Investigation of Knock in Gaseous Fuels in the Presence of Diluents

Roshan Ashok Rodrigues
Western Michigan University

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Recent energy security and environmental concerns have prompted growing interest into utilization of alternative fuels such as, natural gas and landfill gas. These gaseous fuels contain significant amount of diluents in the fuel composition, such as carbon dioxide, nitrogen, water vapor and other trace gases, which vary by geographical location. Successful engine operation is limited by a phenomenon called "knock", which occurs due to auto-ignition of the end gas ahead of the flame front, and therefore, needs to be investigated with the utilization of these gaseous fuels.

The present contribution discusses the experimental set-up, procedure and results of the investigation of knock in binary mixtures of methane and hydrogen with the presence of varying amounts of diluents, to closely represent the general composition of such gaseous alternative fuels. The knock characteristics were investigated using two methods namely, knock limited spark timing and knock limited compression ratio. From the empirical analysis, it was determined that, the addition of diluents, such as carbon dioxide and nitrogen to the binary mixtures, augmented the knock resistance characteristics to extend the engine operating limits.
INVESTIGATION OF KNOCK IN GASEOUS FUELS
IN THE PRESENCE OF DILUENTS

by

Roshan Ashok Rodrigues

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Roshan Ashok Rodrigues
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CHAPTER I

INTRODUCTION

Preface

Fossil fuels currently supply more than 83% of all the energy consumed in the United States and 78% of all the energy consumed in the world. In United States alone oil provides the primary contribution (35%) followed by natural gas (26%) and coal (22%). Presently, U.S. produces approximately 8.69 million barrels of oil per day while consuming 20.5 million barrels of oil per day approximately. To meet the energy demands and consumption U.S. now imports over half (58%) of its oil supply and this trend is expected to increase (68%) by 2025 based on economics and population growth.

The Energy Policy Act (EPAct) of 2005 was signed into law by President Bush more than a decade later since the enactment of the EPAct of 1992 by congress. The bill focuses on increasing domestic production, reducing foreign dependency on oil and improving air quality by promoting the use of clean burning alternative fuel sources. Natural gas, Hydrogen and Bio-gas are few of the “gaseous” alternative fuels that are defined by the 1992 EPAct.
It is evident that the ratification of the EPAct has further strengthened the production and utilization of alternative fuels as U.S. alone produced 22% of the world’s natural gas. Alternative fuels such as natural gas is a vital component in the nation’s energy supply as it has many applications and can serve a wide variety of sectors such as industrial, residential and transportation. Additionally, these gaseous alternative fuels can be classified as clean burning fuels with characteristics that generate significantly lower harmful emissions. Also, recent technological advancements in exploration and production sector can provide the industry the necessary means to increase production to meet the rising demand. As a result, the extensive use of alternative fuels is a trend that will continue to increase steadily in the coming years as an economical source of energy.

Objective of Study

The current rapidly growing interests on utilization of various alternative fuels, including low heating value fuels such as land filled gases and biogases, are prompted due to the energy security concerns and the environmental advantages. It is nevertheless augmented due to the recent high price of the conventional petroleum based fuels. Generally, the low heating value (Btu) fuels contain substantial amounts of the diluents such as carbon dioxide, nitrogen, water vapor and other trace gases in the fuel
composition. This paper describes experimental set-up and the results of the investigation of knock in a single cylinder variable compression ratio spark ignition engine fueled with gaseous fuels such as natural gas, which is primarily, methane and hydrogen in the presence of different amounts of diluents specifically carbon dioxide and nitrogen in the fuel mixture in order to represent closely the general composition of land filled and biogases in practice. The knock characteristics of the fuels were quantitatively evaluated and presented in terms of the Methane Number using various methods namely knock limited spark timing (KLST) and knock limited compression ratio (KLCR). Additionally, an algorithm was developed to provide general guidelines and optimization of the operation of the SI engines fueled by fuel-diluent mixtures through knock modeling.

Outline of Thesis
The main focus of the thesis is to determine the effect of knock in clean burning alternative fuels such as natural gas (predominantly methane) and hydrogen with the addition of diluents such as nitrogen and carbon dioxide. Chapter 2 discusses the background of alternative fuels while providing a deeper insight into alternative fuel properties and current technology.
Chapter 3 describes “knock” phenomenon and the various factors that affect its onset. Also, knock rating, which refers to the numerical classification of anti-knock, along with knock detection methods is mentioned.

Chapter 4 describes the experimental set-up which includes the equipment and data acquisition software. The set-up validation and experimental procedure is also discussed in this section.

Chapter 5 explains the set-up of the knock detector, the method and algorithm used to evaluate knock, and the validation procedure.

Chapter 6 evaluates the onset of knock in the presence of varying amounts of diluent in binary mixtures of methane and hydrogen fuel.

Chapter 7 presents the algorithm developed to model the knock limited spark timing and knock limited compression ratio using baseline data.

Chapter 8 briefly outlines the research study, summarizes the results and provides recommendations for future research.
CHAPTER II

BACKGROUND

Alternative Fuels

Natural gas, hydrogen, propane, bio-diesel, ethanol and methanol are all classified as “alternative fuels” and can be identified as fuels that are not extensively petroleum but yield substantial energy while providing significant environmental benefits.

There are several advantages to alternative fuels which directly impact a nation’s economy and energy security. Some of the more widely recognized are cost, emissions and foreign dependency. Alternative fuels on average are 15 to 40% less expensive than gasoline and diesel which when implemented can facilitate substantial savings rapidly as most of these fuels are domestically produced. Such fuels also burn cleaner thereby emitting less toxic exhaust emissions such as NO\textsubscript{x} and CO and pollutants such as particulate matter. Finally, significantly reduced foreign dependency on petroleum based fuels can be realized.

The current research deals specifically with “gaseous” alternative fuels such as natural gas, hydrogen, land-fill/bio-gas; therefore this paper will limit the discussion topics to the aforementioned fuels.
Gaseous Alternative Fuels

The 1992 EPAct recognizes several gaseous fuels as alternative fuels such as natural gas, hydrogen and bio-gas. The underlying characteristic of these fuels is that at standard conditions these fuels are of a gaseous form. This trait has empirically displayed enhanced combustion properties over conventional liquid fuels, with excellent combustion stability and cleaner burning consequently releasing less harmful emissions. Listed in table 2.1 and 2.2 are some of the properties compared with conventional fuels.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Heating Value (Mass basis)</th>
<th>Heating Value (Volume basis)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>51,500 Btu/lb (119.93 KJ/g)</td>
<td>270 Btu/ft³ (10,050 KJ/m³)</td>
</tr>
<tr>
<td>Methane</td>
<td>21,500 Btu/lb (50.02 KJ/g)</td>
<td>875 Btu/ft³ (32,560 KJ/m³)</td>
</tr>
<tr>
<td>Gasoline</td>
<td>19,000 Btu/lb (44.50 KJ/g)</td>
<td>836,000 Btu/ft³ (31,150,000 KJ/m³)</td>
</tr>
<tr>
<td>Diesel</td>
<td>18,250 Btu/lb (42.50 KJ/g)</td>
<td>843,700 Btu/ft³ (31,435,800 KJ/m³)</td>
</tr>
</tbody>
</table>

Table 2.1: Heating values of gaseous and conventional fuels

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Flammability Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>4.0% - 75%</td>
</tr>
<tr>
<td>Methane</td>
<td>5.3% - 15%</td>
</tr>
<tr>
<td>Gasoline</td>
<td>1.0% - 7.6%</td>
</tr>
<tr>
<td>Diesel</td>
<td>0.6% - 5.5%</td>
</tr>
</tbody>
</table>

Table 2.2: Flammability limits of gaseous and conventional fuels
Natural Gas

Natural gas is a non-renewable fossil fuel like coal and oil that is non-toxic, colorless, odorless, lighter than air and highly flammable. It predominantly consists of methane (CH₄) and is one of the world’s most abundant fossil fuel next to coal. Natural gas can either be stored on board a vehicle in tanks as compressed natural gas (CNG) at 3000 psig or cryogenically cooled to a liquid state, liquefied natural gas (LNG) typically at 20-150 psig. The primary composition of natural gas varies by geographical location but the typical composition is outlined in table 2.3 below.

<table>
<thead>
<tr>
<th>Name</th>
<th>Chemical Formula</th>
<th>Range (mole %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>CH₄</td>
<td>70.0 – 90.0</td>
</tr>
<tr>
<td>Ethane</td>
<td>C₂H₆</td>
<td></td>
</tr>
<tr>
<td>Propane</td>
<td>C₃H₈</td>
<td>0.0 – 20.0</td>
</tr>
<tr>
<td>Butane</td>
<td>C₄H₁₀</td>
<td></td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>CO₂</td>
<td>0.0 – 8.0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O₂</td>
<td>0.0 – 0.2</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N₂</td>
<td>0.0 – 5.0</td>
</tr>
<tr>
<td>Hydrogen Sulphide</td>
<td>H₂S</td>
<td>0.0 – 5.0</td>
</tr>
<tr>
<td>Rare gases</td>
<td>A, He, Ne, Xe</td>
<td>Trace</td>
</tr>
</tbody>
</table>

Table 2.3: Chemical Composition of natural gas
Natural Gas Outlook

Natural gas is currently being implemented by US to power fleets of vehicles and provide heat in homes. US has already begun to set-up up the next 900 of the next 1000 power plants will use natural gas. Its abundance and characteristics make it a feasible option. US boast’s approximately 3% of the world’s natural gas reserves at 189 trillion cubic feet.

Advantages of Natural Gas

Natural gas is designated as one of the cleanest burning alternative fuels when compared to gasoline or diesel as it emits relatively low levels of harmful by-products into the atmosphere. Current statistics reveal that the 60-70% of urban air pollution is attributed to the release of emissions by the transportation sector. The emissions recognized as a result of incomplete combustion are in the form of carbon monoxide (CO), and oxides of nitrogen (NO\textsubscript{x}). Carbon dioxide (CO\textsubscript{2}) is also identified as a pollution concern which is the emission as a result of complete combustion. Since, natural gas burns very efficiently a 90% and 60% respective reduction in smog-producing gases such as CO and NO\textsubscript{x} is observed. Also, CO\textsubscript{2} emission which is an acknowledged greenhouse gas is reduced significantly by as much as 30-40%. Further volatile organic compound (VOC) emissions is also reduced which is a result of evaporative emissions observed during fueling and use.
Apart from the environmental characteristics there exists a favorable operational and combustion advantage over liquid fuels such as enhanced power production efficiency, good combustion stability and greater tolerance to lean mixture operation.

**Landfill Gas / Biogas**

Landfill gas is a renewable fuel which is the result of the decomposition of organic waste by anaerobic microorganisms. It has a distinct rotten smell due to the presence of sulfides which at low concentrations is still quite potent. It is predominantly composed of methane and carbon dioxide along with traces of non-methane organic compounds (NMOC’s).

The primary composition of landfill gas (LFG) varies by geographical location but the typical composition is outlined in table below.

<table>
<thead>
<tr>
<th>Name</th>
<th>Chemical Formula</th>
<th>Range (Volume %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>CH₄</td>
<td>45.0 – 60.0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>CO₂</td>
<td>40.0 – 60.0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N₂</td>
<td>2.0 – 5.0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O₂</td>
<td>0.1 – 1.0</td>
</tr>
<tr>
<td>NMOC’s</td>
<td>NH₃, H₂ etc.</td>
<td>Trace</td>
</tr>
</tbody>
</table>

**Table 2.4:** Chemical Composition of landfill gas [18]
Landfill Gas Outlook
Currently, in the United States there exists 340 Landfill Gas to Energy (LFGTE) projects. Environmental Protection Agency (EPA) estimates that implementation of 600 additional LFGTE projects could significantly reduce the dependence on coal generated energy by providing electricity to power approximately one million homes [21]. As the costs of crude oil keeps continually increasing and living space becoming limited due to steady population growth, the use of landfill sites will be necessitated for the generation of power and also recycling.

Advantages of Landfill Gas
One of the biggest advantages of landfill gas is the reduction of emissions. Methane as a greenhouse gas is twenty-one times stronger than carbon dioxide and the utilization of landfill gas (LFG) as an energy source prevents methane from escaping into the atmosphere. It has also reduced the use of coal as an energy source which in turn has also helped decrease emissions. It also prevents surface water from being contaminated as the landfill sites used for LFGTE projects contain a plastic membrane that aid in gas extraction which is not present at conventional dumping sites. It has also helped to reduce the foreign dependence on oil by facilitating the generation of heat and electricity without the use of conventional fuels.
Hydrogen

Hydrogen is the most plentiful element in the universe and in recent years has been heavily pursued and researched to harness it as a cheap renewable source of energy. $H_2$ is a colorless, odorless and tasteless gas. It is also non-toxic but in excessive quantities when it displaces oxygen in air it can act as an asphyxiant. It also has exceptional properties such as a wide flammability range of 4% - 75%, low ignition energy, high auto-ignition temperature and high flame speed [1]. These characteristics make it an excellent fuel for S.I applications but there are certain limitations which makes it utilization limited such as generation by electrolysis which is quite expensive and its susceptibility to knock.

Hydrogen Outlook

With crude oil prices rising and increased global warming hydrogen is being actively pursued for implementation in hydrogen internal combustion engines (HICE) and fuel cells for the transportation sector. HICE has several benefits over fuel cells which is technology, cost and operation. HICE technology already exists whereas fuel cells are still being developed and optimized. A HICE application cost ten times less than a fuel cell application. From an operational aspect, HICE can be started in cold weather where as fuel cells are not capable. The establishment of a hydrogen infrastructure is
being heavily pursed along with hydrogen-powered vehicles. HICE is being acknowledged as the world’s cleanest combustion engine and it is only a matter of time until the technology is available to the consumer sector.

**Advantages of Hydrogen**

When utilized in S.I engines it can be used to run on lean mixtures and high exhaust gas recirculation (EGR) which enhances efficiency and reduces greenhouse gas emissions such as CO₂ and CO. Also, increased EGR reduces toxic NOₓ emissions. Hydrogen enhanced combustion (HEC) is also being pursued as a concept for ultra lean combustion. When added as an enrichment agent to conventional fuels with narrow flammability and mixture operational range it can significantly optimize the conventional fuel characteristics through improved flame propagation, mixture ignitability and combustion stability.
CHAPTER III

LITERATURE SURVEY

Introduction

Knock
Technically known as detonation, knock in spark-ignition engines occurs when the fuel-air mixture in the end gas region ignites ahead of the flame front that originates from the spark of the spark plug. As a result multiple flame fronts collide creating a shock wave [2] that reverberates in the combustion chamber which thereby creates a characteristic metallic “pinging” sound. The high pressure waves excite the resonance modes of the cylinder which can be heard as the distinct metallic “pinging” sound. The resonance frequency of the pressure oscillations is usually between 5 KHz - 20 kHz depending on the engine application [3].

Under normal operating conditions the fuel-air mixture is ignited by the spark generated by the spark plug. This causes the flame front to propagate through the combustion chamber until it reaches the cylinder walls and disperses. In a knock condition the end gas which is the unburned gas ahead of the flame front ignites thereby causing the flame fronts to collide which is known to create adverse effects.
Knock is extensively researched as it is a major barrier to achieving higher thermal efficiency and increased power output. The onset of knock due to auto-ignition causes sudden pressure changes in the cylinder and generates extremely high temperature spikes due to rapid combustion of gaseous mixture. This is acknowledged to cause potential damage mainly to pistons but is also known to affect piston rings, connecting rods, gaskets, bearings, and even the cylinder heads [4].

The onset of knock is affected by various factors such as:

- Spark timing (ST)
- Compression ratio (CR)
- Equivalence ratio (EQR)
- Fuel grade (Low BTU <600)
- Mixture temperature and kinetics
- End gas temperature, pressure and volume.
- Heat transfer

The factors that have the greatest impact such as ST, CR and EQR are briefly mentioned below to provide a better understanding.

**Spark Timing**

The goal of the ignition system is to ignite the fuel at a point where maximum amount of work can be achieved from the expanding gases and therefore
spark timing is a critical factor in preventing engine knock and also reducing power loss, gas consumption and emissions. The timing of the spark is usually advanced a certain number of degrees before the piston reaches top dead center (TDC) in order to maximize the required temperature and pressure in the cylinder during the power stroke (see Figure 3.1).

**Figure 3.1:** Schematic of cylinder displaying point of spark.

The spark timing can either be advanced or retarded depending on conditions. As engine speed increases more advance is required since the spark has to occur earlier as the speed of the pistons increase. Knock can be eliminated to an extent when the spark timing is retarded (moving the spark closer to the top of the compression stroke), since achievement of maximum temperature and pressure in the cylinder can be lowered also reducing the formation of harmful pollutants such as nitrogen oxides (NO\textsubscript{x}).
Compression Ratio

It is defined as the ratio of the volume of the cylinder at the beginning of the compression stroke (when the piston is at BDC) to the volume of the cylinder at the end of the compression stroke (when the piston is at TDC) and is an important parameter (Figure 3.2) of an engine. It is validated that higher compression ratios increase the air temperature in the cylinder at the end of the compression stroke to a point that leads to increasing thermal efficiencies and fuel economies. Diesel engines operate with high CR’s in order to generate the high temperatures required for fuel auto-ignition. In contrast, gasoline engines operate with lower compression ratios in order to avoid fuel auto-ignition, which is engine knock, often heard as a pinging sound.

Figure 3.2: Schematic of cylinder displaying top and bottom dead center.
**Equivalence Ratio (φ)**

It is defined as the actual air/fuel ratio divided by the stoichiometric air/fuel ratio. For a stoichiometric mixture $\phi = 1$, fuel-lean mixture $\phi < 1$ and fuel-rich mixture $\phi > 1$. The equivalence ratio is a critical factor in determining the NO$_x$ emissions since in a fuel-lean mixture the excess oxygen reacts with nitrogen to form nitric oxide (NO). In contrast a fuel-rich mixture lacks oxidizing agents and therefore NO formation is reduced resulting in negligible NO$_x$ emissions.

**Knock Rating**

In spark-ignition engines knock is a trait characterized by a pinging sound that results in loss of engine performance, increased emissions and potential damage to engine components. Auto-ignition of the end gas ahead of the propagating flame is responsible for the knock condition [5]. Therefore, the resistance of the fuel to the incidence knock is the most critical factor in the consideration of knock and consequently an experimental procedure for rating of gaseous fuels was established through the use of octane number (ON), methane number (MN) and the less widely used butane number (BN). Hence, knock rating refers to a numerical classification of motor fuel anti-knock that is established empirically with a specialized set of operating conditions.
**Octane Number (ON)**

Liquid fuels such as gasoline and diesel that are used to run an internal combustion engine specifically utilize octane number (ON) to determine the knock rating. Octane number is defined as a measure of the resistance of a fuel (typically liquid) to auto-ignition ("knock") when ignited in an internal combustion engine. The reference fuels utilized to establish the ON as specified by the ASTM procedure are iso-octane (2, 2, 4 tri-methyl pentane) and n-heptane where 100 percent iso-octane equals “100 ON” and 100 percent n-heptane equals “0 ON” [6].

The ON of certain blends of liquid fuels such as gasoline or diesel is determined by operating the CFR engine with the particular fuel at a specific set of operating conditions and subsequently comparing the onset of knock to a similar condition as tested with the reference fuels. Therefore, gasoline with an ON of 92 has the same knock characteristics as a mixture of 92 percent iso-octane and 8 percent n-heptane. Since, iso-octane displays minimal knock characteristics, a high iso-octane concentration would result in a higher ON indicating more anti-knock quality. The ON can also be utilized to classify gaseous fuels but due to their significantly lower sensitivity (more resistive) to knock than iso-octane the ON was replaced with methane number (MN) which is specifically designed to handle gaseous fuels.
**Methane Number (MN)**

Gaseous fuels such as natural gas or hydrogen when utilized to run an internal combustion engine instead of gasoline or diesel can create an entirely different variation of knock parameters. The methane number (MN) is defined as a measure of the resistance of a gaseous fuel to auto-ignition ("knock") when ignited in an internal combustion engine. The reference fuels utilized to establish the MN are methane and hydrogen where 100 percent methane equals “100 MN” and 100 percent hydrogen equals “0 MN” respectively.

The MN of a certain blend of gaseous fuel is determined by operating the CFR engine with the particular fuel at specific operating conditions and comparing the onset of knock to a similar condition as tested with the reference fuel to determine the knock rating.

**Knock Intensity**

To accurately determine the MN of a specific fuel blend an established measure is required to quantify the onset and intensity of knock which will identify a knock condition within an engine run. This parameter is acknowledged as the knock intensity and the empirical value employed as the threshold to define a knock condition varies from author to applications as it is very subjective.
Knock Detection

The accurate determination of the MN of a fuel relies on a reliable and repeatable knock detection method. Several methods exist in both industry and research that can be employed such as human ear, engine vibrations and cylinder pressure which are described below briefly as being some of the more common methods. Additionally, less sparingly used detection methods are the ion current and wall loss. Ion current is a recent technology but generates a lot of noise to be reliable and wall loss is still a principle [7].

**Human Ear**

The first knock detector to exist was the human ear and was established as the gold standard for a long time. The human ear is capable of detecting sounds in the 20 Hz to 20 kHz range but cannot accurately determine the knock intensity due to subjectivity. Therefore, more reliable methods were developed where the knock intensity and threshold could be clearly defined to identify a knocking condition.

**Engine Vibrations**

For individual engine applications knock is known to occur within a certain frequency range. An accelerometer with a piezo-ceramic element is utilized to measure the engine block or cylinder vibrations. The accelerometer generates electric signals that measure the vibration of the mechanical components due
to valve closing, piston slap and knock where the amplitude and frequency generated is relative to the engine vibrations and intensity of knock.

The low cost of accelerometers and ease of installation make this method prevalent and therefore, it has been extensively used in research and series production engines for knock detection [8]. Though these characteristics make it an excellent knock detector, a high level of expertise is required to perform frequency analysis such as Fast Fourier Transform (FFT) or Wavelet Transform (WT) to isolate the knocking signals [9].

Cylinder Pressure
It is a known attribute that during a knock condition the in-cylinder pressure rises to significantly high levels abruptly. This method utilizes a piezoelectric pressure transducer to measure the in-cylinder pressure. The pressure transducer generates an electric signal that determines the in-cylinder pressure where the pressure generated is relative to the combustion and intensity of knock.

This method is mainly used in research applications due to the high costs of piezoelectric pressure transducers and set-up. Additionally, these transducers also require additional equipment such as charge amplifiers and frequency filters. Even though the high investment cost, this method has been widely preferred due to the significant reliability and repeatability [9, 10] of the data.
generated to determine the onset of knock. Also, after conducting significant literature survey stating the direct link between knock and pressure oscillations [6, 9 - 17] the in-cylinder pressure knock detection method was determined to be a more feasible option as it provides a quantifiable metric not always seen in other methods described earlier. Therefore, for this current research the in-cylinder pressure method was adopted as the knock detector.

Knock Rating Procedure

The general method used to investigate knock for a particular composition of fuel when run under a constant set of operating conditions is to vary either spark timing or compression ratio. The knock limited spark timing (KLST) is determined by varying only spark timing (while keeping all other parameters constant) until the onset of borderline knock. Similarly, the knock limited compression ratio (KLCR) is determined by varying only compression ratio (while keeping all other parameters constant) until the onset of borderline knock.
CHAPTER IV

EXPERIMENTAL SET-UP, VALIDATION AND PROCEDURE

Introduction

To simulate landfill gas operation, the engine laboratory had to be initially set-up. Also, empirical data had to be generated prior to conducting knock analysis. This chapter provides a detailed description on the equipment and data acquisition software utilized for the experimental set-up. In addition, the experimental validation and procedure is discussed.

Experimental Set-up

Engine

An ASTM-CFR engine was utilized to conduct the knock investigation which is a single-cylinder, overhead valve, constant rpm, four-stroke, spark ignition engine with continuously variable compression ratio and spark timing. This engine is approved by the ASTM and is specifically designed and extensively used throughout the world for research and testing of fuels for the IC engine. The specifications for the ASTM-CFR engine are described in table 4.1 below as per the ASTM manual:
Table 4.1: Technical specifications of the ASTM-CFR engine

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>CFR-48</td>
</tr>
<tr>
<td>Type</td>
<td>Research</td>
</tr>
<tr>
<td>Displacement</td>
<td>611.72 cm³ (33.73 in³)</td>
</tr>
<tr>
<td>Stroke</td>
<td>11.43 cm (4.50 in)</td>
</tr>
<tr>
<td>Bore</td>
<td>8.25 cm (3.25 in)</td>
</tr>
<tr>
<td>Rpm</td>
<td>600 ± 6</td>
</tr>
<tr>
<td>Spark Timing</td>
<td>40ºCA BTDC to 40ºCA ATDC</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>4.5 to 16.0</td>
</tr>
</tbody>
</table>

The engine also features a three phase synchronous motor which is essentially a starter. The role of the synchronous motor is to run or in technical terminology “motor” the engine continuously. When the engine is operated with fuel, power is produced and the continuously running synchronous motor also works to absorb the power.

The engine utilized was originally designed to research and conduct tests on liquid fuels such as gasoline and diesel to determine ON and consequently for the current research, the engine intake system had to be modified to allow for the ability to run gaseous fuels in order to determine MN. The subsequent sections will describe the air and fuel metering system which was designed to permit gaseous fuel intake.
Air Metering Panel

The air metering panel was designed separate from the fuel and diluent metering panel as the requirements were significantly distinct. It essentially consisted of an electronic mass flow-meter to measure intake flow and a 0.075 m$^3$ (20 gallon) surge tank (Figure 4.1) to reduce the high intensity pressure pulsations generated during engine operation. The surge tank also provided a high volume charge of air to meet the cyclic intake demands of the engine. The components of the air metering panel are described in detail below.

**Mass Flow-meter**

The flow-meter is the most essential component in the air metering panel. This device was coupled to the engine data acquisition system and monitored via software though the analog output option of the flow-meter to allow the accurate delivery of air to acquire the required air-fuel mixture ratio to the engine intake. The TSI 4000 flow-meter with a 300 LPM range was used to quantify air volume. The range was selected by calculating the theoretical airflow (TAF) of the engine which is 183.51 LPM as per the formula below:

$$TAF = \left(\frac{ED \times RPM \times VE}{ES \times K}\right)$$  \hspace{1cm} (4.1)

- **TAF** = Theoretical airflow [ft$^3$]
- **ED** = Engine displacement [in$^3$]
- **RPM** = Engine Speed [rpm]
- **VE** = Volumetric Efficiency [%]
- **ES** = Engine Stroke (rotations per power stroke) [#]
- **K** = Conversion coefficient [in$^3$ to ft$^3$]
Surge Tank

The surge tank is a critical component of the air metering system subsequent to the flow-meter. Initially, the air flow-meter was installed to measure flow in the air supply line connected directly to the engine intake manifold. The high intensity cyclic pressure pulses generated from the four (4) strokes during engine run were skewing the air flow data and the installation of a surge tank facilitated to maintain the pulse intensity at a minimum. Also, the surge tank provided a high volume charge of air to meet the cyclic intake demands of the engine.

Check Valve

A flap check valve was utilized to ensure that fuel or diluents did not back flow and accumulate into the air metering panel during the non-intake strokes. Since, the fuels and diluents are metered to the engine above atmospheric pressure through the use of highly pressurized cylinders it was critical to contain the gases within the engine intake manifold to prevent any leakage into the surroundings.

Filter

The filter is the first component in the metering panel to ensure that the air delivered to the engine is free of debris and any contaminants. A paper filter was utilized to achieve the required filtration.
Fuel and Diluent Metering Panel
The fuel and diluents metering panel was developed in order to safely and accurately meter the desired mixture ratios prior to engine intake. The panel consisted of four (4) sets of electronic mass-flow meters to regulate the desired concentrations of four types of gases namely methane, hydrogen, carbon dioxide and nitrogen. The Omega FMA series and TSI 4000 mass flow-meters utilized were specifically calibrated for the individual gases. Additionally, the panel consisted of flashback arrestors, gas filters, flow controller, pressure gages, check valves and a mixing manifold. The components of the fuel metering panel are described below and listed chronologically as per the figure 4.1 set-up.

Filter
The filter is the first component in the fuel and diluents metering panel to ensure that the fuel/diluents delivered to the engine is free of debris and any contaminants. A paper filter was utilized and achieved the required filtration.

Mass Flow-meter
The flow-meter is the most essential component in the fuel and diluents metering panel. This device was coupled to the engine data acquisition system and monitored via software though the analog output option of the flow-meter. This set-up allowed the accurate delivery of fuel to acquire the
required air-fuel mixture ratio to the engine intake mixture. Omega FMA series and TSI 4000 mass flow-meters were utilized that were selected and calibrated specifically for the individual gases (see Table 4.2).

<table>
<thead>
<tr>
<th>Model</th>
<th>Gas</th>
<th>Flow Rate (LPM)</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>TSI 40241</td>
<td>Methane (CH$_4$)</td>
<td>30</td>
<td>Fuel</td>
</tr>
<tr>
<td>Fathom GR111</td>
<td>Hydrogen (H$_2$)</td>
<td>100</td>
<td>Fuel</td>
</tr>
<tr>
<td>Fathom GR111</td>
<td>Carbon Dioxide (CO$_2$)</td>
<td>35</td>
<td>Diluent</td>
</tr>
<tr>
<td>Fathom GR111</td>
<td>Nitrogen (N$_2$)</td>
<td>77</td>
<td>Diluent</td>
</tr>
</tbody>
</table>

**Table 4.2:** Fuel and diluent mass flow-meter specifications

The mass flow meters selected were calibrated for standard conditions to eliminate any discrepancies. A brief overview of the calibration procedure is explained in the set-up validation section of this chapter.

**Flow Controller**

To accurately dispense the individual fuels and diluents needle valves were incorporated into the design that could be manually operated through the use of the adjustment knobs. Four sets of coarse and fine flow controllers were installed. The coarse controllers were used to bring the individual gases to the vicinity of the required volumetric flow percentage and then using the fine controllers the desired mixture ratio was precisely set.
Pressure Gauge
A diaphragm type 0-30psi pressure gauge was employed to monitor the metering pressure of the individual fuels and diluents. The gauge was also used to ensure that the fuels and diluents were not metered at a pressure that could cause potential engine or metering panel damage. Additionally, it also verified the proper functioning of the check valve of the flashback arrestor to ensure that the threshold value of 22psig was not exceeded.

Check Valve
The fuel/diluent metering panel consisted of individual check valves that were rated to the specific gas characteristics in order to prevent any reverse flow during metering of single or multiple fuels into the engine intake. The check valves essentially prevented reverse flow in the individual fuel lines that were not being metered.

Flash Back Arrestors
The experimental analysis consisted of motoring" the engine with highly flammable gases such as H₂ and CH₄. In order to avert potentially dangerous situations, flash back arrestors were installed on the high pressure gas cylinders. Western FA-10 arrestors were used on the individual cylinders containing flammable gases. The arrestors house a flame trap that by design restricts flow to stop a potential flashback situation.
**Fuel and Diluent Mixing Manifold**

The final critical component that the fuel and diluent metering panel encompasses is the mixing manifold which enables the individually metered gases to appropriately mix prior to engine intake. When metering multiple gases it is important that suitable mixing occur to prevent generation of inaccurate test data due to combustion as a result of inconsistent gas mixture or an excess of a particular fuel or diluent at a given instant. The manifold was designed in-house to accept all four gases within in the same location at the highest point to allow ample time for proper mixing prior to engine intake.

**Figure 4.1:** Schematic of engine set-up with air, fuel and diluent metering panels.
Data Acquisition (DAQ) Hardware

In order to analyze the various engine related parameters such as crank angle, cylinder pressure, exhaust temperature, intake temperature and flow rates of gases a data acquisition system was utilized. Therefore, it was necessary to procure hardware that could be compatible with the DAQ system. The following section describes in detail the equipment that was coupled to the DAQ system in order to gather the necessary engine data.

Pressure Sensor

The sensor used for the empirical application was the KISTLER 7061B ThermoComp® Quartz (See Figure 4.2) which is a water-cooled piezoelectric transducer specifically designed to operate in IC engines. When utilized in a combustion chamber where severe temperature variations occur, the sensor provides highly-precise thermodynamic measurements. It is also highly insensitive to thermal shock as it features a double diaphragm which increases accuracy.

The measurement was acquired through the piezoelectric element or quartz crystals contained in the sensor which generates an electrical charge (coulomb) that is proportional to the mechanical loading. The measuring range of the sensor was 0 to 250 bars with a sensitivity of -80 pC/bar. Additionally, the sensor selected also had a high natural frequency of 45 kHz.
to ensure that it would not interfere with the natural frequency of knocking. The high impedance charge signal generated from the sensor was then transmitted to a charge amplifier using a highly insulated low noise cable.

![Figure 4.2: KISTLER ThermoComp® piezoelectric pressure transducer.](image)

**Charge Amplifier**

The primary function of the charge amplifier is to convert the high impedance charge signal generated by the pressure sensor to a low impedance voltage signal that can be easily employed in the DAQ system. A PCB model 462A charge amplifier was used to couple the Kistler pressure sensor to the DAQ
system (See Figure 4.3). Since, the resonance frequency of the pressure oscillations due to knock varies by engine and application in a range up to 40 kHz the charge amplifier was coupled to a 180 kHz low pass filter to ensure that significant knock frequencies are captured by the DAQ system. Additionally, the output of the pressure sensor was amplified using the charge amplifier by a factor of 5000. The sensitivity of the charge amplifier was 100 pC/volt and therefore the calculated sensitivity of the pressure sensor was -1.25 bar/volt.

Figure 4.3: Set-up of charge amplifier with pressure sensor.

Rotary Encoder

For the knock study it was necessary to generate in-cylinder pressure data with respect to crank angle. A BEI model HS35 incremental optical encoder was utilized to relay this information to the DAQ system (See Figure 4.4). It featured a hollow shaft which enabled the encoder to be installed on the externally extended crank shaft of the CFR engine.
The encoder works by transmitting light through a code disc (rotated inside the encoder allowing it to act like a shutter that alternately transmits and shuts off light) to a photo-detector. As a result a series of square waves are produced as it rotates. The 4096 disc resolution of the encoder selected allowed 4096 square wave cycles to be captured in one revolution of shaft turn. Therefore, a 0.0879° crank angle resolution was achieved. The encoder was also used as an external clock to appropriately display the pressure curve with respect to crank angle.

Figure 4.4: Image of BEI rotary encoder.
Mass Flow-meter
The air, fuel and diluents metering panel consisted of mass flow-meters that were utilized to determine the flow rate of the individual gas metered. As described earlier the air flow meter used was TSI model 40241 which featured a fast response time of 4 milliseconds to ensure accuracy due to fluctuating flow observed during normal engine operation. The operating principle of the TSI flowmeter is heat transfer and it incorporates a platinum film and a thermistor. The platinum film is continuously heated and maintained to a constant temperature while the thermistor is used to measure the flow temperature. When a flow stream is present the heat is transferred from the platinum film proportional mass flow rate.

Figure 4.5: Image of TSI mass flow-meter.

The fuel and diluents were metered using the Fathom model GR111 which is also based on a thermal principle. The flow stream is passed through a capillary tube that contains heated resistance temperature detectors (RTDs).
This creates temperature differential that is proportional to the mass flow rate (See Figure 4.6). This meter featured a response time of 1 second which was quite acceptable due to the pressurized delivery of fuels and diluents. Both mass flow-meters were coupled to the DAQ system using the voltage analog output option of the device.

Figure 4.6: Working principle of FATHOM mass flow-meter.

Thermocouple
The inlet and exhaust temperatures were measured using J-type Omega thermocouples in the respective manifolds. The 0 to 480 °C range of the thermocouple made it well suited for the experimental application. The operating principle of the thermocouple is the junction of dissimilar metals (Iron and Constantan) which produces a temperature dependent voltage.

Terminal Block
A National Instruments (NI) model SCB-68 terminal block was utilized to
connect the output signals of all the sensors to be coupled to the DAQ system. The terminal block contains 68 shielded input/output (I/O) in a connector block with screw terminals for easy installation (See Figure 4.7).

![SCB-68 terminal block](image)

**Figure 4.7:** Image of SCB-68 terminal block.

**DAQ Card**

The final device incorporated in the DAQ hardware is the DAQ card which interfaces with the PC by featuring an analog to digital converter (ADC). This enables the PC to couple the signals to LABVIEW software in order to display results numerically or graphically (see Figure 4.8). To acquire the sensor data efficiently a 12 bit resolution and 500 kS/s sampling rate was utilized.
Figure 4.8: Schematic of data acquisition set-up.

Data Acquisition (DAQ) Software

National Instruments graphical programming language “LabVIEW VI” was used for data acquisition. LabVIEW operates on various platforms (Windows, Mac etc.) and is used extensively for data acquisition, measurement analysis and instrumentation control. LabVIEW is quite sophisticated in which it provides a user the ability to create programs using graphical tools and icons as opposed to the conventional text code.

Virtual instruments are programs created in LabVIEW which are also called VI’s in short. These VI’s are stand alone or can further contain sub-VI’s which are similar to sub-routines in regular programming languages such as C++. The software has two main windows which are the Front Panel and Block Diagram.
The front panel is used to create and display the instrumentation, graphs or numerical data. It consists of controls and indicators which are user inputs and program outputs respectively. The block diagram is where the user inputs the graphical code such as functions (like addition, subtraction etc.) or execution structures (like while loops, for loops etc.). In order to acquire and analyze data for the current experimental set-up three VI’s were utilized which are as follows:

- Acquiring Flow Data
- Recording Pressure Data
- Detect Knock

The following section describes each of the VI’s briefly.

**Acquiring Flow Data VI**

In order to ensure the accurate mixture delivery of air, fuels and diluents during engine operation the Acquiring Flow Data VI had to be utilized. This VI essentially displays the flow rate of intake air, fuels and diluents that are delivered to the engine intake manifold. Apart from displaying the mixture ratio of the various fuels and diluents along with air in order to simulate different gaseous fuel composition the VI was extensively used to monitor and set the EQR. All data was displayed in real-time which was an important aspect to aid in adjusting and fine tuning the mixture ratio’s that were subject to a highly dynamic environment (see Figure 4.9).
Due to the dynamic nature of flow the real-time data had to be analyzed in order to ensure that the proper mixture ratio was being delivered. This was achieved with the use of a sub-VI called composition solver. The composition solver VI was used to calculate the mixture ratio required to run the engine in order to generate empirical data. To detect knock in different compositions of landfill gas the air-fuel mixture had to be simulated with the proper proportions of air, CH\textsubscript{4}, H\textsubscript{2}, CO\textsubscript{2} and N\textsubscript{2}. Due to the number of being experiments conducted it was not feasible to determine the proper ratios by trial and error method. Therefore, a mathematical approach to
accurately determine the flow rate was utilized which consisted of solving linear equations solver. Since, the study investigates different compositions of landfill gas, the variation in delivery composition of methane, hydrogen, carbon dioxide or nitrogen had a significant effect on EQR as a change in volume of any one variable affected the overall mixture ratio. The baseline fuel for landfill gas was CH$_4$ and the addition of H$_2$ impacted the EQR as it was now dependent on the volume of both the fuels at any given time since both are combustible gases. The equations and the various variables involved to determine the correct volumetric proportions are described below.

Here the variable “x” is the methane flow rate, “y” is the hydrogen flow rate, “h” is the air flow rate and “Φ” is the equivalence ratio use to define lean, rich or stoichiometric condition.

$$\frac{x + y}{h} = \phi \cdot \frac{x + y}{S_a}$$

(4.2)

“S$_a$” is the stoichiometric air flow which is variable due to the presence of two fuels namely methane and hydrogen and is determined by:

$$S_a = 9.52x + 2.38y$$

(4.3)

In equation 4.3 above, 9.52 is the stoichiometric volume of air for one mole of CH$_4$ and similarly 2.38 is the stoichiometric volume of air for one mole of H$_2$. 
Further, to calculate the required mixture proportion to simulate landfill gas and bio-gas the following equations were necessary:

\[
\frac{x}{x + y} = mp. \tag{4.4}
\]

\[
\frac{y}{x + y} = hp. \tag{4.5}
\]

\[
\frac{z}{x + y + z + p} = co2p. \tag{4.6}
\]

\[
\frac{p}{x + y + z + p} = np. \tag{4.7}
\]

The appropriate air-fuel mixture ratio is required for combustion. The make-up of the fuel mixture simulating landfill gas is composed of combustible and incombustible (diluent) gases. Now, since methane and hydrogen are the only combustible fuels, equations 4.4 and 4.5 display the required percentage of CH\(_4\) (mp) and H\(_2\) (hp) individually with respect to combustible fuels only. The required percentage for carbon dioxide (co2p) and nitrogen (np) are displayed in equations 4.6 and 4.7 respectively and being incombustible represents an individual percentage in the entire fuel and diluent mixture.

To provide further understanding take for example a composition with 80 MN in the presence of 10 percent CO\(_2\) only. The fuel make-up of 100 percent would consist of 90 percent combustible fuel and 10 percent incombustible
fuel which is CO$_2$. To get the required 80 MN the 90 percent of combustible fuel would consist of a mixture ratio of 80 percent CH$_4$ and 20 percent H$_2$ which means the overall 100 percent fuel composition would consist of 72 percent CH$_4$, 18 percent H$_2$, and 10 percent CO$_2$.

Finally, equation 4.8 displays total flow rate ($T_{LPM}$) of the engine intake which has a TAF value of 183.51 LPM. The flow rates of all variables should equal $T_{LPM}$ to establish the correct mixture proportions. Now, the $T_{LPM}$ varies by engine set-up, variables being applied and is never constant. Therefore, the $T_{LPM}$ is a variable that is generated during engine run using real-time data acquisition.

$$h + x + y + z + p = T_{LPM}$$ (4.8)

From equations 4.2 to 4.8 six linear equations are generated, which when solved for the unknown variables ($x$, $y$, $z$, and $p$) gives the percentage or flow rate for a desired fuel composition. These values which are displayed in real-time are then set manually from the fuel control panel.

\[
\Phi h - 9.52x - 2.38y + 0z + 0p = 0
\]

\[
0 h + (mp - 1) \cdot x + mp \cdot y + 0z + 0p = 0
\]

\[
0 h + hp \cdot x + (hp-1) \cdot y + 0z + 0p =0
\]

\[
0h + co2p \cdot x + co2p \cdot y + (co2p-1) \cdot z + co2p \cdot p=0
\]

\[
0h + np \cdot x + np \cdot y + np \cdot z + (np-1) \cdot p=0
\]

$$h + x + y + z + p = T_{LPM}$$ (4.9)
The composition solver sub-VI helped eliminate the tedious task of calculating the flow-rate and was critical to the experimental set-up. The VI is displayed in figure 4.10 below.

**Figure 4.10**: Front Panel of Composition Solver sub-VI

**Recording Pressure Data VI**

With the flow VI functioning to allow proper engine operation it was then required to record the engine pressure data with respect to crank angle to perform the knock analysis. The front panel of the VI (see Figure 4.11) was set-up so that certain variables namely atmospheric pressure, compression...
ratio, spark timing, intake and exhaust temperature would be entered prior to data acquisition. Before acquiring any pressure data, the engine was operated at the desired fuel composition for a minimum of 10 minutes to ensure that the readings would be repeatable. This was to avoid any situations where the engine is not completely warmed up to its operating temperature or the flow rates not being stabilized to the desired values. An external counter was used to track the time and after 10 minutes the VI was activated to acquire. The in-cylinder pressure data was then acquired for 100 consecutive engine cycles to account for cyclic variability of the engine.

![Front panel of Recording Pressure Data VI](image)

**Figure 4.11:** Front panel of Recording Pressure Data VI
After acquisition the average of the 100 cycles was calculated and exported to a LMV data file. Apart from the in-cylinder pressure data the VI calculated the averages of power generated per cycle and work done per cycle while displaying P-V and pressure versus crank angle data graphically.

**Detect Knock VI**

This VI was developed specifically to detect knock from the in-cylinder pressure data that was exported to LMV data file. Ideally this VI would be a sub-VI in the Recording Pressure Data VI to acquire real-time knock indication. But, due to the specification of the computer (Intel Pentium III and 256 MB RAM) it was difficult to run it as a sub-VI without causing high CPU usage. The next chapter will describe the knock detector VI in more detail.

**Experimental Set-up Validation**

**Background**

The CFR engine and its components were calibrated and validated to ensure that the empirical data obtained is accurate. In any research the most important factor in obtaining good results is ensuring the set-up is well calibrated and documented. With the engine set-up coupled to the DAQ hardware and software to obtain data it was necessary to perform additional validations to ascertain reliable and repeatable conditions.
The following procedures were performed on variables such as cylinder height, spark timing and top dead center of the CFR engine and DAQ software to validate the engine set-up to provide accurate data.

**Cylinder Height**

The continuously variable compression ratio on the CFR-ASTM engine is achieved by changing the cylinder height while referring to the micrometer indicator to determine compression ratio desired. The initial reference cylinder height position is essential to the experimental set-up and needs to be carefully calibrated as it establishes the proper relationship between the micrometer setting readout and the compression ratio.

![Figure 4.12](image)

**Figure 4.12:** The variation of the compression pressure curve at 0.352 micrometer reading for the CFR engine during motoring at intake temperature 303 K, intake pressure 98 kPa and 600 rpm.
The first step in determining the basic cylinder height was to install a CFR compression pressure gage and run the CFR-ASTM engine at normal operating conditions (see Figure 4.12). The compression pressure gage available from Waukesha Motor Co. was equipped with a check valve assembly fitted with TFE-fluorocarbons wafer seals. The basic cylinder height setting for the research method was set by referring to the ASTM-CFR manual Figure 11-(b) which displays graphically the compression pressure (psig) for prevailing barometric pressure (in-Hg) at time of validation test. Using the compression pressure gage the cylinder height was gradually adjusted to display 1358 kPa (197 psig) as determined per the graph for a barometric pressure of 741.6 mm-Hg (29.2 in-Hg). The concluding step was to adjust only the micrometer indicator to display a reading of 0.352 without further changing the cylinder height setting.

**Spark Timing**

The ability of the flame front originating from the spark plug to progress into the end gas region dictates combustion occurrence in an engine. The spark timing is of the utmost importance as it is the parameter used to establish maximum power for a given set of engine conditions. The spark timing can be advanced to achieve maximum engine efficiency or retarded to eliminate engine detonation during high engine loads. Therefore, the functional testing
was carried out to validate correct spark timing using the flashing neon light on the spark timing scale, SNAP ON computerized tach advance strobe light and also through LabVIEW using the Spark Timing VI. The Snap-on digital tachometer model MT1261A helped expedite the setting of the spark timing as opposed to flashing neon light indication method. The digital tachometer has an accuracy of ± 1° as opposed to the neon tube indication method where multiple flashes are prevalent and hard to read under bright conditions. The VI also was used to validate the ST by observing the in-cylinder pressure curve with respect to CA. During a spark the in-cylinder pressure at that given instant displays noisy data which is the result of a voltage spike. This was used as an indicator to determine if the ST was set correctly (Figure 4.13).

![Graph of Pressure vs. Crank Angle (deg)](image)

**Figure 4.13:** Spark timing validation. The variation of pressure vs. CA in the CFR engine with methane operation at compression ratio 12, spark timing of 16° BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Top Dead Center

The rotary encoder was coupled to the pressure recording VI and the trigger point to being acquiring data was set for TDC. If the trigger point is incorrectly set or is not activated at TDC the data generated would be inaccurate. It is known that maximum pressure occurs at TDC and using that information the trigger point was verified by differentiating in-cylinder pressure with respect to crank angle. When plotted the differentiation at TDC should be zero which is displayed in Figure 4.14.

![Figure 4.14: TDC validation. The variation of \( \frac{dP}{d\theta} \) vs. crank angle in the CFR engine during motoring at compression ratio 8:1, spark timing of 30° BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.](image)

With the variables validated the experiments were conducted with high confidence to generate accurate, reliable and repeatable data. The next section discusses the experimental procedure utilized for the generating data.
Experimental Procedure

Bio-gas and landfill gas on an average have a composition of 54 percent methane, 42 percent carbon dioxide, and 4 percent nitrogen [18]. The gas composition varies with time and geographical location and therefore in order to closely represent the landfill and bio-gas compositions the experiments were conducted for various compositions of fuel mixtures and with different percentage’s of carbon dioxide and nitrogen as the diluents. The main objective of the experiments performed was to determine the effect of diluents (CO₂ and N₂) especially carbon dioxide on the fuel mixture composition as it accounts for a significant portion of the diluent in a landfill gas composition.

To investigate the onset of knock in the presence of diluents, the KLST and KLCR had to be determined with different volumetric compositions of diluents. This involved the variation of spark timing for KLST while keeping all other parameters such as equivalence ratio, compression ratio and intake temperature constant. Unless otherwise specified, the KLST values were determined for a constant compression ratio of 12:1, equivalence ratio of 1.0 and an intake temperature of 303K. The spark timing was varied from 40° BTDC to 40° ATDC which is based on the fuel/diluent composition and operating conditions. With the SNAP-ON tachometer the ST was easily adjusted until the onset of borderline knock.

Similarly, the compression ratio was varied for KLCR while keeping all other parameters such as equivalence ratio, spark timing and intake temperature constant. Unless otherwise specified, the KLCR values were determined for a constant spark timing of 13° BTDC, equivalence ratio of 1.0 and an intake
temperature of 303K. The compression ratio was varied from 4.5 to 16.0 for the various fuel/diluent compositions and operating conditions with the use of the installed micrometer indicator until the pre-determined knock intensity was achieved.

The initial set of experiments conducted were to determine the baseline knock characteristics, specifically KLST and KLCR for binary mixtures of methane and hydrogen at MN 0, 20, 40, 60, 80 and 100. The baseline was critical to the determination of optimum spark timing and compression ratio to cover the range of parameters in order to conduct useful knock analysis. Once the baseline data was generated, the KLST and KLCR was further investigated for different volumetric compositions of binary mixtures of methane and hydrogen in the presence of 10, 20, 30, 40 and 50 percent CO\textsubscript{2} and 5, 15, 25 and 40 percent N\textsubscript{2}.

The general procedure utilized to conduct the experiment and generate empirical data is briefly described in this following section with the first step being to open all the LabVIEW VI’s. Then, all the gas cylinders and cooling water flow valves are opened. Based on the rating method KLST or KLCR, either compression ratio or spark timing respectively would be set initially. Compression ratio can be adjusted before the engine is motored or while it is motoring, but spark timing can only be set while the engine is motoring. Once, either parameter is set the Acquiring Flow Data VI’s is activated where the desired volumetric concentrations are keyed in. The flow controllers are then manually adjusted until the desired flow is achieved after which the engine is operated for a minimum of ten minutes to ensure stabilization of cooling water and lubricant oil temperatures.
Once the engine warms up and stabilizes all necessary information is keyed into the Record Pressure Data VI and is then activated. The VI records 100 cycle pressure data and saves the readings it into a data file. To generate data for a different composition the Acquiring Flow Data VI is activated once again and the process is repeated until all required data is generated for analysis. With the conclusion of the experiment(s) all gas cylinder valves are first shut while the engine is still motoring to ensure that all gases are purged from the fuel lines. Lastly, the VI’s and the engine is shutdown and the cooling water valve closed.

Now, prior to analyzing knock from the generated empirical data a critical element which is the knock detector had to be programmed using LabVIEW data analysis software and experimentally validated. The Detect Knock VI was designed and developed to analyze the saved pressure data file in order to determine variables such as knock intensity and number of knock. Detailed information on the development and validation of the VI is discussed in the next chapter.
CHAPTER V

KNOCK DETECTION AND VALIDATION

Background
With the experimental set-up complete it was necessary to set-up the knock detection VI in LabVIEW to analyze and accurately determine the knock rating or MN of a fuel. Unlike peak pressure data acquisition setting up a knock detector is quite expensive. It requires high end transducers to ensure suitable filtering of the noise which is mainly generated during ignition, piston slap, closing of valves and also from the use of inexpensive transducers. Also, a high level of expertise is required in frequency analysis and acoustic mode detection applicable during the onset of knock [9, 10].

Knock Detection Method
For the current research and with the experimental set-up, the in-cylinder pressure knock detection method was adopted as a feasible option without the procurement of any expensive equipment. Also, after conducting significant literature survey stating the direct link between knock and pressure oscillations [10, 11, 12, 13, 14, 15, 16, 17] the in-cylinder pressure knock detection method was adopted as shown in figure 5.1 as it provides a quantifiable metric not always seen in other methods.
The knock was detected and quantified by using an algorithm developed by M. D. Checkel and J. D. Dale [19] which calculates the first, second and third differential of in-cylinder pressure (See Figure 5.2 - 5.4) and then in addition verified by the audible pinging sound heard during a knock condition. It is a known attribute that during a knock condition the in-cylinder pressure rises to significantly high levels abruptly [20] and the third differential of this abrupt pressure rise generates a large negative value (See Figure 5.4) that can be directly related to flame front collision due to end gas ignition.

The knock indicator algorithm used was essentially a cubic spline fit differentiator which uses nine points around a centered point to calculate each point’s derivative as a local slope of the best fit line [19].

\[
dP(\theta) = \frac{86[P(\theta+4) - P(\theta-4)] + 142[P(\theta+3) - P(\theta-3)] + 193[P(\theta+2) - P(\theta-2)] + 126[P(\theta+1) - P(\theta-1)]}{1188*d\theta}
\]  

(5.1)

As with any digitized data a certain degree of inherent noise always exists and therefore the knock indicator algorithm also included a low pass filter to smooth out the noise.

\[
F(\theta) = \frac{2[S(\theta-4) + S(\theta+4)] + 3[S(\theta-3) + S(\theta+3)] + 4[S(\theta-2) + S(\theta+2)] + 5[S(\theta-1) + S(\theta) + S(\theta+1)]}{33}
\]  

(5.2)
The 100 cycle in-cylinder pressures were then acquired for a knock and non-knock conditions and were used to calculate and plot the respective third derivatives using the knock indicator algorithm (See Equation 5.1 and 5.2) that was set-up in the Detect Knock VI. The resulting third derivative data was filtered using a low pass filter and plotted against crank angle to determine the negative amplitude. After successful functioning of the knock indicator algorithm, the knock threshold value had to be determined that would distinguish a knock condition and validated to ensure accurate results. The Detect Knock VI helped establish the threshold value to indicate a knock condition as it allowed for user inputs of critical values such as knock region and knock amplitude which was set by trial and error method.

![Figure 5.1](image-url)  
*Figure 5.1: Average of 100 cycle pressure curve for knock and non-knock at compression ratio 14:1, spark timing 25° BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.*
Figure 5.2: 1\textsuperscript{st} derivative of the average of 100 cycle pressure curve for knock and non-knock conditions at compression ratio 14:1, spark timing 25\degree BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 5.3: 2\textsuperscript{nd} derivative of the average 100 cycle pressure curve for knock and non-knock conditions at compression ratio 14:1, spark timing 25\degree BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Figure 5.4: 3rd derivative of the average of 100 cycle pressure curve for knock and non-knock conditions at compression ratio 14:1, spark timing 25° BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Detect Knock VI

This VI was developed specifically to detect knock from the in-cylinder pressure data that was exported to LMV data file from the pressure data VI. Ideally, the Detect Knock VI would be a sub-VI in the Recording Pressure Data VI to acquire real-time knock indication. But, due to the specification of the computer (Intel Pentium III and 256 MB RAM) it was difficult to run it as a sub-VI without causing high CPU usage which would eventually cause the program to hang-up or freeze. The front panel of the VI displayed plots of in-cylinder pressure with respective first derivative, second derivative and third derivative (See Figure 5.5).
Figure 5.5: Front Panel of Detect Knock VI displaying in-cylinder pressure with 1st, 2nd and 3rd derivative graphs. Also, displayed is the user input fields which are the knock region (time to start/end) and threshold knock value.
The front panel also contained user input fields which allowed to set the
knock region (time to start/end) and threshold knock value. Also, an analysis
feature was added to the VI that contained a user defined time constant. This
permitted a wait time of usually 500-1000 milli-seconds prior to calculating
the third derivative of the subsequently cycle which allowed for the graphical
analysis of each of the 100 cycles by slowing it down to a viewable level.
Additionally, the cycle number, the number of knock detected and a visual
indicator (that would light up green when knock was detected) were
displayed for quick observation and user convenience.

Knock Validation
A knock condition was validated using the knock indicator algorithm set-up
in the Detect Knock VI by running a number of iterations to determine the
maximum negative amplitude of 3rd derivative of pressure in a normal non-
knock, slight-knock, moderate-knock and heavy-knock condition run. This
information was then coupled with the audible pinging noise of knock and
was used to establish the threshold value for a knock condition per each of
the 100 cycles. The threshold value for the current set-up was determined to
be -750 kPa/°CA³ and will vary from author to application due to its
subjective nature. To validate the knock analysis, in figure 5.6 is an audibly
confirmed knock cycle displaying the 3rd derivative’s amplitude exceeding
the threshold value to depict a knock condition.

**Figure 5.6:** 3rd derivative of one (1) actual cycle displaying a knock condition at compression ratio 12:1, spark timing 10º BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

**Figure 5.7:** A 20 percent of knock cycles displayed from a 100 cycle run in the CFR engine with methane operation at compression ratio 12:1, spark timing 10º BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Also, in order to acquire repeatable and accurate results a knock limit of 20 percent was established to define a condition of knock. Therefore, if within the 100 consecutive cycle run, 20 cycles exceed the threshold value, that run would constitute as being in a knock condition. Figure 5.7 displays graphically in a 100 cycle run where such a condition exists.

To further validate the knock indicator empirical data was generated for six consecutive (100-cycle) runs by operating the CFR engine at an established parameter which would provide a 20 percent knock limit. Analyzing the data a knock variation from 20% - 29% was observed (See Figure 5.8) with a 14% coefficient of variation which is quite acceptable and expected due to the cyclic variations and the non-predictive nature of combustion itself.

![Graph](image)

**Figure 5.8:** Knock variation per six consecutive runs in the CFR engine with methane operation at compression ratio 12:1, spark timing 10° BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
The variation can also be attributed to the minute fluctuations in the flow of gaseous fuel from the high pressure cylinders into the engine intake, which is relatively difficult to control without the use of self-adjusting automatic flow regulators.

But, with the Detect Knock VI and its experimental validation the knock analysis was conducted with significant confidence. The VI was opened and the essential parameters such as knock region (which is essentially the range of crank angle where knock is likely to occur) and threshold value were entered. The LMV data file containing the 100 cycle pressure data saved from the Recording Pressure VI was loaded on to the Detect Knock VI and initiated to determine the number of knock cycle in that particular run. The next chapter discusses the results generated from the knock analysis.
CHAPTER VI

EXPERIMENTAL RESULTS AND DISCUSSION

Results

The initial sets of experiments conducted were oriented towards determining the baseline KLST and KLCR for binary mixtures of methane and hydrogen for 0, 20, 40, 60, 80 and 100 MN. Once, the baseline parameters were established, the experiments were conducted for different compositions of diluents, namely CO\textsubscript{2} and N\textsubscript{2}. The findings for KLST and KLCR are separated into two sections and discussed individually.

Knock Limited Spark Timing

The variations in KLST for binary mixtures of hydrogen and methane were determined in the presence of varying percentages of diluents. Two sets of empirical data were generated as mentioned earlier for the addition of the individual diluents, which are carbon dioxide and nitrogen. The KLST results at a constant CR of 12:1 are displayed in figure 6.1 and 6.2.

With the addition of either diluent the KLST decreases for increasing percentage of H\textsubscript{2} additive to a point of beyond 40\textdegree\ ATDC, which was the maximum limit at which the spark timing could be varied based on the current experimental set-up.
**Figure 6.1:** Variation of KLST with for binary mixtures of CH₄ and H₂ in the presence of varying percentage of CO₂ diluent at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

**Figure 6.2:** Variation of KLST with for binary mixtures of CH₄ and H₂ in the presence of varying percentage of N₂ diluent at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Generally, the addition of incombustible diluent augments the KLST since a part of the fuel composition is replaced by the diluent thereby lowering the heating value of the fuel and also due to the change in overall concentration of the fuel which affects the chemical kinetics rate. Therefore, under those conditions greater spark advance would be required to incite a knock condition compared to a fuel composition without diluents. It can be noticed from figures 6.1 and 6.2 that with the addition of CO₂ diluent, a 2-3 °CA increase in KLST is accomplished as opposed to N₂ diluent which only provides a 1 °CA increase for a given mixture composition when evaluated against the baseline curve.

When KLST is plotted with respect to either diluent (CO₂ or N₂) in the fuel and diluent mixture it can be observed that the KLST increases 20 - 45 °CA for incremental CO₂ addition depending on H₂% (See Figure 6.3). Likewise, incremental N₂ addition can only provide about a 6 - 23 °CA increase in KLST based on a particular H₂% (See Figure 6.4) which is due to the relatively low impact of the diluent on the fuel mixture mixing with air that is composed of 79% N₂. The lower the CH₄% the greater the KLST increase was observed for either diluent. In both cases, the KLST span figures are determined from a range of 0% – 80% H₂ beyond which at 100% H₂ insufficient data was available due to heavy knock and a KLST value beyond 40 °CA ATDC.
Figure 6.3: Variation of KLST with for varying percentage of CO₂ diluent for 0% - 100% H₂ fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 6.4: Variation of KLST with for varying percentage of N₂ diluent for 0% - 100% H₂ fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
But, at 100% H₂ operation, CO₂ diluent presented KLST improvement, while even 40% N₂ diluent provided no improvement. This can be confirmed by the missing curve for 100% H₂ fuel with N₂ addition, which was beyond the experimental limits of 40 °CA ATDC (See Figure 6.4).

From the KLST experiments the indicated power was also monitored to determine the effects of the addition of diluents. It can be observed from Figure 6.5 with the addition of CO₂ the indicated power decreases for a given binary mixture. As the percentage of CO₂ diluent is increased, the binary mixtures percentages are lowered thereby reducing the overall heating value of the fuel. The effect of the incombustible diluent and the lowered heating value of the fuel results in power drop. The indicated power decreases to a maximum value of approximately 0.3 kW with the addition of 50% CO₂ diluent and this is applicable between 0 – 60% H₂ in the binary mixture beyond which an increase in indicated power is observed. At 100% H₂ it can be clearly identified that addition of CO₂ diluent increases power as a result of combustion which ordinarily would be limited due to knocking. Similarly, from figure 6.6 it can be observed that addition of N₂ diluent causes a maximum power drop of 0.2 kW with the addition of 50% N₂ between 0 – 60% H₂ in the binary mixture. Unlike CO₂ diluent at binary mixtures of 80% H₂ and above, no significant increase or decrease of power is observed.
Figure 6.5: Variation of Indicated Power with for varying percentage of CO₂ diluent for 0% - 100% H₂ fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 6.6: Variation of Indicated Power with for varying percentage of N₂ diluent for 0% - 100% H₂ fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
The decrease in power while motoring with N\textsubscript{2} diluent is not very evident as compared to CO\textsubscript{2} diluent, due to the fact that air, which is vital for combustion is already composed of 79\% N\textsubscript{2}. When utilizing N\textsubscript{2} as a diluent, the fuel mixture composition only realizes an excess of N\textsubscript{2} diluent, which slightly reduces the heating value of the fuel being an incombustible gas. Additionally, N\textsubscript{2} diluent does not act as a heat sink like CO\textsubscript{2} diluent, as a result only a minor drop in power is observed.

The peak in-cylinder pressure was also monitored in order to closely determine the effects of the addition of the individual diluents. Figure 6.7 and 6.8 which displays CO\textsubscript{2} and N\textsubscript{2} diluent addition respectively to the binary mixtures illustrates that, the peak in-cylinder pressure increases with increasing diluent concentration. Due to the unpredictable nature of the combustion process an average of 185 kPa increase in pressure is observed with increasing CO\textsubscript{2} diluent concentration up to 60\% H\textsubscript{2} as stated from earlier graphic illustrations beyond which, a much higher in-cylinder pressure increase is noticed. This can be accounted to the greater advance in spark timing at that fuel-diluent mixture allowing combustion to occur earlier which provides the mixture ample time to completely burn thereby generating a higher in-cylinder pressure. Similarly, N\textsubscript{2} diluent offers a 142 KPa increase only, since it acts almost like excess air for the fuel mixture.
Figure 6.7: Variation of peak in-cylinder pressure with for varying percentage of CO\textsubscript{2} diluent for 0\% - 100\% H\textsubscript{2} fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 6.8: Variation of peak in-cylinder pressure with for varying percentage of N\textsubscript{2} diluent for 0\% - 100\% fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Lastly, the exhaust gas temperature was also monitored and revealed important information regarding the behavior of the fuel in the presence of the diluents. Figure 6.9 clearly display that as the percentage of CO₂ diluent is increased the exhaust gas temperature is reduced. There are several factors that cause this phenomenon but the most significant are the reduction in the heating value of the fuel as diluent is added and the heat sink effect of CO₂ diluent gas itself. It is obvious that, as the percentage of diluent added is increased, the concentration of the binary fuel mixtures reduce thereby decreasing the overall heating value of the fuel. Also, CO₂ gas when released into the manifold from its compressed state expands, thereby absorbing the surrounding heat energy, which in this case is supplemented by the process of combustion occurring in the cylinders. At 0% H₂ combustion additions of up to 40% CO₂ diluent displays a 42°C drop in exhaust gas temperature and at 100% H₂ a temperature drop of 133°C can be observed. Since, at 100% H₂ the heating value of the fuel is very low due to 100% H₂ gas concentration and also excessive wall losses due to improper combustion. N₂ diluent also displays a similar trend where at 0% H₂ a temperature drop of 27°C is displayed and at 100% H₂ a maximum temperature drop of 51°C occurs (See Figure 6.10). Between the two diluents, the effect of CO₂ is more significant as it has a greater heat sink property when compared to N₂.
Figure 6.9: Variation of exhaust gas temperature with for varying percentage of CO\(_2\) diluent for 0\% - 100\% H\(_2\) fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 6.10: Variation of exhaust gas temperature with for varying percentage of CO\(_2\) diluent for 0\% - 100\% H\(_2\) fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Knock Limited Compression Ratio

The variations in KLCR for binary mixtures of hydrogen and methane were also determined in the presence of varying percentages of diluents. The KLCR results at a constant spark timing (ST) of 13° CA BTDC as per the ASTM method are displayed in figure 6.11 and 6.12. Similar to the KLST experiments, two sets of empirical data were generated for the individual diluents, which are carbon dioxide and nitrogen.

For binary mixtures of CH₄ and H₂ only, the KLCR decreases for increasing percentage of H₂ as a fuel additive. The decrease in KLCR can be accounted to the fast flame propagation of H₂ which is responsible for the high temperature at the end gas region known to cause detonation. As either diluent is added and the percentage of CO₂ or N₂ is increased the KLCR is augmented for both 0 and 100% H₂ fuel mixture (See Figure 6.11 and 6.12). The addition of diluent to the binary fuel mixture reduces the combustion temperature as it acts as a heat sink being an incombustible gas.

From Figure 6.11, it can be asserted that for every 10 percent increase of CO₂ in the fuel diluent mixture the compression ratio was augmented by a value of one up to 20 percent of CO₂ and increased even more drastically with addition of higher percentage of CO₂. Similarly, with the addition of up to 25 percent N₂ diluent the compression ratio was augment only by a value of 0.5 beyond which the increase was significantly higher.
Figure 6.11: Variation of KLCR with for binary mixtures of CH₄ and H₂ in the presence of varying percentages of CO₂ diluent at constant spark timing of 13° CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 6.12: Variation of KLCR with for binary mixtures of CH₄ and H₂ in the presence of varying percentages of N₂ diluent at constant spark timing of 13° CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
The indicated power displayed in Figure 6.13 and 6.14 while determining the KLCR values shows a very erratic power loss pattern with the addition of either diluent when compared to the binary mixture. This can be explained to the effect that determining the KLCR is a much more difficult process than KLST. Unlike spark timing adjustment which is quite easily set, the compression ratio adjustment consists of turning a hand crank which is not easily rotated while the engine is motoring and utilizes significant time to dial into a pre-determined value. Also, the basic methodology for determining the KLCR as described in chapter 4 consists of several repeated runs at a composition while varying the CR to determine a condition with 20% knocking cycles. Due to this time consuming process the compression ratio adjustment was performed in 0.5 increments. This helped to conserve the fuel as fewer runs were required to determine the KLCR for a specific composition. This explains the erratic indicated power figures for both diluents. The CO$_2$ diluent when added to 20 and 40% H$_2$ fuel composition displayed a ± 0.1 kW power variation. Also, for 60 and 80% H$_2$ fuel composition a maximum power variation displayed was ± 0.2 kW. With N$_2$ the trend observed is significantly different where only a power loss is displayed. An average of 0.1 kW power loss was observed in exception of 60% H$_2$ fuel composition which displayed a 0.2 kW power loss.
Figure 6.13: Variation of Indicated Power with for varying percentage of CO\textsubscript{2} diluent for 0\% - 100\% H\textsubscript{2} fuel mixture at constant spark timing of 13\textdegree\ CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 6.14: Variation of Indicated Power with for varying percentage of N\textsubscript{2} diluent for 0\% - 100\% H\textsubscript{2} fuel mixture at constant spark timing of 13\textdegree\ CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
The peak in-cylinder pressure was also monitored for KLCR experiments in order to closely determine the effects of the addition of the individual diluents. Figure 6.15 and 6.16 which displays CO₂ and N₂ diluent addition respectively to the binary mixtures illustrates that, the peak in-cylinder pressure generally increases with increasing diluent concentration but significant variation was also present where peak in-cylinder pressure was lower. Again, this variation can be accounted to the incremental value utilized to determine the KLCR for a specific composition.

Since, spark timing was held constant, the compression ratio was the factor utilized to determine the peak conditions. Due to the time consuming process of determining KLCR, it was not very feasible to reduce the incremental value below a 0.5 increment. This would require a constant and unlimited supply of fuel along with considerable time for repeat runs to determine the optimum values for each composition. Due to the constraints of fuel and time the KLCR was determined by a run that closely represented the 20% knocking cycle’s criteria with a tolerance of ± 5% knocking cycles. Since, the set-up was validated; high confidence can be applied to the empirical data acquired.

Also, the in-cylinder pressures are displayed for up to 80% H₂ fuel composition beyond which, the KLCR value was below the specified limit of 4 and only values for high diluent concentration of 30% and over is graphed.
Figure 6.15: Variation of peak in-cylinder pressure with for varying percentage of CO₂ diluent for 0% - 100% H₂ fuel mixture at constant spark timing of 13° CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 6.16: Variation of peak in-cylinder pressure with for varying percentage of N₂ diluent for 0% - 100% H₂ fuel mixture at constant spark timing of 13° CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Lastly, while conducting the KLCR experiments the exhaust gas temperature was also simultaneously monitored and revealed important information regarding the behavior of the fuel in the presence of the diluents. Figure 6.17 clearly display that as the percentage of CO\textsubscript{2} diluent is increased the exhaust gas temperature is reduced. Similar to the trend observed in the KLST experiments, the heating value of the fuel is reduced with the addition of diluent and also contributing to the drop in exhaust temperature is due to the heat sink effect of CO\textsubscript{2} diluent gas itself. At 0\% H\textsubscript{2} combustion additions of up to 30\% CO\textsubscript{2} diluent displays a 20\(^\circ\)C drop in exhaust gas temperature and at 100\% H\textsubscript{2} a temperature drop of 53\(^\circ\)C can be observed. Again, the heating value of the fuel is very low due to 100\% H\textsubscript{2} gas concentration and also excessive cylinder wall losses due to improper combustion. Also, with the addition of 40\% diluent concentration for 0, 20 and 40 percent H\textsubscript{2} fuel concentration the compression ratio was increased to above the maximum specified limit of 16 and therefore no data was recorded. Now, N\textsubscript{2} diluent also displays a similar trend where at 0\% H\textsubscript{2} a temperature drop of 25\(^\circ\)C is displayed and at 100\% H\textsubscript{2} a temperature drop of 57\(^\circ\)C occurs (See Figure 6.18). But, an interesting trend is observed for both the diluents where the maximum temperature drop occurs at 80\% H\textsubscript{2} concentration by a value of 67\(^\circ\)C and 81\(^\circ\)C for CO\textsubscript{2} and N\textsubscript{2} diluent respectively.
Figure 6.17: Variation of exhaust gas temperature with for varying percentage of CO₂ diluent for 0% - 100% H₂ fuel mixture at constant spark timing of 13° CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 6.18: Variation of exhaust gas temperature with for varying percentage of N₂ diluent for 0% - 100% H₂ fuel mixture at constant spark timing of 13° CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
In summary, both KLST and KLCR experiments displayed that in the presence of either diluent the operating limitations of a particular fuel composition could be extended significantly. CO$_2$ diluent was very effective to augment combustion at higher H$_2$% fuel compositions that ordinarily would have high knock or have a tendency to not occur at all. N$_2$ also displayed a similar trend but at a lower performance level than CO$_2$ diluent. The addition of diluents to the binary compositions of CH$_4$ and H$_2$ displayed a slight power loss due to lowered heating value of the fuel but is negated due to the process of combustion augmentation at compositions where combustion would normally not occur.
CHAPTER VII

KNOCK MODELING

Background

Data generated from experimental research can be utilized to determine a baseline, which can then be simulated to predict the operating limits in the presence of specific diluents. Based on the current research, the data was modeled for predicting of KLCR and KLST for binary mixtures of CH\textsubscript{4} and H\textsubscript{2} with the presence of varying percentages of either CO\textsubscript{2} or N\textsubscript{2} diluent. For successful modeling, baseline data had to be first determined, and then used to generate an algorithm to closely represent the data that has been acquired as a result of varying conditions such as mixture composition, compression ratio, spark timing etc. The following sections discuss the procedure involved to model the KLST and KLCR for varying percentages of CO\textsubscript{2} or N\textsubscript{2} diluent.

KLST Modeling

Displayed in figure 7.1 is the baseline KLST data for binary mixtures of CH\textsubscript{4} and H\textsubscript{2} determined from the experimental research. A third order polynomial fit was generated in order to closely represent the trend, which was established at engine operating conditions of constant compression ratio of 12:1, intake temperature of 303K, intake pressure of 98 kPa and 600 rpm.
Figure 7.1: Baseline KLST with third order polynomial fit for 0% - 100% H₂ fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 7.2: Baseline KLST with linear fit for 0% - 100% H₂ fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
The baseline KLST for varying percentages of $H_2$ can be displayed by a third order polynomial fit (Equation 7.1) or a linear fit (Equation 7.2) as:

\[
B_{(KLST \text{ poly wrt } H_2)} = -0.0001*(H_2\%)^3 + 0.01*(H_2\%)^2 - 0.35*(H_2\%) + 10.00 \tag{7.1}
\]

\[
B_{(KLST \text{ linear wrt } H_2)} = -0.19*(H_2\%) + 10.2 \tag{7.2}
\]

Now, with the experimental data generated for binary mixtures in the presence of either diluent, the KLST equations for varying compositions were modeled by linear regression for $N_2$ and $CO_2$ diluent as the following:

\[
N_2_{(KLST \text{ wrt } H_2)} = [-0.19 \ (H_2\%) + 10.2 + (N_2\%)^{(m)}] \text{ where } m = N_2\% / 100 \tag{7.3}
\]

\[
CO_2_{(KLST \text{ wrt } H_2)} = [-0.19 \ (H_2\%) + 10.2 + (CO_2\%)^{(n)}] \text{ where } n = CO_2\% * 0.15 \tag{7.4}
\]

The modeled and the actual KLST data with respect to $H_2$ are displayed in Figure 7.3 and 7.4 for $N_2$ and $CO_2$ respectively.

**Figure 7.3**: Actual KLST values with modeled 5% and 40% $N_2$ diluent for 0% - 100% $H_2$ fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Figure 7.4: Actual KLST values with modeled 10% and 40% CO₂ diluent for 0% - 100% H₂ fuel mixture at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Now, figure 7.3 and 7.4 displays KLST values for increasing percentage of N₂ and CO₂ diluents respectively. For N₂ modeling a minimum deviation of 2.57% was observed at H₂ concentration of 0% and a maximum deviation of -88.37% was observed at H₂ concentration of above 60%. The linear model is valid only up to 60% H₂ concentration and 40% diluent addition as higher values displayed a significant KLST increase and would require a polynomial fit model. Beyond 60% H₂ concentration the KLST values are enhanced significantly and therefore no longer follow a linear trend, which is why only 60% H₂ concentration KLST values are displayed. Similarly, CO₂ model displayed a minimum deviation of 5.57% at H₂ concentration of 0% and a maximum deviation of -78.75% was observed at 60% H₂ concentration.
The KLST values were also modeled for increasing percentages of H\textsubscript{2} addition for both N\textsubscript{2} and CO\textsubscript{2} diluents. The baseline was initially determined using a linear fit and the model equations were derived for the individual diluents.

N\textsubscript{2}(KLST wrt N\textsubscript{2}) = \[0.1495 (N\textsubscript{2} \%) + 10.058 - (H\textsubscript{2} \%)(p)\] where p = H\textsubscript{2} \%/100 \hspace{1cm} (7.5)

CO\textsubscript{2}(KLST wrt CO\textsubscript{2}) = \[0.300 (CO\textsubscript{2} \%) + 8.800 - (H\textsubscript{2} \%)(p)\] where p = H\textsubscript{2} \%/100 \hspace{1cm} (7.6)

The modeled and the actual KLST data with respect to diluents (N\textsubscript{2} and CO\textsubscript{2}) are displayed in Figure 7.5 and 7.6 for varying H\textsubscript{2} concentration.

**Figure 7.5**: Actual KLST values with modeled 20% and 60% H\textsubscript{2} concentration for 0% - 40% N\textsubscript{2} diluent addition at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

It can be observed for both diluents from figures 7.5 and 7.6 that as the H\textsubscript{2} concentration is increased beyond 60% the KLST values are enhanced significantly.
Figure 7.6: Actual KLST values with modeled 20% and 60% H$_2$ concentration for 0% - 40% CO$_2$ diluent addition at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Now, figure 7.5 and 7.6 displays KLST values for increasing percentage of N$_2$ and CO$_2$ diluents respectively. For N$_2$ modeling a minimum deviation of 9.36% was observed at H$_2$ concentration of 20% and a maximum deviation of -45.34% was observed at H$_2$ concentration of 60%. Similarly, CO$_2$ model displayed a minimum deviation of -0.11% at H$_2$ concentration of 20% and a maximum deviation of -86.52% was observed at concentration of 60% H$_2$. As stated earlier, the linear model is valid only up to 60% H$_2$ concentration and 40% diluent addition as higher values displayed a significant KLST increase and requires a polynomial fit model. Also, it can be observed from figure 7.6, at 80% H$_2$ concentration the trend is deviating significantly from the linear model of the lower H$_2$ concentrations.
KLCR Modeling

Similar to the methodology described for KLST, displayed in figure 7.7 and 7.8 are the baseline KLCR data for binary mixtures of CH\textsubscript{4} and H\textsubscript{2}. Again, a third order polynomial fit was generated in order to closely represent the trend (Figure 7.7) and additionally, a linear fit (Figure 7.8), which were established at engine operating conditions of constant spark timing of 13\textdegree CA BTDC, intake temperature of 303K, intake pressure of 98 kPa and 600 rpm. The baseline KLCR for varying percentages of H\textsubscript{2} can be displayed by the following model equations:

\begin{align*}
B_{\text{KLCR poly wrt H2}} &= -0.00002(H_2\%)^3 + 0.002(H_2\%)^2 - 0.136(H_2\%) + 9.971 \quad (7.7) \\
B_{\text{KLCR linear wrt H2}} &= -0.06(H_2\%) + 9.9 \quad (7.8)
\end{align*}

\[ y = -2\times10^{-5}x^3 + 0.0026x^2 - 0.1363x + 9.9714 \]

**Figure 7.7:** Baseline KLCR with third order polynomial fit for 0\% - 100\% H\textsubscript{2} fuel mixture at constant spark timing of 13\textdegree CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Using the baseline equation, the model was derived to display the KLCR values for varying percentages of N\(_2\) and CO\(_2\) as per equations 7.7 and 7.8 respectively.

Now, with the experimental data generated for binary mixtures in the presence of either diluent, the KLCR equations for varying compositions were modeled by linear regression for N\(_2\) and CO\(_2\) diluent as the following equations 7.9 and 7.10:

\[
\text{N}_2 (\text{KLST wrt H}_2) = [-0.06*(H_2\%) + 9.9 + (N_2\%)/100] \quad \text{where} \quad q = N_2\% / 100 \quad (7.9)
\]

\[
\text{CO}_2 (\text{KLST wrt H}_2) = [-0.06*(H_2\%) + 9.9 + (CO_2\%)/100] \quad \text{where} \quad r = CO_2\% / 100 \quad (7.10)
\]

Figure 7.9 and 7.10 show KLCR values for varying percentage of N\(_2\) and CO\(_2\) diluent respectively with respect to varying H\(_2\) concentration.
Figure 7.9: Actual KLCR values with modeled 5% and 25% N₂ diluent for 0% - 100% H₂ fuel mixture at constant spark timing of 13° CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 7.10: Actual KLCR values with modeled 10% and 30% CO₂ diluent for 0% - 100% H₂ (100 - 0 MN) fuel at constant spark timing of 13° CA BTDC, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
Now, figure 7.9 for N$_2$ modeling displayed a minimum deviation of -0.43% at H$_2$ concentration of 20% and a maximum deviation of 10.29% was observed at 80%H$_2$ concentration. Similarly, figure 7.10 for CO$_2$ model displayed a minimum deviation of 0.8% at H$_2$ concentration of 60% and a maximum deviation of % was observed at 0% H$_2$ concentration with the addition of 30% CO$_2$ diluent. The linear model is valid only up to 80% H$_2$ concentration and 30% diluent addition as higher values displayed a significant KLCR increase and requires a polynomial fit model.

The KLCR values were also modeled for increasing percentages of H$_2$ addition for both N$_2$ and CO$_2$ diluents. The baseline was initially determined using a linear fit and the model equations were derived for the individual diluents as displayed in equations 7.11 and 7.12 respectively.

\[
\text{N}_2\text{(KLCR wrt N}_2\text{)} = [0.140 \times (\text{N}_2\%) + 8.99 - (\text{H}_2\%)] \text{ where } s = \text{H}_2\% / 200 \tag{7.11}
\]

\[
\text{CO}_2\text{(KLCR wrt CO}_2\text{)} = [0.165 \times (\text{CO}_2\%) + 9.40 - (\text{H}_2\%)] \text{ where } s = \text{H}_2\% / 200 \tag{7.12}
\]

The modeled and the actual KLCR data with respect to diluents (N$_2$ and CO$_2$) are displayed in Figure 7.11 and 7.12 for varying H$_2$ concentration. For N$_2$ modeling, the minimum KLCR deviation observed was 2.53% at H$_2$ concentration of 20%. As the concentration of H$_2$ increased to 80% a maximum deviation of -35.62% was observed. Similarly, for CO$_2$ modeling, the minimum deviation was observed at lower H$_2$ concentrations of 20% and a maximum deviation was -27.42 observed at 80% concentration of H$_2$. 
Figure 7.11: Actual KLCR values with modeled 20% and 80% H₂ concentration for 0% - 40% N₂ diluent addition at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.

Figure 7.12: Actual KLCR values with modeled 20% and 80% H₂ concentration for 0% - 30% CO₂ diluent addition at constant compression ratio of 12:1, intake temperature 303K, intake pressure 98 kPa and 600 rpm.
CHAPTER VIII

SUMMARY AND CONCLUSIONS

Summary
Alternative fuels are being extensively explored as the world’s source of petroleum slowly depletes. Additionally, this drive has also been sparked to promote the use of cleaner burning fuels in order to protect the environment. The abundant availability of natural gas (which is predominantly CH₄) makes it a primary candidate for the use in alternative fuel technology. Being a gaseous fuel, favorable operational and combustion advantage over liquid fuels such as enhanced power production efficiency, good combustion stability and greater tolerance to lean mixture operation exists.

Knock is an inherent characteristic during combustion, which is a major barrier to achieving higher thermal efficiency and increased power output. Auto-ignition causes sudden pressure changes in the cylinder and generates extremely high temperature spikes due to rapid combustion of the gaseous mixture and is acknowledged to cause potential engine damage. The onset of knock which is affected by various factors such as spark timing and compression ratio among others has been extensively investigated in this current research to determine the optimum operating limits of a specific fuel composition especially in the presence of diluents.
In order to investigate the knock characteristics of various parameters for varying fuel and diluent compositions, an alternative fuel research laboratory was set-up, which mainly consisted of an ASTM-CFR engine and a metering panel for air, fuel and diluent that was collectively linked to a data acquisition system. Using LabVIEW software VI’s were developed to monitor engine parameters and detect knock. For the current research, the in-cylinder pressure knock detection method was adopted as it provides a quantifiable metric not always seen in other methods. The experimental set-up was validated for both the engine operation and data acquisition prior to acquiring empirical data for knock analysis.

Initially, the baseline KLST and KLCR had to be determined for binary mixtures of CH\textsubscript{4} and H\textsubscript{2} to investigate onset of knock. Using the baseline, addition of different volumetric compositions of diluents was then investigated. This involved the variation of spark timing for KLST and similarly, the variation of compression ratio for KLCR, while keeping all other parameters such as equivalence ratio, compression ratio and intake temperature constant. Addition of either diluent extended the operating limitations of a particular fuel composition. CO\textsubscript{2} diluent was very effective to augment combustion at higher H\textsubscript{2}\% fuel compositions that ordinarily would have high knock or have a tendency to not occur at all. N\textsubscript{2} diluent also displayed a similar trend but at a lower performance level than CO\textsubscript{2} diluent.
Lastly, the KLST and KLCR were modeled for the binary mixtures in the presence of varying compositions of either diluent. Empirical relations were established to predict KLCR or KLST for a specific binary fuel mixture in the presence of a particular diluent composition. The model was validated by conducting an analysis and comparing against the empirical data. Using the equations derived for the model, the engine operating limitations can be investigated without conducting any experiments.

**Conclusions and Recommendations**

With the KLST experiments, the addition of CO$_2$ or N$_2$ diluent augmented the knock resistance and extended the engine operating limits by permitting a greater spark advance. Addition of CO$_2$ diluent displayed a 2-3 °CA increase in KLST and similarly, N$_2$ diluent displayed a 1 °CA increase for a given mixture composition of 0 - 60% H$_2$ when evaluated against the baseline curve. The KLST indicated power decreased by 0.3 kW for CO$_2$ diluent and 0.2 kW for N$_2$ diluent. The KLST peak in-cylinder pressure also increased, due to increased spark advance, by an average value of 185 kPa and 142 kPa for CO$_2$ and N$_2$ diluent addition respectively. Lastly, the KLST exhaust gas temperature for up to 40% CO$_2$ addition displayed a temperature drop of 42°C - 133°C from 0% H$_2$ - 100% H$_2$ and likewise, addition of up to 40% N$_2$ displayed a temperature drop of 27°C - 51°C from 0% H$_2$ - 100% H$_2$. 
With KLCR experiments, the knock resistance was also augmented and extended the engine operating limits with the addition of CO₂ or N₂ to binary mixtures of CH₄ and H₂. It was observed that for 10% addition of CO₂ the compression ratio could be raised by a value of one and increased even more drastically with higher percentage of diluent. Similar trend was observed with N₂ diluent where an increase in compression ratio by a value of 0.5 was observed for 10% addition. Now, the KLCR indicated power and peak in-cylinder pressure displayed a very erratic pattern which can be accounted to the KLCR procedure which was timing consuming. Therefore, the compression ratio was determined in 0.5 increments due to constraints of fuel. The KLCR indicated power displayed a power variation of ± 0.1 kW power variation with CO₂ addition to 0% - 40% H₂ and ± 0.2 kW power variation with CO₂ addition to 60% - 80% H₂. With addition of N₂ diluent an average power loss of 0.1 kW was observed. The average KLST peak in-cylinder pressure was quite erratic but displayed a general trend of increasing pressure with higher diluent concentration of CO₂. Lastly, the KLCR exhaust gas temperature for up to 30% CO₂ addition displayed a temperature drop of 20°C - 53°C from 0% H₂ - 100% H₂ and likewise, addition of up to 25% N₂ displayed a temperature drop of 25°C - 57°C from 0% H₂ - 100% H₂. But, a trend is observed where the maximum temperature drop occurs at 80% H₂ by a value of 67°C and 81°C for CO₂ and N₂ diluent.
Both the KLST and KLCR were modeled in order to provide an easy way to determine the knock limited operating parameters for the addition of either CO$_2$ or N$_2$ diluent (to binary mixtures of CH$_4$ and H$_2$) without performing any experiments. The baseline empirical data was utilized to determine a linear fit and an exponential constant was added to the equation which was dependent to H$_2$% in the fuel composition.

The modeled KLST for CO$_2$ addition displayed a minimum deviation of -0.11% at H$_2$ concentration of 20% with a maximum deviation of -86.52% at 60% H$_2$. Similarly, N$_2$ diluent displayed a minimum deviation of 9.36% at lower H$_2$ concentrations of 20% and a maximum deviation of -45.34% was observed at 60% H$_2$. The deviation increased with diluent addition to higher percentage H$_2$% and in order to reduce the margin of error a polynomial fit would be required to closely resemble the trend.

Also, the modeled KLCR displayed an analogous trend where the minimum deviation was observed at lower concentrations of H$_2$ and increased with higher H$_2$ concentrations. The minimum deviation for CO$_2$ addition was 5.02% at H$_2$ concentration of 20% and the maximum deviation of -27.42% for 80% H$_2$ concentration. With N$_2$ diluent the minimum and maximum deviation observed was 2.53% and -35.62% for H$_2$ concentrations of 20% and 80% respectively. But, overall the modeled data provides an estimate of the knock operating limits without conducting actual experimentation.
For future investigations of alternative fuels, this research can be extended to determine the operating limitations as a result of knock for different fuels such as landfill gas or bio-gas along with various other diluents and diluent compositions.

Additionally, the MN can be determined for the binary mixtures in the presence of diluents. From this research it can be observed that, the addition of diluents augments the knock resistance properties. Therefore, certain binary compositions in the presence of diluents will exceed the 100MN knock rating. An investigative study can be conducted to determine the impact of diluent addition on MN in order to augment the knock limited operating conditions.


