8%, increased brake specific HC emissions by 73.9%, increased brake specific CO emissions by 105.6%, increased brake specific CO2 emissions by 55.9%, reduced brake specific PM emissions by 80.7%, and reduced brake specific fuel consumption by 3.6%. These results correspond to those achieved by Wagner, Sluder and coworkers at Oak Ridge Nationals Laboratory, where the HECC mode was developed. Major operational parameters and emissions results of the three modes tested are given in Table 5.23.
On an energy basis, hydrogen was substituted for diesel fuel at 0%, 2.5%, 5%, 7.5%, 10%, and 15% by aspirating the hydrogen into the engine’s intake air, after the turbocharger. The effect of hydrogen substitution on the advanced combustion mode, HECC, was similar in results to the study in which hydrogen was substituted for diesel fuel in conventional combustion modes. In general, the effect of hydrogen substitution on the HECC mode was to increase brake specific NOX emissions from 4.0% to 21.6%, which was a result of the increase in combustion temperature caused by hydrogen. Hydrogen had little effect on the brake specific NO emissions of the HECC mode unlike in the conventional modes where an increase of hydrogen was seen to decrease NO. The brake specific NO2 emissions increased trend from 14.7% to 52.0%, with an increase of hydrogen. The brake specific HC emissions first increased with 2.5% and 5% then decreased from 7.5% to 15% hydrogen substitution. The brake specific CO emissions decreased trend from 3.7% to 29.4%, with an increase of hydrogen, due to more complete

<table>
<thead>
<tr>
<th></th>
<th>Baseline</th>
<th>LTC</th>
<th>HECC</th>
</tr>
</thead>
<tbody>
<tr>
<td>EGR Total (%)</td>
<td>11</td>
<td>48</td>
<td>50</td>
</tr>
<tr>
<td>Engine produce EGR (%)</td>
<td>11</td>
<td>16</td>
<td>16</td>
</tr>
<tr>
<td>Simulated EGR (%)</td>
<td>none</td>
<td>32</td>
<td>34</td>
</tr>
<tr>
<td>BSFC (g/kW.hr)</td>
<td>253</td>
<td>253</td>
<td>244</td>
</tr>
<tr>
<td>NOx (g/kW.hr)</td>
<td>1.74</td>
<td>0.68</td>
<td>0.79</td>
</tr>
<tr>
<td>PM (g/kW.hr)</td>
<td>0.98</td>
<td>1.57</td>
<td>0.42</td>
</tr>
<tr>
<td>THC (g/kW.hr)</td>
<td>0.76</td>
<td>1.06</td>
<td>1.65</td>
</tr>
<tr>
<td>Intake Temp (C)</td>
<td>59</td>
<td>70</td>
<td>75</td>
</tr>
<tr>
<td>ExhTemp (C)</td>
<td>342</td>
<td>357</td>
<td>336</td>
</tr>
<tr>
<td>Main Timing (°BTDC)</td>
<td>-2.9</td>
<td>-2.9</td>
<td>4.0</td>
</tr>
<tr>
<td>Pilot Timing (°BTDC)</td>
<td>17.4</td>
<td>17.4</td>
<td>none</td>
</tr>
<tr>
<td>Rail Pressure (bar)</td>
<td>450</td>
<td>450</td>
<td>490</td>
</tr>
</tbody>
</table>

Table 5.23: Major operational parameters and emissions result of the three modes tested.
combustion. The brake specific CO$_2$ emissions had a decreasing trend from 0.9% to 8.5%, with an increase of hydrogen, due to a decrease of hydrocarbon input to the engine. The brake specific PM emissions had an increasing trend from 25.5% to 14.2%, with an increase of hydrogen, due to the increase in localized combustion temperature. The brake specific fuel consumption had an increasing trend from 0.8 % to 3.4%, with an increase of hydrogen, due to the reduction of intake air.

Hydrogen increased the amount of premixed fuel added to the HECC mode, which was hoped to further enhance this PCCI mode. The reductions on the HECC modes emissions with hydrogen substitution were modest. As legislative emission restrictions on diesel engines increase advanced combustion modes will continue to be studied as a part of a solution. In this study, hydrogen substitution has been demonstrated in an engine running an advanced combustion mode up to 15% hydrogen fuel substitution, without penalty. Further benefits can be projected when hydrogen is utilized in an engine optimized for PCCI combustion.
Chapter 6
Conclusion

6.1 Conclusion

The aim of the studies presented in this Thesis were to examine the benefits of aspirating small quantities of hydrogen gas into the air intake of a diesel engine, while the engine was running in conventional combustion modes and advanced combustion modes. The following conclusions were drawn from the experimental worked conducted on the conventional combustion modes.

• Aspirating hydrogen into the air intake of an unmodified diesel engine will result in retarded injection timing, based on the engine’s ECU injection timing map, given the reduction of diesel fuel. Significant changes in emissions will occur due to the retarding of injection timing which can be repeated by manually retarding the injection timing without aspirating hydrogen.

• Depending on engine operation parameters, up to 30% of the fuel energy demand of a diesel engine can be from aspirated hydrogen. At 35%, the engine will choke from lack of oxygen.

• Hydrogen substitution for diesel fuel, by aspiration, resulted in a modest increase in brake specific NO\textsubscript{X} emissions. However, hydrogen substitution results in a significant decrease of brake specific NO emissions and a significant increase of brake specific
NO$_2$ emissions. The NO/NO$_2$ trade off caused directly from hydrogen substitution can be advantageously used in after treatment systems.

- Hydrogen substitution for diesel fuel, by aspiration, resulted in a modest decrease in brake specific CO emissions.
- Hydrogen substitution for diesel fuel, by aspiration, resulted in a modest decrease in brake specific CO$_2$ emissions.
- Hydrogen substitution for diesel fuel, by aspiration, resulted in a modest decrease in brake specific HC emissions at high load operation and a modest increase at low load operation.
- Hydrogen substitution for diesel fuel, by aspiration, resulted in a decrease in brake specific PM emissions at high speed operation and an increase at low speed operation.
- Hydrogen substitution for diesel fuel, by aspiration, resulted in an increase in brake specific fuel consumption. This increase is inherently due to the reduction of air via hydrogen substitution.

The following conclusions can be drawn from the experimental worked conducted on the advanced combustion modes.

- The advanced operation condition known as HECC was achieved on Penn State’s Detroit Diesel 2.5L TD DI-4V using simulated EGR. The resulting emissions corresponded to those of Wagner, Sluder and coworkers at Oak Ridge National Laboratory.
• The coefficient of variance of the indicated mean effective pressure was not affected by the substitution of hydrogen, beyond what can be achieved through a repeatability study without using hydrogen.

• The high concentration of EGR used in the advanced combustion modes reduced the brake specific NO emissions, such that hydrogen substitution had no reducing effect.

• Hydrogen substitution for diesel fuel, by aspiration, resulted in an increase in brake specific NO\textsubscript{2} emissions, resulting in an overall increase of NO\textsubscript{X}.

• Hydrogen substitution, by aspiration, for the advanced combustions modes caused trends similar to the conventional combustion modes for the brake specific HC, CO, CO\textsubscript{2} and PM emissions at low speed and low load conditions.

6.2 Future Work

The studies reported in this Thesis have generated questions to be answered in future work. The following areas of future work are recommended based on experimental worked conducted conventional combustion modes.

• In this study, the injection timing of diesel fuel was not optimized for the addition of hydrogen through aspiration. The engine was operated with the engine’s default injection timing locked. Increased emission benefits may be possible through the optimization of diesel injection timing.
• Aspiration of hydrogen into the air intake of a diesel engine is an inexpensive and simple method to retrofit an engine to combust hydrogen. This study has shown hydrogen substitution, via aspiration, to be limited to 30% hydrogen on an energy basis, before the engine is choked by lack of oxygen. Direct injection of pressurized hydrogen into the engine cylinders would allow for the majority of the fuel energy needed to operate a CI engine to come from hydrogen. A minimal amount of diesel fuel would be required to ignite the hydrogen as a pilot fuel. According to literature, higher percentages of hydrogen substitution yield emissions benefits.

The following recommendations for future work are based on experimental worked conducted on the advanced combustion modes.

• Combustion simulation and Computational Fluid Dynamics (CFD) modeling would provide insight into the localized concentrations of hydrogen in the pre-mixing combustion phase of the HECC mode. Furthermore, such modeling would provide accurate indication of local combustion temperatures which would aid in the explanation of the resulting emissions.

• The SMPS indicated the formation of nano-particles formed from the organic fraction of PM. The nano-particles were found while searching for the HECC mode at -2 °ATDC. When the thermal denuder was used to burn off the organic fraction of PM, trace levels of soot remained. This data indicates the possibility of nearly eliminating soot in a further optimized HECC mode.
• Simulated EGR constituted the majority of the EGR concentration needed to operate in the advanced combustion modes. Refinement of the EGR loop and a rebuild of the engine should allow the engine to run in the advanced combustion modes using actual EGR. A comparison between the emissions of the HECC mode entered using simulated EGR and actual EGR would be insightful.
Bibliography


Appendix A

Brake Specific Calculations

A.1 Brake Specific Calculations

In subsequent equations the method used to convert from part-per-million (ppm) emissions into brake specific emissions for the cases of CO is given. The NOx, NO, CO2, NO2, HC and PM emissions were converted to brake specific units using an identical method.

\[
\text{CO} \quad \frac{g}{kW\cdot h} = \frac{\text{CO} \quad \frac{g}{hr}}{(\text{load} \cdot kW)} \quad \text{A.1}
\]

Where:

\[
\text{CO} \quad \frac{g}{hr} = \left( \text{CO density} \quad \frac{kg}{m^3} \right) \left( \text{Exhaust flow, volumetric} \quad \frac{L}{hr} \right)
\]

\[
\left( \text{CO density} \quad \frac{kg}{m^3} \right) = \frac{(\text{CO ppm})}{1000000} \left( \frac{101325 \text{ Pa}}{8314 \text{ Pa} \cdot \text{m}^3 \cdot \text{mol} \cdot \text{K}} \right) \left( \frac{\text{CO MW}}{(273\text{ K}) + \text{Exhaust temp} \cdot \text{C}} \right) \quad \text{A.3}
\]

\[
\left( \text{Exhaust flow, volumetric} \quad \frac{L}{hr} \right) = \left( \frac{\text{Air} \quad \frac{M}{hr}}{\text{Exhaust Density} \quad \frac{kg}{m^3}} \right) + \left( \frac{\text{Fuel} \quad \frac{M}{hr}}{\text{Exhaust Density} \quad \frac{kg}{m^3}} \right) \quad \text{A.4}
\]
\[
\text{Exhaust Density}_{\text{kg/m}^3} = \frac{[300^\circ C \cdot (\text{Exhaust Density at 300C})]}{(\text{Exhaust temp} \ C + 273 \ K)}
\]

A.5

\[
\text{Exhaust Density at 300C} = 1.2 \frac{\text{kg}}{\text{m}^3}
\]

A.6
Appendix B

Error Analysis

B.1 Error Analysis

The error analysis method used in this Thesis was based on the error analysis method used by Hess[12]. Error is characterized in four main classes, instrument measurement errors, systematic errors, personal errors and random errors. Instrument measurement errors, also referred to as zeroth order uncertainty, are associated with the uncertainty that arises from the precision of measurement equipment. Systematic errors, also referred to as first order uncertainty, are associated with the uncertainty that arises from the accuracy of measurement equipment. Personal error is due to the judgment of an observer while recording the data. Random error is the error that remains after the instrument measurement errors, systematic errors, and personal errors are accounted for. The overall combination of all error is characterized as the Nth order uncertainty which can be quantified as the root-sum-square of the fore mentioned uncertainties [12, 56].

The value of error can be reported as absolute error, relative error or percentage error. The absolute error is the value given by the difference between the measured results and the actual results. The relative error is calculated by dividing the absolute error by the mean of the measured value. The percentage error is defined by multiplying the relative error by 100%.
Data acquisition was conducted under steady-state, with instrumentation measuring speed, load, temperatures, pressures, mass air flow, fuel mass, and emissions from the AVL bench, over a 15 minute sampling period, with a data point taken every 10 seconds. Though the engine operated at steady state, the AVL emission bench was placed in a standby mode until data sampling was enabled. The individual analyzers which comprise the bench often required an unpredictable period of time to stabilize. Thus, selections of 25 sequential data points were selected, those points having the lowest standard deviation of the recorded data. The points were then analyzed using the Student t-test to calculate the error between the 25 data points sampled at steady-state, as given in Eq. B.1. The Student t-test multiple used was 1.96, due to the 25 samples taken, based on a 95% confidence interval.

\[
\text{Percentage Error}_{\text{Student}} = \frac{t_{\alpha/2,v} \cdot \sigma}{\sqrt{n \cdot \chi}} \cdot 100\%
\]

Where:

\( t_{\alpha/2,v} \), Student t-test multiplier (1.96)

\( n \), number of data points (25)

\( \chi \), Mean

\( \sigma \), Standard deviation

The gaseous and PM emissions were the data of most concern in this Thesis. All other data have been taken used to better explain the resulting gaseous and PM emissions results. Thus, the gaseous and PM emissions data points were rigorously analyzed and
presented with error bars. The instrumental and systematic errors which affected gaseous and PM emissions measurements are presented in Table B.1, Table B.2 and Table B.3.

Table B.1: Major sources of instruments error which affect gaseous emission results in percent error.

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Equipment</th>
<th>Percent error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>HC%_Inst</td>
<td>HC analyzer error of linearization</td>
<td>1.570</td>
</tr>
<tr>
<td>NOX%_Inst</td>
<td>NOX analyzer error of linearization</td>
<td>0.308</td>
</tr>
<tr>
<td>NO%_Inst</td>
<td>NO analyzer error of linearization</td>
<td>0.308</td>
</tr>
<tr>
<td>NO2%_Inst</td>
<td>NO2 analyzer error of linearization</td>
<td>0.308</td>
</tr>
<tr>
<td>CO%_Inst</td>
<td>CO analyzer error of linearization</td>
<td>0.909</td>
</tr>
<tr>
<td>CO2%_Inst</td>
<td>CO2 analyzer error of linearization</td>
<td>0.714</td>
</tr>
<tr>
<td>FCE%_Inst</td>
<td>Fuel scale</td>
<td>0.136</td>
</tr>
<tr>
<td>RME%_Inst</td>
<td>Engine rotational speed measurement</td>
<td>0.111</td>
</tr>
</tbody>
</table>

Table B.2: Major sources of instruments errors which affect PM emission results in percent error.

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Equipment</th>
<th>Percent error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>BME%_Inst</td>
<td>BG-1 measurement</td>
<td>3.441</td>
</tr>
<tr>
<td>PSE%_Inst</td>
<td>PM scale</td>
<td>0.001</td>
</tr>
<tr>
<td>FCE%_Inst</td>
<td>Fuel scale</td>
<td>0.136</td>
</tr>
<tr>
<td>RME%_Inst</td>
<td>Engine rotational speed measurement</td>
<td>0.111</td>
</tr>
</tbody>
</table>

Table B.3: Major sources of systematic error which affect gaseous and PM emission results in percent error.

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Measurements</th>
<th>Percent error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>ERSM%_sys</td>
<td>Engine rotational speed measurement</td>
<td>0.032</td>
</tr>
<tr>
<td>ELM%_sys</td>
<td>Engine load measurement</td>
<td>0.227</td>
</tr>
<tr>
<td>MAFM%_sys</td>
<td>Mass air flow measurement</td>
<td>0.739</td>
</tr>
<tr>
<td>FM%_sys</td>
<td>Fuel measurement</td>
<td>0.812</td>
</tr>
</tbody>
</table>
Hess explains that the proper method for combining instrument and systematic errors for brake specific calculations in which multiplication occurs is to root-sum-square (RSS) the error in the percent error form. By doing so only large values of error are necessary to consider, since the RSS calculation will not be affected by errors which are 5 times smaller [12]. An example of the RSS calculation for gaseous NOx is given in Eq. B.2.

$$RSS_{\text{Percent}} = \left( \%\text{Error}_{\text{student}}^2 + \text{NO}_x^2 \cdot \text{Inst}^2 + FCE\%_\text{Intr}^2 + RME\%_\text{Inst}^2 + ERSM\%_\text{sys}^2 + ELM\%_\text{sys}^2 + MAFA\%_\text{sys}^2 + FM\%_\text{sys}^2 \right)^{\frac{1}{2}}$$  \hspace{1cm} \text{B.2}

The resulting percent error value was then divided by 100% to be converted back to a relative error value, as in Eq. B.3

$$\text{Error}_{\text{Relative}} = \frac{RSS_{\text{Percent}}}{100\%}$$  \hspace{1cm} \text{B.3}

The error bars were then finally calculated by converting the relative error into absolute error by multiplying by the mean value of the given brake specific value, as in Eq. B.4.

$$\text{ErrorBar} = \overline{X} \cdot \text{Error}_{\text{Relative}}$$  \hspace{1cm} \text{B.4}
Appendix C

Repeatability Study

C.1 Repeatability Study

To confirm the integrity and reliability of the data presented in the thesis, a repeatability study was preformed. The repeatability study consisted of three separate operations of the DDC 2.5L engine at 1800 rpm at 25% of maximum output with out hydrogen aspiration. Exhaust, intake air and oil temperatures noted in the data to confirm the consistency of engine operation condition. The indicators of the repeatability study are the gaseous emissions data in brake specific units, which are presented in Table C.1.

<table>
<thead>
<tr>
<th>Trial</th>
<th>Speed (rpm)</th>
<th>Power (Kw)</th>
<th>Exhaust (oC)</th>
<th>Intake Air (oC)</th>
<th>Oil (oC)</th>
<th>HC (g/kW.h)</th>
<th>NOx (g/kW.h)</th>
<th>NO (g/kW.h)</th>
<th>NO2 (g/kW.h)</th>
<th>CO (g/kW.h)</th>
<th>CO2 (g/kW.h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7/2/2007  12pm</td>
<td>1798.09</td>
<td>15.66</td>
<td>332.52</td>
<td>22.40</td>
<td>93.07</td>
<td>-</td>
<td>1.93</td>
<td>1.51</td>
<td>0.42</td>
<td>2.16</td>
<td>844.97</td>
</tr>
<tr>
<td>8/14/2007  8am</td>
<td>1805.27</td>
<td>15.67</td>
<td>339.47</td>
<td>21.48</td>
<td>91.47</td>
<td>0.83</td>
<td>1.93</td>
<td>1.50</td>
<td>0.42</td>
<td>2.28</td>
<td>838.26</td>
</tr>
<tr>
<td>8/14/2007  5pm</td>
<td>1805.14</td>
<td>15.66</td>
<td>342.30</td>
<td>21.89</td>
<td>91.70</td>
<td>0.76</td>
<td>1.88</td>
<td>1.48</td>
<td>0.40</td>
<td>2.21</td>
<td>845.21</td>
</tr>
</tbody>
</table>

Standard Deviation 4.11  0.01  3.04  0.46  0.87  0.05  0.03  0.01  0.01  0.06  3.94

The repeatability study confirms the repeatability of the data in this thesis by comparing the standard deviation of the three trials to the standard deviation of the engine operating at 1800 rpm and 25% of maximum output with 0% and 15% hydrogen substitution on an energy basis, given in Table C.2.
The 15% increase of hydrogen substitution seen in Table C.2 indicates an increase in the standard deviation compared to the standard deviation of the repeatability study, in all emission except for HC. The difficulties in recording HC emissions were discussed in the results sections of this thesis. The repeatability study shown here added confidence to the data presented in this thesis, even though hydrogen substitution resulted in modest changes in emission data.