THESIS

EXPERIMENTAL & ANALYTICAL EVALUATION OF KNOCK CHARACTERISTICS OF PRODUCER GAS

Submitted by

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WE HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER OUR SUPERVISION BY APARNA ARUNACHALAM ENTITLED EXPERIMENTAL & ANALYTICAL EVALUATION OF KNOCK CHARACTERISTICS OF PRODUCER GAS BE ACCEPTED AS FULFILLING IN PART REQUIREMENTS FOR THE DEGREE OF MASTER OF SCIENCE.

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ABSTRACT OF THESIS

EXPERIMENTAL & ANALYTICAL EVALUATION OF KNOCK CHARACTERISTICS OF PRODUCER GAS

Amongst the popular gaseous bio-fuels is producer gas. Evaluation of knock properties of producer gas enhances efficient utilization of this renewable energy resource in an internal combustion engine. A literature review revealed that producer gas is formed from a set of combustion-reduction reactions in a gasifier and is typically composed of 18-20% H_2, 18-20%CO, 2-3% CH_4, 12% CO_2 and 48-50%N_2. It is seen that a production process where the combustion and reduction reactions are effectively separated yields a gas rich in hydrogen. Hence based on the production method and range in gas composition five different producer gas compositions are chosen for knock evaluation.

Knock evaluation for gaseous fuels has been done by previous researchers using the Methane Number method. This method requires the use of a Cooperative Fuel Research (CFR) F2 engine installed in Colorado State University's Engines and Energy Conversion Laboratory. It was seen that the methane number of producer gas ranged from 54-131. Further it was quantitatively evaluated that addition of CO_2 increases the critical compression ratio while H_2 decreases it. Overall, the effect of CO_2 on changing the critical compression ratio was found to be over twice that of H_2.

It was attempted to evaluate the methane number of producer gas using chemical kinetics software CHEMKIN. A Methane Number evaluation process was developed using CHEMKIN's internal combustion engine model. There were significant differences between model and experiment. Recommendations for future work are discussed.

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Table of Contents

List of Figures

Page No.

List of Tables **Page No.**

Abbreviations

1. CHP- Combined heat and power
2. FICFB – Fast Internal Circulating Fluidized Bed
3. IISc – Indian Institute of Science, Bangalore
4. CPC – Community Power Corporation, Colorado
5. LHV – Lower Heating Value
6. SI – Spark Ignited
7. ON – Octane Number
8. MON – Motor Octane Number
9. RON – Research Octane Number
10. MN – Methane Number
11. CFR – Cooperative Fuel Research
12. ASTM – American Standards for Testing and Methods
13. CR – Compression Ratio
14. MFC – Mass flow Controller
15. AFR – Air Fuel Ratio
16. KI – knock Intensity

Chapter 1 – Literature Review

1.1 Motivation & Role of Biomass as a sustainable source of energy

Biomass can be defined as any organic or plant derived matter than can be used directly or indirectly as a source of energy. It includes wood, woody residue from timber based industries, agricultural residues as well as animal manure.

Biomass is considered to be carbon neutral. In effect, the amount of carbon dioxide plants utilize during photosynthesis is what they give out upon their combustion. Hence, they do not add any extra carbon dioxide to the atmosphere when used as a fuel. Also, the present energy security issues faced by most nations have prompted us to look at bio-fuels and bio-energy as a sustainable energy resource. For Instance, the United States envisions a replacement of 30% of its petroleum consumption with bio-fuels by 2030 **[1]**. Amongst the Organization for Economic Co-operation and Development (OECD) countries such as Austria, Finland, Germany and Sweden, bio-fuels are increasingly used for the generation of electricity. In the case of developing countries in South Asia, use of biomass as a source of cooking and heating fuel is not new. But improving the efficiency of their processes in order to reduce environmental pollution and better utilize their biomass resources is a key issue. The focus for these countries is technological advancement in sync with favoring rural economies via social and economic development.

Though bio-energy programs have a great potential to provide a sustained energy source for global needs, it is important to understand the positive and negative implications of large scale use of forestry resources. Although current wood fuels are being derived from residues and by-products, the future will insist on fuel wood directly from forests and tree plantations. It is indeed necessary for energy industries to work hand in hand with forestry organizations in making sure they do not over exploit natural resources and damage the already sensitive ecological balance. This is not entirely impossible but needs a concerted effort by energy engineers, forestry personnel, governments, law makers and consumers alike to create a well integrated bio-based economy.

One such biomass based energy fuel being used now for several decades has been Producer Gas (also known as Wood Gas). It is a combustible gas obtained from the thermo chemical conversion of woody biomass. The use of producer gas started in the early 19th century and took prominence during the World War II when petroleum resources became scarce. Producer gas generators were widely used in internal combustion engines for vehicles. They were rather inefficient at the time and soon the ease and availability of gasoline diminished the use of producer gas. Decades later, producer gas is being rediscovered as a fuel resource and improvements are being made in its production as well as usage in internal combustion engines.

This work is an attempt to aid in the better understanding of the combustion and knock properties of the age old fuel.

1.2 Producer Gas – An Introduction

Producer gas is a combustible gaseous product obtained by the gasification of dry biomass or wood or wood waste. Gasification is a thermo chemical conversion process which involves the heating of the solid woody biomass in an oxygen starved environment. Initially a pyrolysis process leads to the decomposition of solid wood into charcoal and a mixture of volatile gases. The products of pyrolysis undergo combustion and consequently reduction resulting in producer gas, essentially a mixture of carbon monoxide, hydrogen, hydrocarbons, carbon dioxide and nitrogen.

In the case of thermo chemical conversion use of dry woody biomass as fuel is preferred as presence of moisture wastes energy required for its drying. Additionally woody biomass needs to be properly sized in order for it to not clog the gasifier and allow for complete burning. It is often seen that wet biomass (such as plant, sewer, manure) is used for biological conversion processes.

1.2.1 Gasification

The various processes involved in a "gasifier" are outlined here:

1. Drying – Biomass can contain varying amounts of moisture, ranging from less than 10% up to 50-70% on a wet basis **[2]**. Knowing the amount of moisture present in the wood fuel source can be decisive in choosing the type of gasifier/reactor. In some cases external drying processes can be necessary. In the gasifier, there is an intrinsically operated drying process due to the heat of combustion of burning wood. Hence the drying zone is in the upper bunker section of the gasifier.

2. Pyrolysis – This zone is starved of air/oxygen. It utilizes the conducted heat of combustion reducing the wood into volatile gases and solid char. Pyrolysis occurs at 400-800 deg C **[2]** and produces a mixture of CO, CO_2, H_2, CH_4, and H_2O along with tar vapors.

3. Combustion – This is the zone where the intake air is fed. As a result complete combustion takes place in this zone. The char and volatile combustion products from the

pyrolysis zone undergo combustion in order to produce CO_2 and water vapor in an exothermic reaction(at 1200 deg C) **[2]** as shown:

$$C + O_2 \leftrightarrow CO_2 \quad + 401.9\ \text{kJ/mol}$$

$$H_2 + 0.5\ O_2 \leftrightarrow H_2O + 241.1\ \text{kJ/mol}$$

4. Reduction/Gasification – This is the zone wherein the products of combustion undergo a reduction reaction in order to produce a mixture of combustible gases including CO and H_2. The charcoal produced during the pyrolysis process acts as the reducing agent for these reactions to occur **[2]**.

$$C + CO_2 + 164.9\ \text{kJ/mol} \leftrightarrow 2\ CO$$

$$C + H_2O + 122.6\ \text{kJ/mol} \leftrightarrow CO + H_2$$

$$CO_2 + H_2 + 42.3\ \text{kJ/mol} \leftrightarrow CO + H_2O$$

$$C + 2H_2 \leftrightarrow CH_4$$

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O + 205.9\ \text{kJ/mol}$$

The above occurring endothermic reactions are the global routes for the formation of producer gas. They occur at temperatures between 800-1200 deg C. The gas composition is hence dependent on their reaction rates which are in turn a factor of the reaction temperatures.

This process can be summarized in **Figure 1.1**.

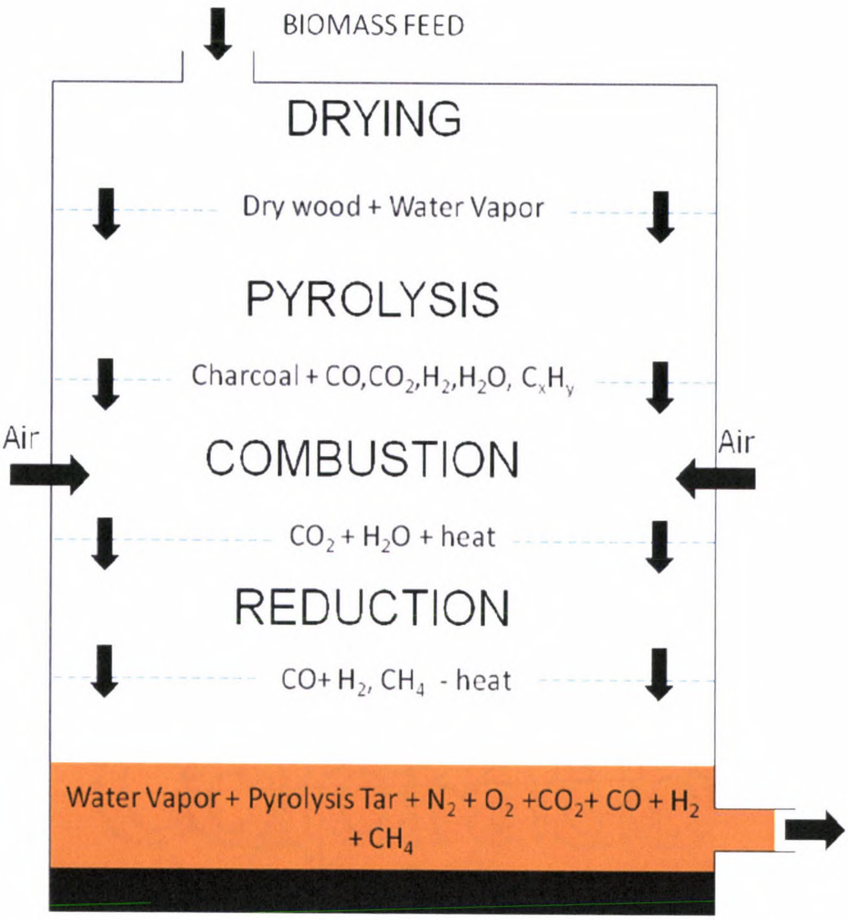


Figure 1.1 Schematic of the reaction processes of gasification (in a downdraft gasifier)

1.2.2 Gasifier

The reactor in which the process of gasification takes place is called a gasifier. Different types of gasifiers have been developed locally and over the years. The difference amongst them is mainly in the way the fuel is introduced and the way it comes in contact with the gasification medium. The gasification media acts as a reaction agent during oxidation and reduction reactions. It can be pure oxygen, atmospheric oxygen, air or water vapor. Also, the order in which the above mentioned processes occur can differ. The main classifications of gasifiers include:

a) Fixed bed gasifiers

b) Fluidized bed gasifiers

c) Entrained flow reactors

The study of gasifiers is in itself exhaustive. A brief description is included with respect to the gasifiers for the chosen case studies in Section **1.3**.

1.2.3 Gasification versus Combustion

a) Gasification converts solid woody mass into gaseous fuel through high temperature oxidation – reduction reactions. On the other hand combustion converts woody mass into gaseous products of combustion during high temperature oxidation reactions.

b) The product of gasification is a fuel which can further be used in varying applications including internal combustion engines, gas turbines and even fuel cells. The product of combustion is hot flue gases whose thermal energy is extracted in a heat exchanger to produce power.

c) Due to the low sulfur content in biomass, formation of sulfur dioxide in the emissions is low as compared to emissions from petroleum based fuels. NO_x formation can be limited due to lower combustion temperatures.

The drawback in gasification though are the cleaning and cooling processes the raw gas needs to undergo before it is let into an internal combustion engine.

1.2.4 Gas Utilization in an Internal Combustion Engine

Prior to utilization of the producer gas in an internal combustion engine, it needs to be cooled and cleansed. The gas when produced is at a temperature of 500-800 deg C **[3]** and needs to be cooled to lower temperatures in order to carry out the downstream cleaning processes. Cooling the gas also helps in condensing tarry residues while increasing its energy density. The produced gas is brought down to 40 deg C before being mixed with air and injected into the engine.

The major impurities are condensable, organic tarry producer gas compounds, inorganic particles and dust. The tarry compounds can condense on engine components and impair its functionality **[3]**. Inorganic particles and dust can corrode and erode engine parts. Producer gas cleaning equipment usually consists of cyclones, filters and electrostatic precipitators for dust. Wet scrubbing and condensation methods are most common for removal of tarry residues.

The selection of these processes can depend on factors such as gas quality requirements, type of woody raw material, pollutants produced, type of gasifier, presence of a turbocharger and load demands.

The schematic in **Figure 1.2** outlines the various process steps involved from the production of the gas to its injection in an internal combustion engine.

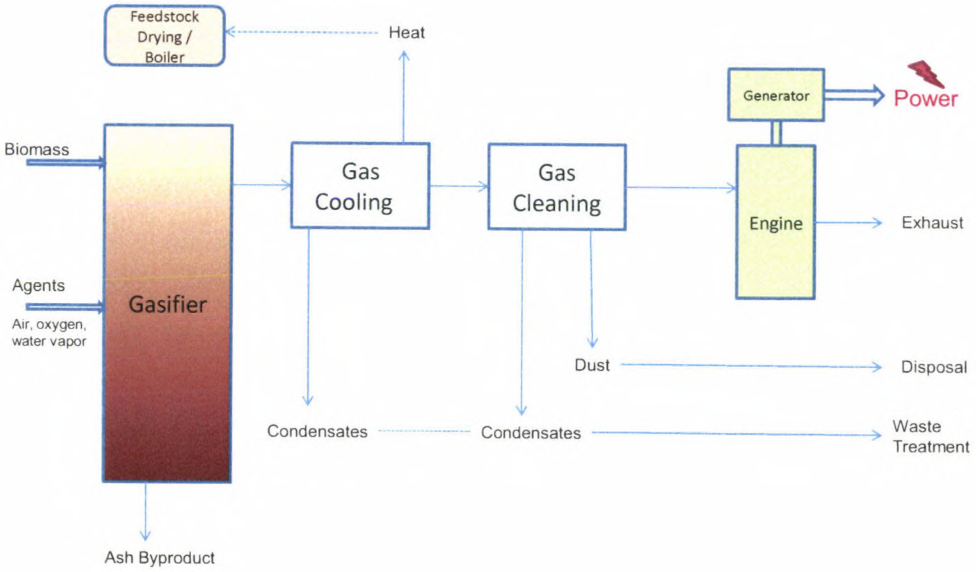


Figure 1.2 Schematic of the processes involved in producer gas utilization for internal combustion engine application

1.3 Producer Gas Compositions

The previous discussions along with the schematic in **Figure 1.3** show how the final producer gas composition is dependent on the various process variables. The producer gas composition is a function of the biomass type, gasifier type, cleaning and cooling processes as well as the mode of end utilization.

For our study it was important to choose producer gas compositions which would provide a range wide enough to analyze the combustion properties and the methane number. With respect to this, the literature survey led to the consideration of the cases discussed henceforth.

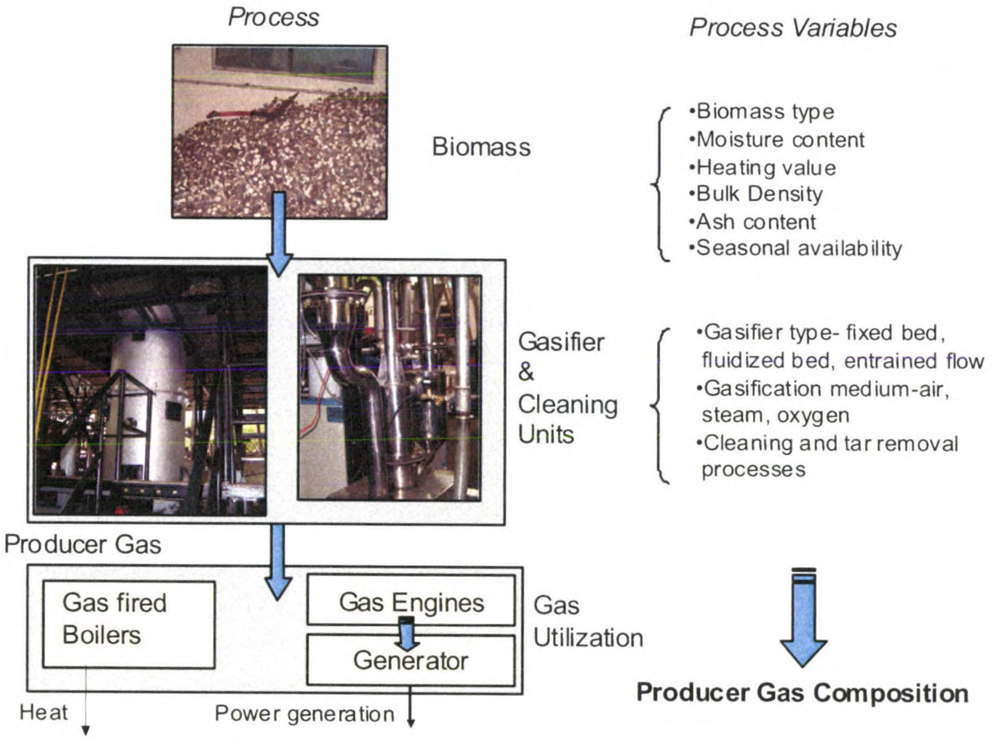


Figure 1.3 Schematic of the process and process variables involved in the formation of producer gas

1.3.1 Case Study 1: The Güssing Gasification Plant [4]

The biomass gasification and CHP (Combined heat and power) plant in Güssing, Austria is an 8MW (thermal) capacity plant which utilizes a technology called Fast Internal Circulating Fluidized Bed (FICFB) gasification **[5]**. It was established as a demonstration plant in 2002 and now runs 8000 hours annually.

Technology Brief – The basic principle of operation of a fluidized bed gasifier involves the fluidization of the bed material and its circulation between two chambers as depicted in **Figure 1.4**. The first chamber is the gasification zone. Biomass and the gasification medium (steam) are fed into this chamber. Bed material such as silica, quartz or dolomite is fluidized by the inflowing gasification medium (steam). The bed material along with char from gasified biomass is removed from the gasification chamber and is led into a cyclonic combustion chamber.

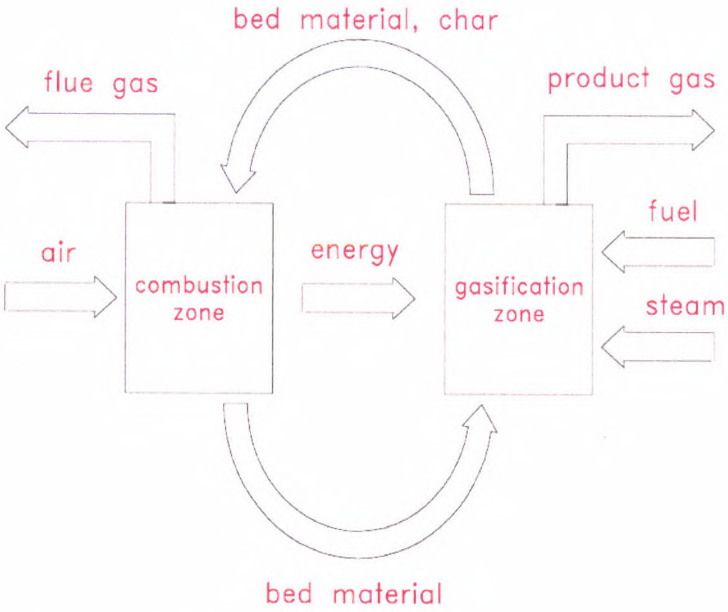


Figure 1.4 Principle of the FICFB process. Source [5]

Air is fed into the combustion chamber and allows for the combustion of the char or non-gasified biomass. The heat from combustion is transferred to the gasification chamber by the bed material which returns through the cyclonic chamber. This heat is utilized for the endothermic reduction reactions and for production of producer gas. By keeping the two processes of gasification and combustion separate, the nitrogen formed in the final gaseous product is reduced and a gas of high calorific value is obtained.

The producer gas at the end of the gasification is cooled and cleaned in a two stage cleaning process. The first stage of cleaning uses a fabric filter which removes the particles and some tar. The particles are resent into the combustion chamber of the gasifier. In the second stage of cleaning, a scrubber is used to remove the tar. Finally the cooled and cleaned gas is fed into a Jenbacher gas engine. The producer gas composition obtained in Güssing is shown in **Table 1.1.**

Table1.1 Producer Gas composition at the Güssing gasification plant [4]

Gas Component	Volume %
H_2	40
CO	24
CH_4	10
CO_2	23
N_2	3

1.3.2 Case Study 2: The "Viking" Gasification Plant [6]

The "Viking" gasification plant is a CHP test plant at The Technical University of Denmark commissioned in 2002. It ran for over 2200 hours until October 2003. It is a 75kW (thermal) plant utilizing the 2 stage gasification process.

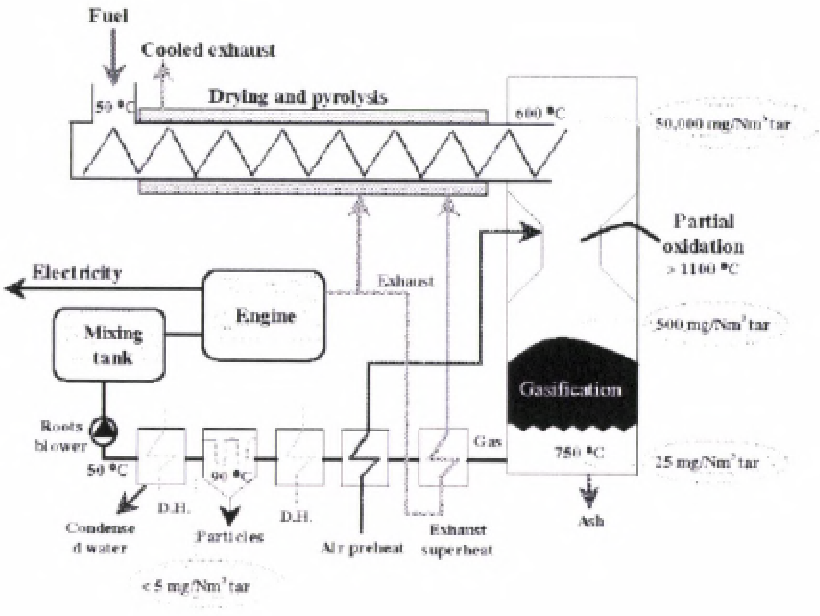


Figure 1.5 Schematic of the 2 stage gasification process. Source [6]

Figure 1.5 shows a schematic of the 2 stage gasifier. The gasifier consists of an external drying and pyrolysis unit with a screw conveyor in order to transfer the pyrolysis products into the gasification unit. The gasification unit consists of a charcoal bed aiding as the reducing agent. In between these two units is a partial oxidation section where air intake is drawn. This section causes oxidation of the pyrolysis products generating enough heat for the gasification process.

Table 1.2 Producer Gas Composition at the Viking Gasification Plant [6]

Gas Component	Volume %
H_2	30.5
CO	19.6
CH_4	1.6
CO_2	15.4
N_2	33.3

It has been shown that high tar reduction is possible through this process as a result of the partial oxidation of the pyrolysis tars and the reactions that follow in the presence of the charcoal bed **[7]**. The composition obtained in Viking is shown in **Table 1.2**.

1.3.3 Case Study 3: The IISc Gasification Technology [8]

The technology developed by the Indian Institute of Science, Bangalore (IISc) is presently being utilized by at least 4MWe equivalent power plants in India. One such plant is of the Energy Service Company (ESCO) near Coimbatore, India. This plant was commissioned in Sep 2003 and has run 7500 hours since then. It consists of a biomass gasifier rated at 150kg/hr and operates a Cummins make 120kWe gas engine.

The gasifier is fed with the vastly available Julifora Prosopis at a rate of 1.1±0.1 kg/kWh. The downdraft gasifier developed by IISc is open top twin air entries re-burn type. A downdraft gasifier is one wherein the flow of the biomass is in the same direction as the final product gas. The biomass is fed at the top and product gas is availed at the bottom. The gasifier consists of a long reactor with air entry both from the top and in the oxidation zone. The process of re-burn at the zone of secondary air entry helps in complete combustion of the volatiles and cracking of tar. Sufficient residence time is given to the reacting mixture in the reactor in order to allow for cracking of high molecular weight molecules **[8]**.

The produced gas has contaminants in the form of particulate matter (1000 mg/Nm^3) and tar (150 mg/Nm^3). Cyclonic cleaners are used to remove the dry particulate dust from the gas and ejector scrubbers cool and clean the gas. The gas is then de-humidified by the

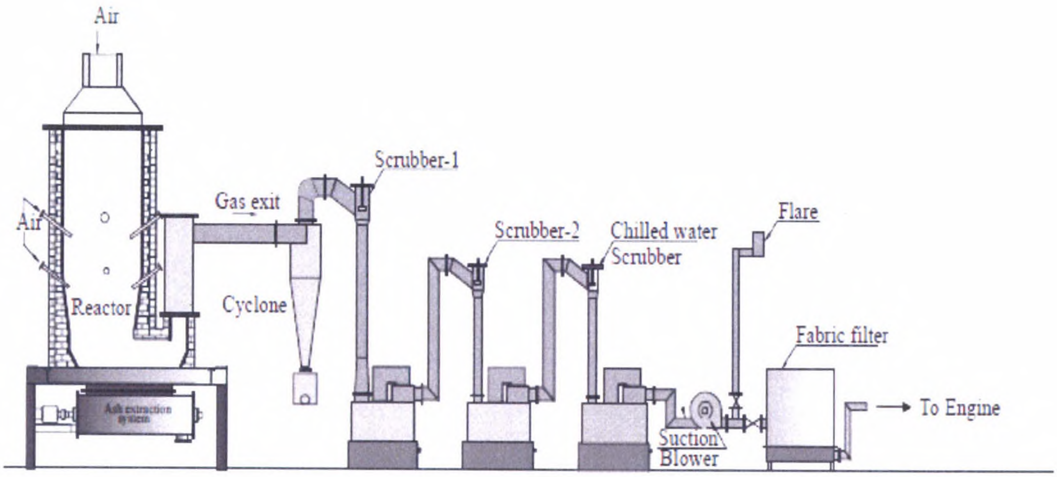


Figure 1.6 Schematic of the gasification plant set up based on IISc technology. Source [8]

principle of condensate nucleation. **Figure 1.6** is a schematic of the IISc gasification process and the gas composition using the IISc technology is provided in **Table 1.3**.

Table 1.3 Producer Gas Composition from the IISc gasification technology [8]

Gas Component	Volume %
H_2	19.0
CO	19.0
CO_2	12.0
CH_4	1.5
N_2	48.5

1.3.4 Case Study 4: The Volund Wilcox Babcock Biomass Gasification at Harboore, Denmark [9]

The producer gas plant at Harboore, Denmark was set up in Dec 1993 but has undergone a series of optimizations thereafter. Two Jenbacher engines of 750 kWe each were installed in the year 2000 and a reverse osmosis based water cleaning system was optimized by mid 2002. Since then the engines have run for over 3000 hours.

An updraft gasifier is installed here which uses steam as the gasification medium. An updraft gasifier differs from a downdraft by way of the direction of the movement of the gas with respect to the woody biomass. In this case, the produced gas is availed at the top of the reactor while the biomass travels downward. The order of the entailing processes in an updraft gasifier is shown in **Figure 1.7**.

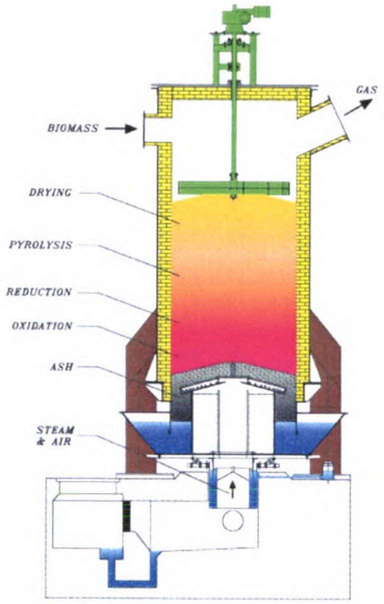


Figure 1.7 Schematic of an updraft gasifier [Source - www.volund.dk/layout]

There is a reversal in the order in which the reduction and combustion processes occur. The pyrolysis products undergo reduction in order to form the product gas which moves upwards. The gas loses part of its heat in drying the incoming biomass. In the combustion zone, remaining char from the pyrolysis process undergoes combustion to provide heat and form carbon dioxide and water vapor. This heat and gas travel upwards providing necessary ingredients for reduction reactions. By using steam as the gasification medium it acts as a reagent in the reduction zone to form hydrogen.

The internal exchange of heat in this process leads to low exit gas temperatures. Biomass with higher moisture contents can be used in this type of gasifier. But since the pyrolysis products do not pass through the combustion zone, there is a possibility of high tar content in the final product gas.

The Harboore gasifier with a capacity of 1880kg/hr uses wood chips with moisture content between 35-55%. The plant has an electrical capacity of 1.5MW and thermal capacity of 4.2MW. The product gas contains about 80000 mg/Nm^3 of particulates and tars before cleaning. It goes through a series of heat exchangers for cooling and gets cleaned by a wet electrostatic precipitator. The final gaseous product has a tar content less than 25mg/Nm^3 at 40deg C **[9]**. The gas composition obtained from the Harboore wood gasification plant is shown in **Table 1.4**.

Table 1.4 Producer Gas Composition obtained at the Harboore Gasification Plant [9]

Gas Component	Volume %
H_2	19.0
CO	22.8
CO_2	11.9
CH_4	5.3
N_2	40.7

1.3.5 Case Study 5: Community Power Corporation's Modular Bio-energy System [10]

Community Power Corporation (CPC) is a Colorado based commercial manufacturer of modular biomass gasification systems. Their research and product development has stretched from 1995. The BioMax^{TM} gasifier systems they manufacture today can provide up to 75kWe of biomass based energy. This utilizes a downdraft gasifier with air as the gasification medium. The company claims that this energy converter can be fed with a variety of agricultural residues including coconut shells, corn, and cardboard pellets apart from wood chips. A 6.8 liter John Deere diesel engine was made use of at the time of this gas composition measurement but a spark ignited engine could also be used.

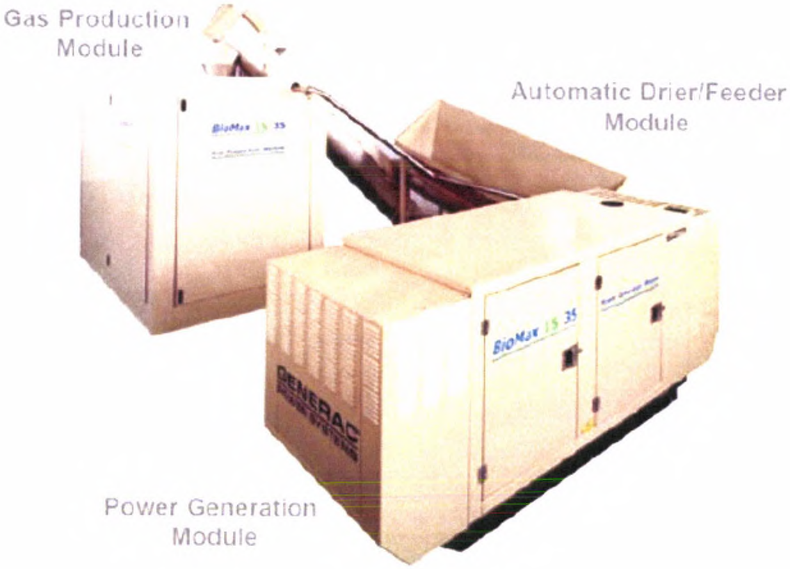


Figure 1.8 Community Power Corporation's Modular bio-energy system

Table 1.5 Gas composition from the CPC BioMax ™ gasifier [10]

Gas Component	Volume %
H_2	18.8
CO	21.0
CO_2	1.3
CH_4	2.2
N_2	56.7

The modular system is a compact arrangement of the biomass dryer, gasifier, cooling-cleaning systems, engine and waste heat recovery sub modules. A dry filter is used for gas cleaning. **Figure 1.8** shows an assembled BioMax gasifier system and the gas composition obtained from this system is presented in **Table 1.5**.

1.4 Producer Gas: Fuel Property Evaluation

Even though producer gas has been used for over a century now, its properties as a fuel for combustion in internal combustion engines are not well defined. One of the reasons for this is the popularity of conventional fuels such as gasoline which attracts more research from auto and engine manufacturers. As the need for alternative fuels is on the rise, producer gas is receiving renewed interest from researchers. New research studies will aid engine manufacturers in improving the efficiency of engines running on producer gas and hence derive maximum benefit from this renewable resource. This section reviews the properties of producer gas as a fuel.

1.4.1 Calorific Value

The calorific value of a substance is defined as the amount of heat released upon complete combustion of a given quantity of the fuel. Since producer gas is a mixture of gases, its calorific value is dependent on that of the constituent gases. For our discussion the Lower Heating Value (LHV) is used, which does not incorporate the heat of vaporization of water. Table **1.6** summarizes the LHV values for the chosen producer gas compositions.

When compared to the LHV of natural gas (~35-40 MJ/m_n^3), the LHV of producer gas is lower by 69-85%. But the more important value for an engine would be the heating value of the mixture of fuel and air entering the cylinder in each combustion cycle. The mixture heating value for natural gas is about 3.32 MJ/m_n^3 **[3]** which means the heating value of producer gas-air mixture is lower to that of natural gas–air by 5-26 % (**Table 1.6**). This indicates that the producer gas engine would be de-rated by 5-26% compared to a natural gas engine of the same displacement.

Table 1.6 Summary of the selected Producer gas compositions with their calorific values

	Comp. #1 Gussing	**Comp.#2 Viking**	**Comp.#3 IISc**	**Comp#4 Harboore**	**Comp.#5 CPC**
H_2	40	30.5	19.0	19.3	18.8
CO	24	19.6	19.0	22.8	21.0
CH_4	10	1.6	1.5	5.3	2.2
CO_2	23	15.4	12.0	11.9	1.4
N_2	3	33.3	48.5	40.7	56.7
LHV[1] (MJ/m_n^3)	10.95	6.32	5.1	6.87	5.49
LHV (MJ/kg)	12.17	6.32	4.60	6.33	5.32
Mixture Cal. Value(MJ/m_n^3)	3.15	2.69	2.46	2.74	2.54

1.4.2 Combustion Properties

There have been many theoretical studies by researchers to evaluate the laminar flame speed and ignition delay time of producer gas such as by Hernandez et al **[11, 12]**. Using the CHEMKIN software, auto ignition delay times and laminar flame speeds have been estimated for various producer gas compositions/equivalence ratios and the effect of

[1] LHV,Lower Heating Value empirically determined in units of MJ/m_n^3 where n represents normal temperature and pressure conditions.

temperature and pressure has been studied. The ignition delay time study suggests that producer gas has the potential to reduce knock tendency in SI engines by means of their lower ignition delay times and hence allowing intake at lower temperatures **[11]**.

The laminar flame speed study suggests that the flame speed of producer gas is lower than that of iso-octane and higher than that of methane. Higher flame speeds have been found for compositions with greater volume contributions of hydrogen and carbon monoxide **[12]**.

1.4.3 Engine Knock

Although it is widely accepted that producer gas has good anti knock properties owing to the diluents in its composition, there have not been many experimental studies evaluating knock properties, such as Methane Number.

Knock is an undesired abnormal combustion process often encountered in SI engines. It occurs in addition to the normal combustion process initiated by a spark plug. A normal combustion process includes the generation of an electrical discharge between the spark electrodes of the ignition system which initiates combustion by the end of the compression stroke. A self sustaining and propagating flame is developed which travels across the cylinder consuming the charge evenly throughout the combustion chamber. **Figures 1.9(a)** and **1.9(b)** show spark initiation and flame propagation in a normal combustion process.

Knock occurs when there is a spontaneous ignition of a portion of the end gas, owing to high temperature and pressure conditions. This auto-ignition process leads to an instantaneous release of energy stored in the end gas fuel. The localized temperature and pressure spike that occurs causes over stressing and wear of critical engine components such as piston and piston rings, valves, cylinder walls, head and head gaskets, valve seats and bearings**[13]**. **Figure 1.10** illustrates the auto-ignition of the end gas leading to knock.

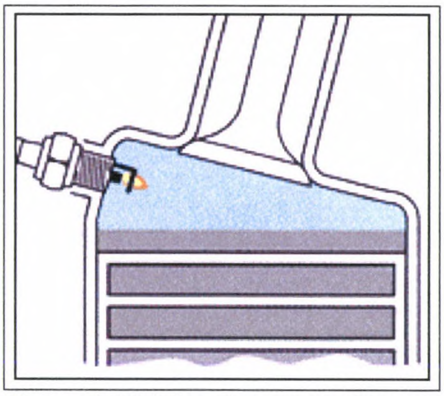


Figure 1.9(a) Spark Initiation Process

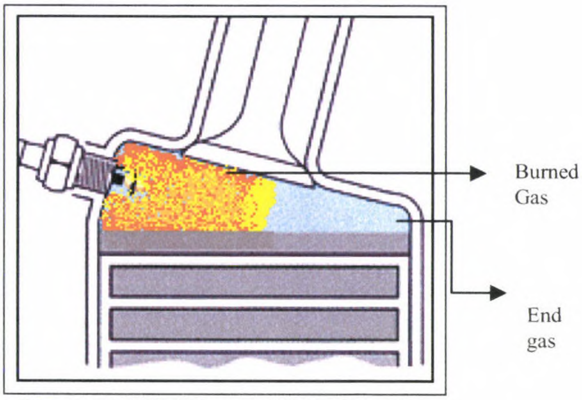


Figure 1.9(b) Normal Combustion

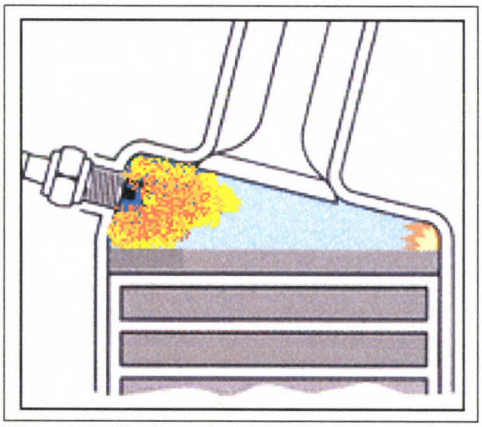
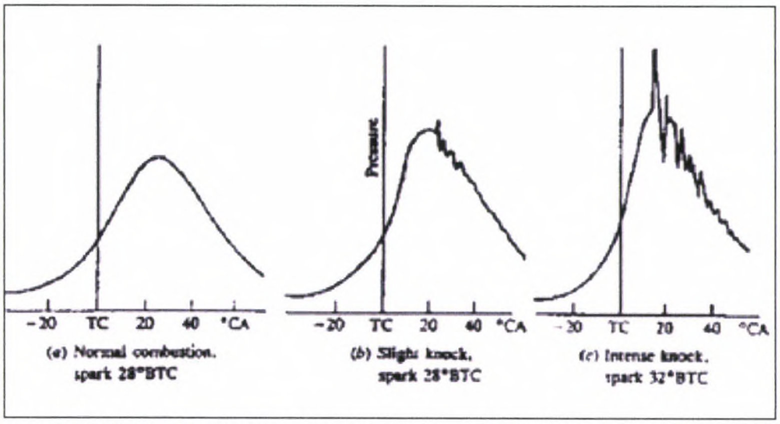


Figure 1.10 Auto Ignition of the end gas

“Knock” is generally identified by its characteristic metallic noise. The noise is a result of the high frequency pressure fluctuations that occur in the engine cylinder. The localized high temperature and pressure conditions generate a shock wave which propagates across the cylinder and is accompanied by an expansion wave. These waves reflect upon the combustion chamber walls and create oscillating pressure pulses **[13]**. **Figure 1.11** illustrates the cylinder pressure traces during various instances of knock.



(a) Normal combustion, spark 28°BTC

(b) Slight knock, spark 28°BTC

(c) Intense knock, spark 32°BTC

Figure 1.11 Cylinder pressure versus crank angle traces – Source [13]

Methane Number

The measurement and characterization of knock assumes importance owing to the detrimental effects it can have on engine performance. Historically knock has been measured for liquid petroleum fuels by the Octane Number (ON) scale. Essentially the knock rating of a liquid fuel is compared to that of a blend of two reference fuels and is assigned a dimensionless number. The ON scale is defined by n-heptane with an ON of zero and isooctane (2,2,4-trimethyl pentane) with an ON of 100. Hence an ON of 90 would imply the tested fuel will exhibit the same knock characteristics as that of a primary reference fuel blend of 90 parts of isooctane and 10 parts of n-heptane when tested in a standard engine under prescribed operating conditions. These procedures have been standardized as the Research method (RON) and Motor method (MON) by the American Standards for Testing and Methods (ASTM).

With the rise of gaseous fuels and alternative gaseous fuels for utilization in SI engines, there was need for a similar standard method of knock characterization for gaseous fuels with gaseous reference fuels. The ON scale ended at 120.34 (an admixture of 6ml TEL/US gal isooctane), which limited the knock rating of fuels with greater resistance to knock. Leikar et al **[14]** has suggested the Methane Number (MN) scale analogous to the

MON method for liquid fuels, based on the work done through 1964-1969 for the Austrian company AVL[2]. They established that methane and hydrogen have the highest and lowest resistance to knock respectively and defined the Methane Number scale as follows **[14]**:

> *"The percentage by volume of methane blended with hydrogen that exactly matches the knock intensity of the unknown gas mixture under specified operating conditions in a knock testing engine. . . For the range beyond 100 MN, methane-carbon dioxide mixtures were used as reference mixtures. In this case, in accordance with the definition, the MN refers to the reference methane-carbon dioxide mixture with a CO_2-content of (MN minus 100) percent volume."*

For this scale, a MN of 90 means the knock intensity of the tested gaseous fuel has the same knock intensity as that of a primary reference fuel blend of 90% by volume of methane and 10% by volume of hydrogen. For a MN beyond 100, for example 125, the reference fuel blend would contain 75% by volume of methane and 25% by volume of carbon dioxide.

Though researchers have scrutinized this existing method thoroughly as well as proposed other means of knock measurement, a 1999 publication by a group of European gas industry leaders concluded that Methane Number is a preferred method for measuring knock intensities of gaseous fuels **[15]**. Further many researchers have used this method for knock characterization of different types of gaseous fuels including reformed natural gas, coal gas, producer gas, digester gas and landfill gas **[10, 15]**.

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[2] AVL is the name of the Austrian company for which Leikar et al completed their work in [14]. The method adopted by Leikar et al is synonymously called AVL method and the software developed based on this method is called METHANE.

Chapter 2 – Experimental Apparatus Development

2.1 The CFR Engine

The CFR F-2 (Cooperative Fuel Research) engine is utilized for the ASTM (American Standards for Testing and Materials) Motor Octane Number rating of a spark ignition engine fuel. It is a single cylinder, four stroke, and variable CR (Compression Ratio) engine equipped with a knock intensity detection system. A 1957 make CFR engine manufactured by the Waukesha Motor Company is installed in the lab and has been duly upgraded and modified for gaseous fuel testing. The engine is coupled to a synchronous AC motor/generator which enables engine start up and maintains a constant speed of 900 rpm. The engine has a bore of 3.25 inches and a stroke of 4.5 inches. Compression ratio can be varied between 4:1 and 18:1 while the engine is running.

The knock intensity detection system consists of a detonation pickup, detonation meter and a knockmeter. The D-1 type detonation pickup shown in **Figure 2.1** is mounted in the combustion chamber wall and reacts to the change in chamber pressure by means of stretching a thin flexible diaphragm at the bottom of the pickup assembly **[16]**. This stretch of the diaphragm causes change in the magnetic field around a magnetostrictive alloy wound with a copper coil wire. The change in magnetic flux around the coil induces a voltage in the coil that connects to an output signal pin.

The Detonation Meter receives this signal and acts as a control panel for the user to adjust the zero point, number of integration cycles and range of knock intensity. The knobs on the detonation meter used to make these adjustments are identified in **Figure 2.2**. The knock meter as shown in **Figure 2.3** has a 0-100 division scale which serves to estimate and compare the knock intensity of the reference and blended fuels. The output signal on the knockmeter is proportional to the rate of change of combustion chamber pressure **[16]**.

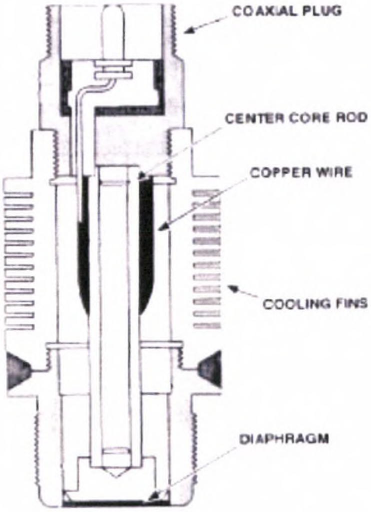


Figure 2.1 Detonation Pickup- Source [16]

Figure 2.2 Detonation Meter

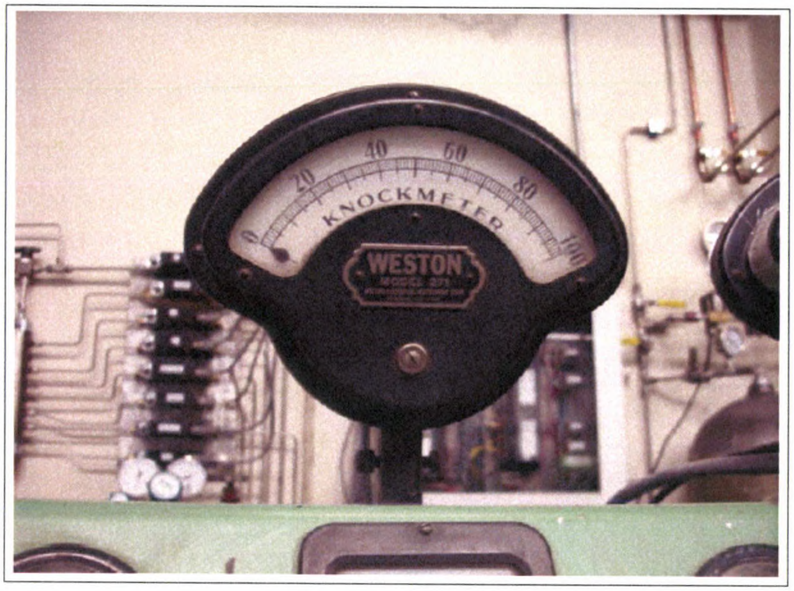


Figure 2.3 Analog Knockmeter

2.2 CFR Engine Modifications and Gas Blending System

The mechanical magneto ignition system originally installed on the CFR was upgraded with a robust Altronic CD200 electronic ignition system. This capacitor discharge system senses the angular position signal from magnetic pickup holes on a camshaft disc. Hence ignition timing is maintained and referenced directly to the crankshaft position. The Altronic set up is shown in **Figure 2.4**.

The engine intake system was enhanced with an Electronic Gas Carburetor (EGC) developed by Continental Controls for air-fuel ratio control. It consists of a venturi mixer and electronic pressure regulator responding to a wide band oxygen sensor located in the exhaust. The carburetor is operated by user friendly *Valve Viewer* software, proprietary of Continental Controls. Using this, the engine can be run at desired O_2 set points and fuel inlet pressures. These two features greatly aid in sweeping equivalence ratio (φ) for maximum knock. The engine has appropriate instrumentation to monitor and record engine speed, intake air temperature, intake air humidity, coolant water temperature and power.

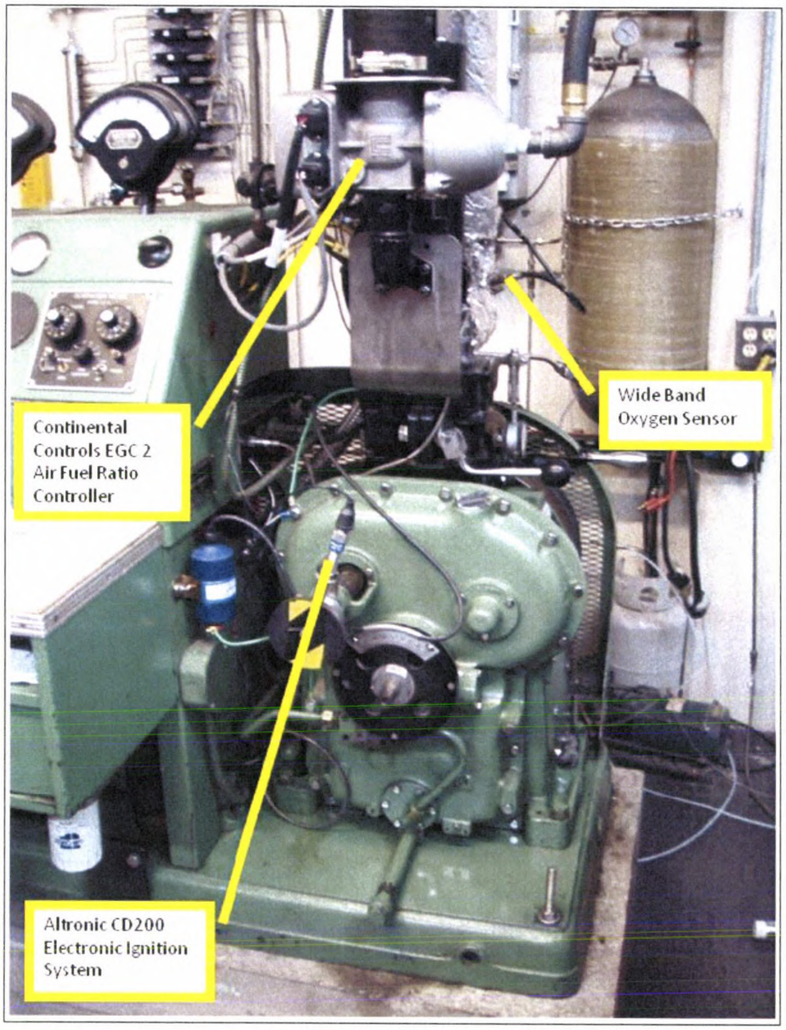


Figure 2.4 Altronic CD200 and EGC set up on the CFR

Gas Blending System: In order to simulate alternative gaseous fuels, a computer controlled gas blending system was developed **[15]**. Eight different gases (hydrogen, methane, carbon dioxide, carbon monoxide, ethane, butane, propane, and nitrogen) which are the general constituents of alternative gases can be blended in this system. By interfacing Mass Flow Controllers (MFCs) with the Lab View software and enabling communication through the National Instruments Field Point modules, the operator can input desired fuel blend into the system. **Figure 2.5** is a schematic of the gas blending system **[15]**.

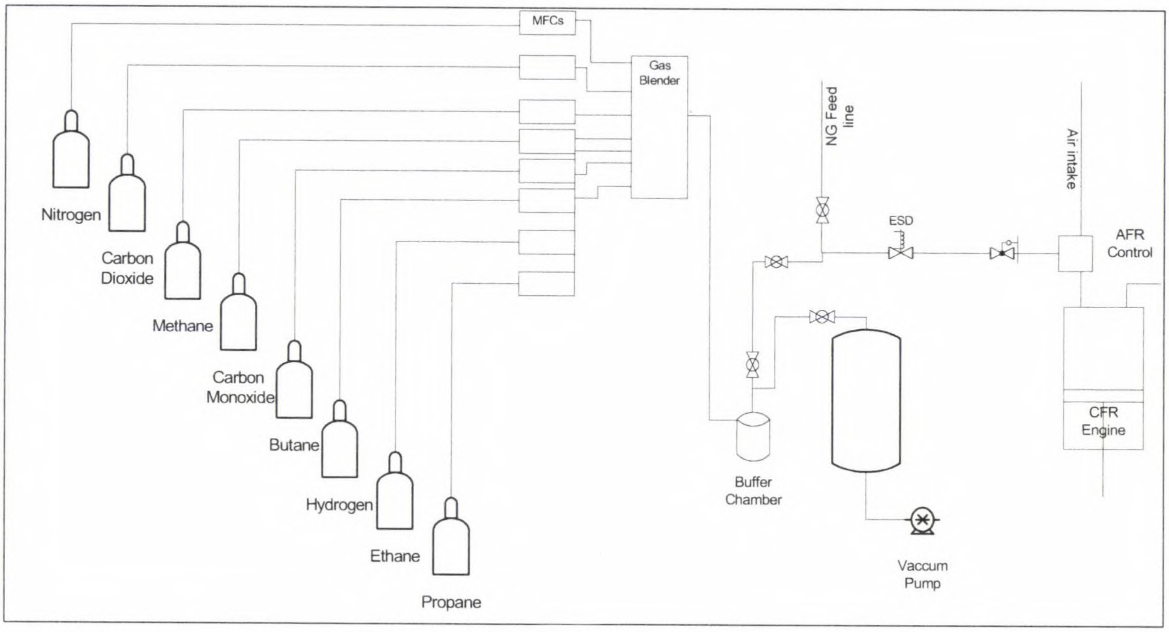


Figure 2.5 Gas Blending System [15]

For the case of testing producer gas, some changes were incorporated in the existing system. Producer gas is a low calorific value fuel (owing to huge volumetric content of N_2 and CO_2) and operates on low air-fuel ratios (AFR ranging between 1 and 2). The MFCs previously installed for N_2 and CO_2 were of lower range mass flows as compared to those required for producer gas. Rotameters were added to allow the required N_2 and CO_2 flowrates. However, when high N_2 or CO_2 flowrates into the fuel flow were established, the carburetor maximum fuel flowrate was not high enough to achieve stoichiometric air-fuel ratio. To achieve stoichiometric air-fuel ratio using the existing carburetor N_2 and CO_2 diluents were metered directly into the air intake just before the carburetor.

Two separate fuel feed lines were installed for CO_2 and N_2 flow as shown in the **Figure 2.6**. The flow rates were controlled using rotameters and three way valves that allowed either the mass flow controller route or the rotameter route to be used, depending on the composition. For compositions with high volumetric content of N_2 such as in Viking, IISc, Harboore, and CPC compositions, the N_2 rotameter route was used. Sample calculations for estimating flow-rate of N_2 are shown in **Appendix I**. For diluents' composition variation tests done in the later part of this report, the CO_2 external flow line was used. The Lab view VI was enabled to display and acquire mass flow rates of the fuel gases.

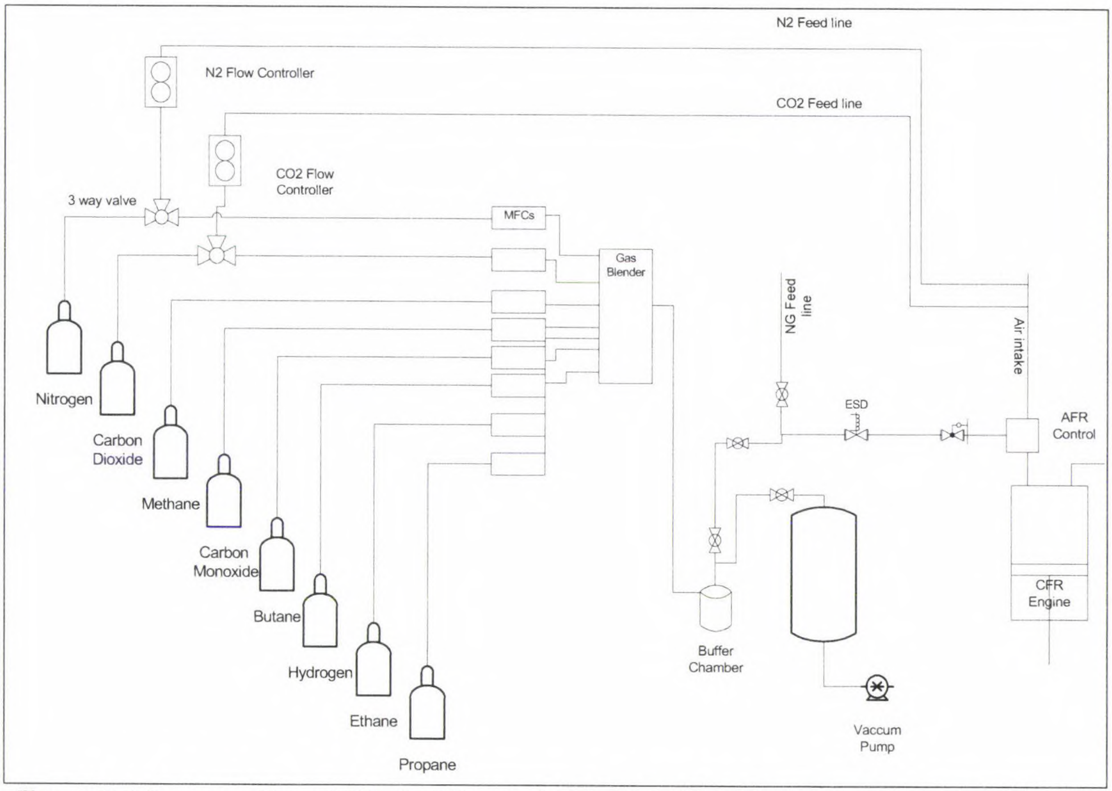


Figure 2.6 Separate N_2 and CO_2 fuel lines added to Gas blending system for Producer Gas Testing

2.3 Experimental Procedure

Although ASTM does not specify any specific testing method for Methane Number measurement, the MON method is considered as an analogous testing method. Work done by Leiker et al. **[14]** was instrumental in defining and documenting the methods for Methane Number measurement. This was adapted and developed further by Ryan et al. **[17]**.

The procedure involves the use of hydrogen and methane as reference fuels in a CFR engine at specified conditions. The knock intensity of the test fuel is matched with a blend of these reference fuels. Both Leikar et al. **[14]** and Ryan et al.**[17]** first established a MN calibration curve by testing blends of methane and hydrogen between methane (MN of 100) and hydrogen (MN of 0). This was done by setting the knockmeter to 50 percent of the full scale for pure methane, which represented a MN of 100. Then the methane-hydrogen blends were tested by varying the compression ratio and matching the knock meter reading of 50 percent of the full scale. Hence a calibration curve was established for the reference fuel blend against compression ratio. Further, while establishing MN of blended fuels, compression ratio for knock of same intensity (50 percent of the full scale) was found and MN was matched up on the calibration curve. This approach requires the knock meter to remain stable throughout MN testing.

In the current approach, procedure for MN testing is fairly direct. Here, the knockmeter is first set at known intensity for the blended gas at the compression ratio for light audible knock. Maintaining the same compression ratio, the composition of reference gas is found which knocks at the same intensity as the blended gas. Though this procedure consumes more time and fuel, it eliminates many variables during engine operation such as intake air temperature, ambient pressure and humidity. Additionally, the knock meter is only required to remain stable for the duration of a single MN measurement. Another change in procedure was that the test was conducted at an AFR that produced maximum knock instead of maintaining an equivalence ratio (φ) of 1 as done by Leikar et al. **[14]** and Ryan et al. **[17]**. This method eliminated any errors in measurement of φ. These changes were also incorporated for testing in previous work **[10, 15]**. **Table 2.1** outlines basic operating conditions to be set for the CFR.

Table 2.1 CFR Operating Conditions for Methane Number measurement

Engine Speed	900 rpm
Equivalence Ratio	Maximum Knock
Spark Timing	15 deg BTDC
Intake Air Temperature	21 deg C

The following is a step wise procedure which was followed to establish Methane Numbers for producer gas:

1. Run the CFR engine on natural gas and allow it to reach stable operating conditions outlined in **Table 2.2**.
2. Ensure it is not knocking by running on a low compression ratio and set the knockmeter to read zero at this point.
3. Change the engine fuel supply to blended gas by entering the required volumetric composition in the Lab view VI.
4. Allow engine to run on blended fuel and reach stable operating conditions.

5. Increase the compression ratio until light audible knock is heard. Set the compression ratio at this point.
6. Adjust the knockmeter to read 50. Sweep the AFR to maximize knock. Readjust the knockmeter to 50.
7. Record Engine and blended gas composition data using the LabView VI.
8. Change fuel supply to reference fuel. Run the engine on estimated methane number.
9. Observe KI (knock intensity) and change reference fuel blend in order to achieve a KI of 50. If KI is less than 50, add hydrogen. If KI is more than 50, add methane. If KI does not reduce with 100% methane, use a blend of CO_2 and methane.
10. Record engine and composition data on Lab View VI. Required MN is the volume % of methane in reference blend if methane-hydrogen was used. Required MN is 100+volume % of CO_2 in reference blend if methane-CO_2 was used.

Table 2.2 Stable operating conditions on natural gas for the CFR

Engine Speed	900 rpm
Oil Temperature	54-60deg C
Coolant Temperature	95 deg C

Chapter 3 – Methane Number Measurement of Producer Gas

3.1 Methane Number of Selected Producer Gas Compositions

Table 3.1 Compositions tested and recorded methane numbers

Test Gas Composition	Trial	H_2%	CO%	CH_4%	CO_2%	N_2%	Methane Number	Avg.	Std. Dev
Gussing	Trial 1	39.1	23.0	10.3	22.3	4.89	54.1	55.6	1.56
	Trial 2	38.2	24.1	10.3	22.6	4.76	57.2		
	Trial 3	38.3	24.1	10.3	22.4	4.86	55.4		
Viking	Trial 1	30.0	17.9	2.65	15.0	34.3	56.5	54.6	1.65
	Trial 2	29.4	17.5	2.61	14.8	35.7	53.7		
	Trial 3	29.5	17.6	2.62	14.8	35.4	53.6		
IISc.	Trial 1	17.9	20.2	2.23	13.4	46.4	131.0	125.7	4.78
	Trial 2	20.7	19.0	1.98	12.6	45.7	121.7		
	Trial 3	20.5	18.9	2.07	12.6	45.9	124.4		
Harboore	Trial 1	20.1	23.3	6.13	13.0	37.5	104.9	105.6	0.64
	Trial 2	20.6	22.3	5.95	12.5	38.6	106.0		
	Trial 3	20.7	22.5	5.98	12.6	38.3	106.0		
CPC	Trial 1	20.0	21.3	3.02	2.03	53.6	54.3	57.5	2.84
	Trial 2	19.9	21.3	3.05	2.04	53.6	58.5		
	Trial 3	20.2	21.3	3.01	2.03	53.4	59.7		

Three trials were conducted for each of the selected producer gas compositions. Test gas composition data and reference gas data were both collected when they produced similar knock intensity on the CFR engine. The reported MN is based on the recorded reference gas composition. **Table 3.1** compiles data for compositions tested and the methane numbers obtained.

For representation purposes, the average values from three trials along with the standard deviation amongst them have been shown in **Figure 3.1**. Test data for all the runs is available in **Appendix II**. Results of Trial 2 have been used for all further discussions.

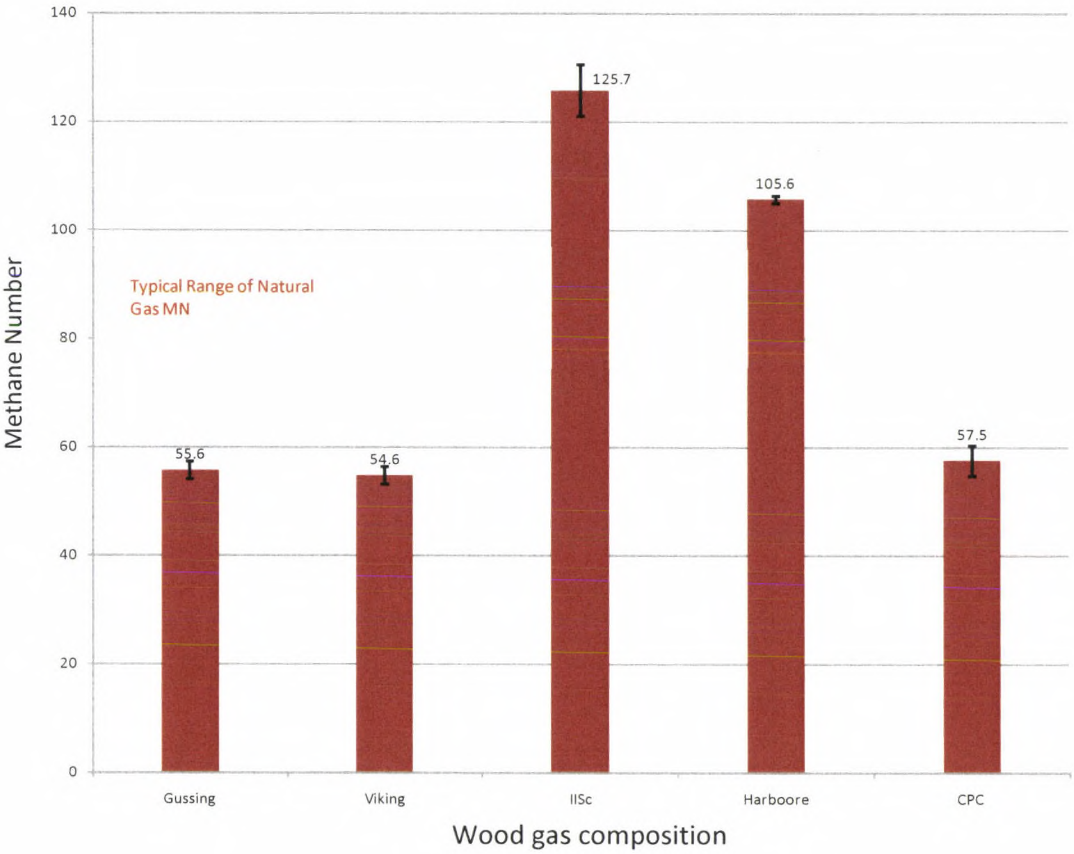


Figure 3.1 Comparison of average Methane Numbers of selected Producer gas compositions

At least three of the selected producer gas compositions have Methane Numbers less than those of typical natural gas. Only two of them have a Methane Number greater than those of typical natural gas. This indicates that if engines running on natural gas (8.5:1 to 10.5:1) were to be directly used for producer gas, only the "IISc" and "Harboore" compositions may be suitable. Hence while designing an engine to run on the other three compositions, one should keep note that their critical compression ratios will be lower than that of natural gas. This compression ratio would have to be ascertained for the engine in question, based on its operating conditions and size.

At this point it is interesting to compare the AVL methane numbers (obtained from the AVL software Methane 3.10a) and the experimental Methane Numbers as shown in **Figure 3.2**.

Figure 3.2 Comparisons of AVL MN and Experimental MN

This shows that although the trends for the methane numbers are similar in both cases, the range of the AVL methane numbers is narrowed to being in between 60 to 90. This is the range of expectant methane numbers for natural gas compositions. The data indicates that Methane 3.10a is not suitable for compositions with higher diluent composition and combustible gas with H_2 and CO such as producer gas.

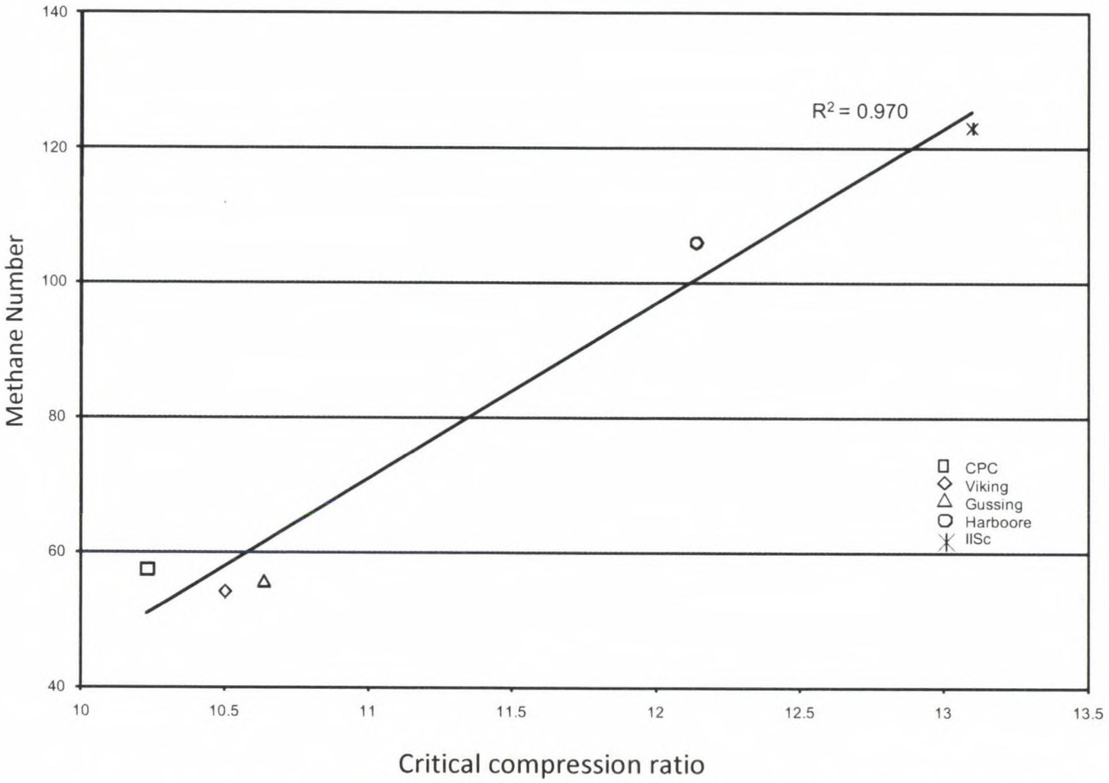


Figure 3.3 Measured Methane Numbers referenced to their critical compression ratios

Figure 3.3 illustrates the relationship between measured Methane Numbers (Trial 2) for each composition and the critical compression ratio. Critical compression ratio refers to the compression ratio at which the fuel mixture experiences 'light audible knock' in the test engine. An examination of this plot reveals a fairly linear trend with an R-squared value of 0.970. It can be deduced that the compositions "Harboore" and "IISc" can be run on compression ratios greater than that of typical natural gas, while compositions "Gussing", "Viking" and "CPC" may require engines to be designed at a compression ratio lower than that of typical natural gas.

3.2 Sensitivity Analysis of Combustible and Diluents Composition

Methane Numbers of producer gas compositions were found to be extremely sensitive to the volumes of combustibles (such as hydrogen) and diluents (such as carbon dioxide) in them. The higher methane numbers have been obtained for compositions "IISc" and "Harboore". These compositions are indeed the most common producer gas compositions obtained in small scale commercial applications. The higher methane numbers are a result of lower hydrogen content (20% volumetric content) and very high diluents (around 45 % nitrogen and 12% carbon dioxide). Higher diluent content effectively reduces the heating value of the fuel producing lower end gas temperatures, which inhibits auto-ignition.

Figure 3.4 shows the correlation between the gas composition and obtained Methane Numbers. There are three compositions which have a Methane Number in the range of 50 to 60. The reason for the composition "Gussing" to have a lower Methane Number of 57.2 could be explained due to its high hydrogen content (around 40% of its volumetric composition). Hydrogen by virtue of its high flame speed increases the end gas temperature and promotes auto-ignition.

Composition "Viking" has a 30% volumetric content of hydrogen and a methane number of 53.7. The reason it has a Methane Number comparable to that of "Gussing" in spite of the lower hydrogen percentage would be the lower carbon dioxide content.

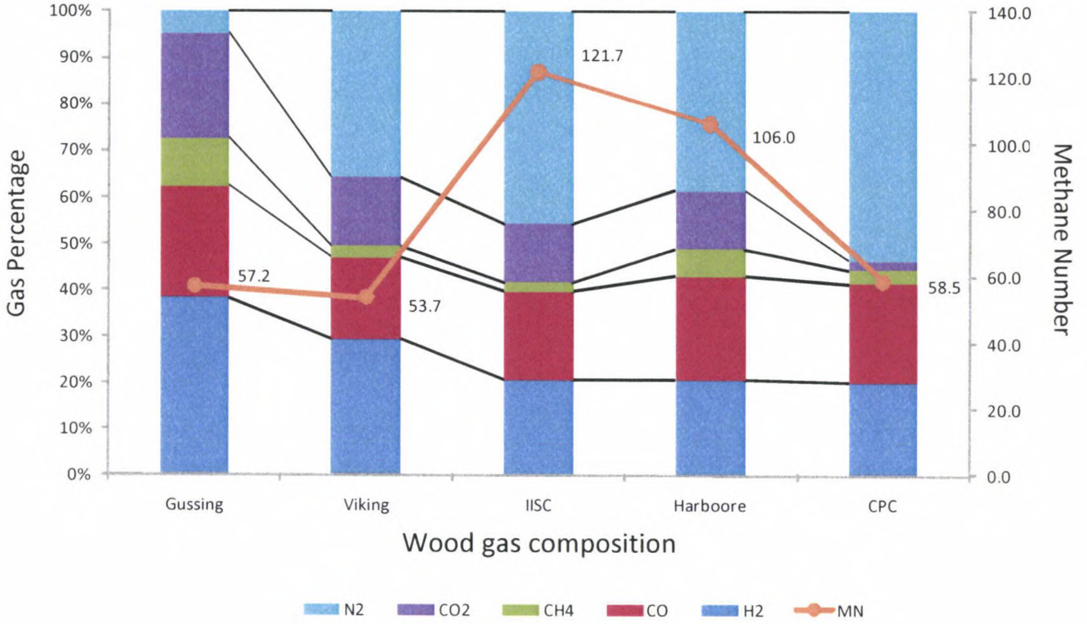


Figure 3.4 Gas Composition Distribution and Methane Numbers

The effect of lower carbon dioxide increasing knocking tendency is evident in the methane number of composition "CPC" as well. This composition has a negligible volume of carbon dioxide, while all the other gases are similar in proportion to "Harboore". This aspect of the effect of carbon dioxide acting as a knock suppressor was studied in detail by testing compositions with varying volumes of carbon dioxide. Similarly the effect of hydrogen acting as a knock inducer was studied by testing compositions with varying volumes of hydrogen.

Constant Combustibles Test - For this test, the volume percentages of combustibles were kept constant at 20% H_2, 20% CO and 5% CH_4. The total diluents amount was maintained constant at 55% by volume. The diluent composition was varied from negligible CO_2 and 55% N_2 to 17% CO_2 and 38% N_2. For each of these compositions the critical compression ratio was determined at the same operating conditions used for Methane Number testing.

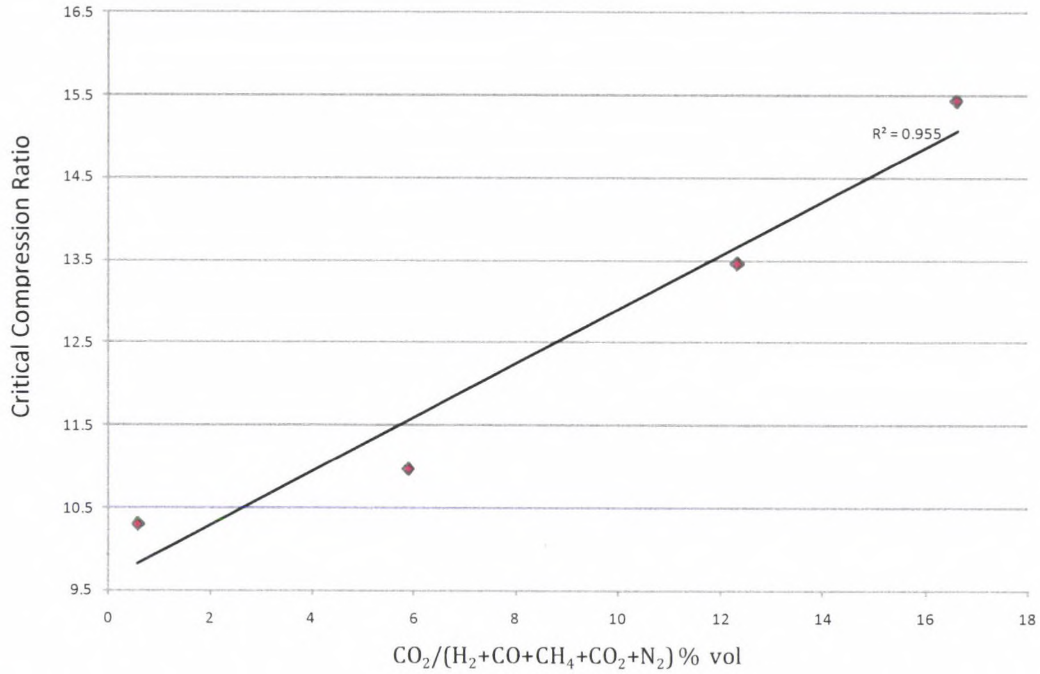


Figure 3.5 Increase in the volume of CO_2 in test gas increases the compression ratio for knock

Figure 3.5 shows that an increase in the volume percentage of carbon dioxide in the test gas acts to increase the critical compression ratio. Within 0-6 % total volume of CO_2 an increase of 0.125 units of compression ratio per % CO_2 is observed. Similarly for the range of 6-13% CO_2 in the test gas, an increase of 0.386 units of compression ratio per % CO_2 is observed and for the range of 13-17% CO_2 in the test gas, a rise of 0.459 units of compression ratio per % CO_2 is measured. This shows that for a higher volume of CO_2 in the gas, small changes in composition can bring about a larger change in critical compression ratio and hence methane numbers. The test results are tabulated in **Table 3.2**.

Table 3.2 Results of Constant Combustibles Test

Volume Percentage of CO_2 in the test gas (Other constituents being 20% H_2, 20% CO, 5% CH_4 and rest nitrogen)	Critical Compression Ratio
0.58	10.3
5.9	11.0
12.3	13.5
16.6	15.4

Constant Diluents Test – For this test, the volume percentages of diluents and methane (which is in low volumes usually) were kept constant at 12% CO_2, 43% N_2 and 5% CH_4. The combustibles composition was varied from 10% H_2 and 30% CO to 25% H_2 and 15% CO. Again, for each of the compositions tested, the critical compression ratio was determined at the same operating conditions used for Methane Number testing. Results from this test are tabulated in **Table 3.3**.

Table 3.3 Results of the Constant Diluents Test

Volume Percentage of H_2 in test gas (Other constituents being 12% CO_2, 43% N_2, 5% CH_4, CO balance)	Critical Compression Ratio
11.1	15.0
15.7	14.6
19.9	13.5
25.8	12.9

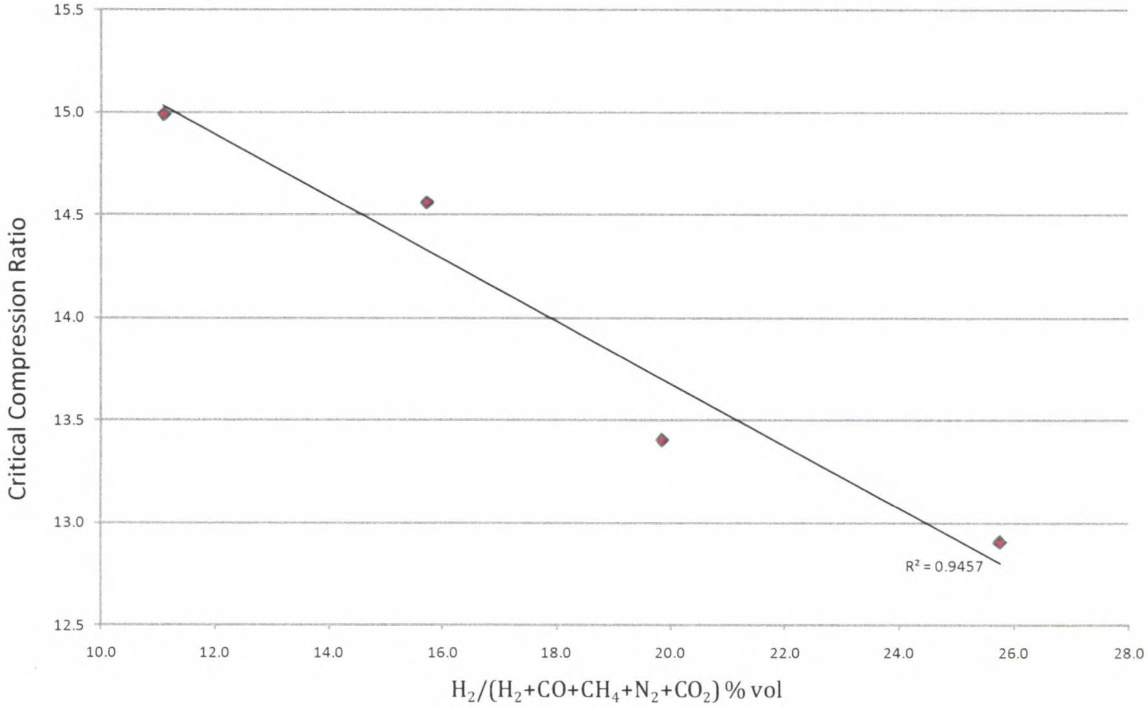


Figure 3.6 Increase in percentage volume of H2 in the test gas decreases the compression ratio for knock

Figure 3.6 shows that there is a decreasing trend for the critical compression ratio as the percentage volume of hydrogen in the composition is increased. If a linear trend was considered for both tests, a 1 % increase in CO_2 increased the critical compression ratio by 0.319 units and a 1% increase in H_2 decreased the critical compression ratio by 0.142 units. The relative impact of CO_2 on critical compression ratio is over 2X that of H_2. Hence the effect of addition of either CO_2 or H_2 was clearly quantified by these tests.

3.3 Estimation of Error in Methane Number

There are three major sources of error in the methane number measurement: procedural error, test gas composition error and reference gas composition error. The procedural error has been previously established by Malenshek et al in **[15]**. In order to find the error in the procedure a chosen composition was tested ten times and the standard deviation was found to be 0.3 MN **[15]**. Error in the duplication of the test gas composition is not relevant, as the achieved composition is only expected to approximate the literature compositions as closely as possible. Matching the literature composition precisely is unimportant. The methane number achieved is hence reported for the tested composition and not for that listed in the literature.

The reported methane number is most dependent on the reference gas composition. An uncertainty in the measurement of the methane or carbon dioxide composition dictates the uncertainty in Methane Number. For single sample experiments, Kline and McClintock **[18]** have suggested a method for determining experimental uncertainty by combining individual uncertainties of all involved variables. The involved variables here are the flow rates of methane or carbon dioxide given by the mass flow controllers. The accuracy specifications of the various mass flow controllers have been taken into account in the calculation of uncertainties **[Appendix IV]**.

A combined, or total, uncertainty for each methane number measurement was computed. The average combined uncertainty was found to be ±4.25 MN. Hence total uncertainty including the procedural standard deviation is ± 4.55 MN. Individual errors are reported graphically in **Figure 3.7**.

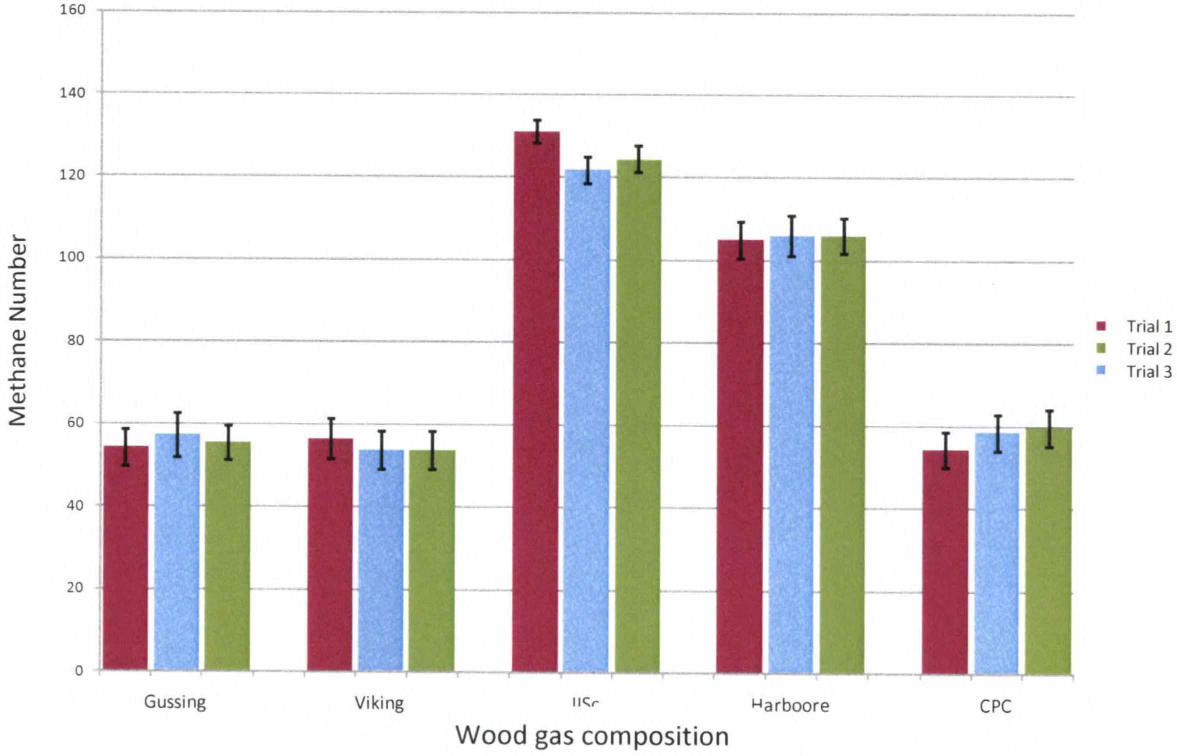


Figure 3.7 Average Error for each MN was found to be 4.55 MN

During experimental work some other sources of error were observed, which could not be quantified. These sources of error along with some methods of process improvement are suggested in **Chapter 5**.

Chapter 4 - Methane Number Determination of Producer Gas using CHEMKIN®

4.1 CHEMKIN Model Setup & Validation

CHEMKIN 4.1.1 software consists of a varied set of applications for solving chemical kinetics problems. The zero dimensional internal combustion engine model of CHEMKIN is a pre-defined reactor model which simulates a combustion cylinder under auto ignition conditions **[19]**. By means of replicating the CFR Engine with the CHEMKIN engine model in the procedure outlined in **Section 2.3**, it is theorized that one can determine the methane number of a producer gas fuel. The following steps were adopted to simulate the experimental procedure in CHEMKIN.

4.1.1 Setting the Engine Parameters

The Closed Internal combustion engine simulator model was selected from the Models palette.

Figure 4.1 Selecting the I.C Engine Simulator

The specifications of the CFR-F2 engine, which was used in the experimental method, were used as the engine input parameters. The "reactor physical properties" are listed in **Table 4.1**.

The engine is simulated to run for one crank revolution and hence the starting crank angle is -180 deg such that zero deg represents TDC (top dead centre). Reactant species or the fuel-air intake to the engine can be input on the "reactant species" tab.

Table 4.1 Modelling the I.C Engine on CHEMKIN

Engine Cylinder Displacement Volume	611 cm^3
Engine Connecting Rod to Crank Radius Ratio	3.71
Engine Speed	900 rpm
Starting Crank Angle	- 180 deg

It is important to note here that the reactant species includes the air intake of the engine as necessary for the desired equivalence ratio (φ). **Appendix V** shows example input parameters for engine physical properties and mole fractions of reactant species. Two different approaches were considered in terms of modelling the heat loss of the system. One case was the simplistic adiabatic model, which assumes no heat loss. The other considered convective heat loss through the engine cylinder walls, in which case a generalized heat transfer correlation Equation 4.1 **[13]** was used.

$$Nu = a\ Re^b\ Pr^c \qquad \text{(Equation 4.1)}$$

The equation includes Nusselt (Nu), Reynolds (Re), and Prandtl (Pr) numbers. The empirical coefficients a, b, and c were assigned typical values of 0.035, 0.8 and 0.333 respectively.

4.1.2 Mechanism Selection

Mechanism selection is an important aspect of CHEMKIN modelling. The collection of chemical data in a given chemistry set is called a reaction mechanism **[19]**. This is generally available as a thermo chemical data file and a file containing the descriptions of the gas phase reactions. Four mechanisms were considered for this work.

1. GRImech 3.0 **[20]**: a compilation of 325 elementary chemical reactions, associated rate coefficient expressions and thermo chemical parameters for 53

chemical species. GRImech has been optimized for natural gas and methane combustion.

2. Pitz et al **[21]**: a compilation of 639 reversible reactions for 126 species involved. This mechanism was developed to study the promotion effect of hydrocarbons on NO-NO2 conversion in a flow reactor.
3. Petersen et al **[22]**: a compilation of 663 chemical reactions among 118 species. This is a methane-propane oxidation model consisting of a comprehensive methane-hydrogen mechanism.
4. USC II **[23]**: a compilation of 784 chemical reactions and 111 species comprehensive of high temperature H2/CO/C1-C4 combustion.

It was attempted to optimize for the mechanism which gave closest results to the experimental producer gas methane numbers.

4.1.3 Procedure

a. The stoichiometric mixture of the test fuel and air is run in the CHEMKIN engine model for compression ratios varying from 4 to 18.

b. The minimum compression ratio at which fuel auto-ignition occurs is identified.

c. At this compression ratio, a mixture containing 50% by volume of hydrogen and 50% by volume of methane is compression ignited in the engine.

d. The goal is to find the minimum % volume of hydrogen required to ignite the reference fuel mixture. The Methane Number is defined as $100-\%H_2$.

e. If the reference fuel mixture ignites for 100% methane, a carbon dioxide – methane blend is used such that the MN range extends beyond 100. In this case, a MN of 120 would correspond to a blend of 80% by volume of methane and 20% by volume of carbon dioxide.

4.1.4 Method Validation

In order to validate this procedure, Methane Number of natural gas compositions was first found. The MN given by the AVL Methane 3.10a model was used as the reference MN.

3 different compositions were used with 2 mechanisms. The results for these tests are shown in **Table 4.2**.

Table 4.2 Results for Methane Number measurement of Natural Gas

Method	69% CH_4,20% C_2H_6,11%C_3H_8	93%CH_4,4.3% C_2H_6,2.7% C_3H_8	49% CH_4, 19% C_2H_6,32% C_3H_8
METHANE 3.10a	56.7	78.5	45
GRImech3.0 (adiabatic)	95.4	96.6	95
Pitz et al. (adiabatic)	63.4	83.9	52

From **Table 4.2** it is clear that GRImech 3.0 overestimates the Methane Number for compositions with lower methane content while Pitz et al. mechanism seems to trend along the numbers obtained from Methane 3.10a. It was found that Pitz et al incorporates more species for its reaction mechanism along with low temperature oxidation reactions, unlike GRImech 3.0. This validation method highlights the importance of choosing a mechanism for the Methane Number measurement which closely approximates chemical reactions pertaining to the chosen fuel composition.

4.2 Results and Discussion

Considering that this method of Methane Number evaluation is procedurally long, it was decided to work on one composition and optimization with different CHEMKIN mechanisms until the Methane Number was found to be acceptably close to the experimental values. The results of this work for composition "Gussing" is shown in **Table 4.3**.

Table 4.3 Results of Methane Number measurement for "Gussing"

Composition	Mechanism/Method	MN
Gussing Composition for Chemkin- 40%H_2,24%CO,10%CH_4, 23%CO_2, 3%N_2	GRImech3.0	28
	Pitz et al.	31
	Petersen et al.	43.5
	USC II	49
	USC II(with heat loss)	**51.5**
	METHANE (AVL method)	61.6
Experimental Gussing Composition – 38.5%H_2,23.8%CO,10.3%CH_4, 22.4%CO_2, 4.8%N_2	Experimental	57.2

From **Table 4.3** it is clear that GRImech 3.0 and Pitz et al. do not work for producer gas as well as they did for natural gas compositions. Petersen et al. worked slightly better, but the best results came from the USC II mechanism. The USC II mechanism has indeed been formulated for high temperature H2, CO, C1-C4 combustion.

The USC II mechanism was then used to evaluate the Methane Numbers for all the other producer gas compositions. Results for this are shown in **Table 4.4**.

Table 4.4 Results of Methane Numbers for producer gas compositions using USC II

Composition	Volume % of gases					Methane Number (USC II with heat loss)	Methane Number (Experimental results for Trial 2)
	H2	CO	CH4	CO2	N2		
Gussing	40	24	10	23	3	51.5	57.2
Viking	30.5	19.6	1.6	15.4	33.3	33	53.7
IISc	19.4	19.4	1.53	12.2	47.5	38	122
Harboore	19.3	22.8	5.3	11.9	40.7	42	106
CPC	18.8	21.0	2.24	1.42	56.5	13	58.5

The data in **Table 4.4** indicates that the USC II mechanism did not give accurate numbers for any other composition except "Gussing". There is also no clear trend in the way the evaluated Methane numbers behaved with this mechanism. **Figure 4.2** displays the trends with two different mechanisms (Petersen-adiabatic and USC II-heat loss) along with the experimental and AVL methods. The USC II mechanism appears to work better for a composition with high H_2 % (up to about 40% by volume) and lower inert gas percentage, but was significantly different than experimental results for those with higher inert gas volumes.

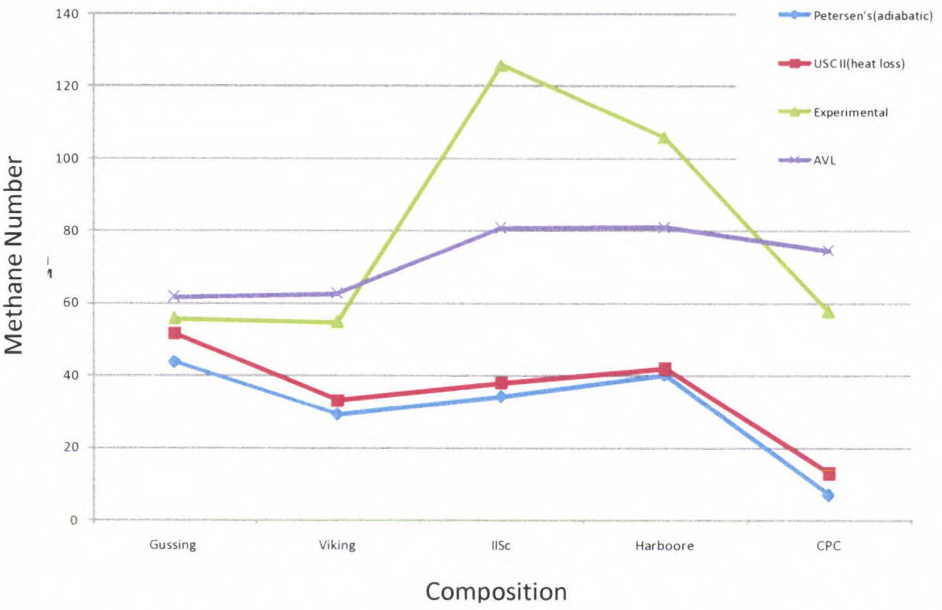


Figure 4.2 Results and trends of Chemkin model compared to experimental MN

4.3 Future Scope of Work

Two aspects need further research. One is the validity of using the CHEMKIN IC engine model for the purpose of predicting knock. The phenomenon of knock is understood to be due to the auto ignition of the end gas and is highly dependent on the temperature and pressure conditions in the cylinder during the power stroke. In the experimental method, the temperature and pressure in the cylinder were influenced by the fact that there was external ignition to the fuel in the cylinder (by means of the spark plug). While in the case of the CHEMKIN model, the fuel is only compression ignited. It simulates “flame” compression by additional piston compression. Consequently, the CHEMKIN model compression ratios in **Figure 4.3** are larger than experiment.

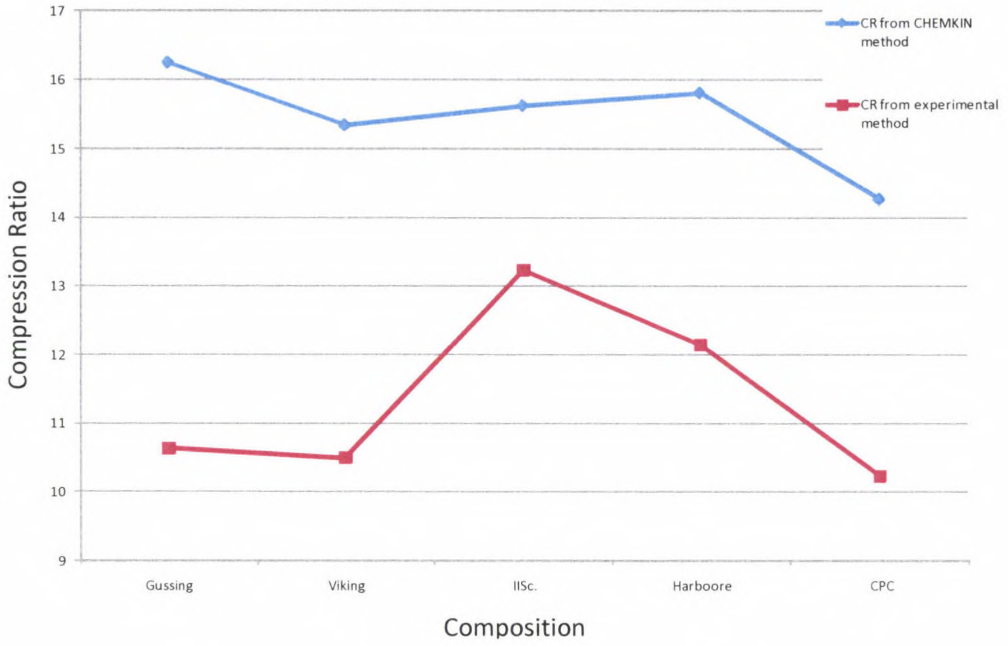


Figure 4.3 Comparison of Compression Ratios of model and experiment

During flame propagation in the experiment, there is significant heat transfer via radiation and turbulent convection between the burned and unburned zones. This physical process is absent in the model. There are other physical differences between model and experiment; the important consideration is whether the impact of these differences is consistent from producer gas to reference blend. The magnitude of heat transfer from burned to unburned gas is likely to be significantly different for producer gas and reference blends, which may account for some of the discrepancy between model and experiment.

The second aspect that could be inspected is that of the CHEMKIN mechanism selection. It would be of use to find or formulate mechanisms specifically for H_2, CO,

CH_4 combustion along with high diluents' volume. It would be of significance to understand if the reaction mechanism suitable for producer gas is indeed suitable for the reference gas as well. A reaction sensitivity analysis on the USC II mechanism would also be insightful. It would highlight key reactions that dictate compression ignition for the conditions modelled. Rate coefficients for key reactions can be modified to match experimental data.

Chapter 5 – Summary & Conclusions

5.1 Summary

With increased use of alternative gaseous fuels in internal combustion engines for power generation, it is apparent their performance optimization is becoming a priority for engine manufacturers. One of the alternative fuels gaining popularity in the alternative power generation market is Producer Gas.

Producer Gas is derived from woody biomass material by subjecting it to combustion-reduction reactions in a gasifier. This process called "gasification" results in a gas consisting of hydrogen, carbon monoxide, methane, carbon dioxide and nitrogen of which hydrogen, carbon monoxide and methane are the gases contributing to the heating value of the gas. By varying process parameters such as gasification medium, biomass material and gasifier type the producer gas composition can be favourably altered to avail high amounts of combustibles. This is observed in compositions of "Gussing" and "Viking" with 40% and 30% hydrogen by volume, respectively. The more commonly availed producer gas compositions (by virtue of lower production costs) are of "IISc" and "Harboore" which have 20% by volume of hydrogen and 20% by volume of carbon monoxide.

One important fuel combustion characteristic is knocking tendency in an internal combustion engine. Knock is an abnormal combustion event that causes engine wear and component damage. The knowledge of knocking tendency of a fuel is important for an engine manufacturer as this limits the compression ratio of operation of the engine. For an engine running on the Otto cycle, higher compression ratios relates directly to higher thermal efficiencies of the engine. Hence knock characterisation of new alternative fuels is highly relevant.

ASTM recommends the use of MON method for knock characterisation of gasoline but no such standard exits for gaseous fuels. Researchers such as Leikar et al have developed the Methane Number scale which is analogous to the Octane Number scale for gasoline. The work of Leikar et al has been further developed by Ryan et al. These two works have been the basis for using the Methane Number scale as an acceptable scale of measurement of knock for gaseous fuels. The Methane Number measurement employs a Cooperative Fuel Research engine. Instead of developing a calibration curve for MN and CR as done by previous researchers, the MN for each composition was measured directly in our work. The procedure followed here differs from that of previous researchers by being more direct and nullifying the effect of ambient and engine operating conditions on knock. Constant equivalence ratio control was avoided by testing the fuel at the AFR which provided maximum knock for both the test gas and reference gas blend.

A theoretical approach was also considered to determine the Methane Number of producer gas using the CHEMKIN software. The zero dimensional internal combustion engine model was used and its parameters set to match that of our test engine. Four chemical mechanisms were tested to determine the mechanism which best simulates conditions for producer gas combustion.

5.2 Conclusions

The key outcomes of the experimental tests are:

1. There are large differences in methane numbers of producer gas compositions.
2. The methane numbers of "Gussing", "Viking" and "CPC" [50-60 MN] are lower than that of typical natural gas [75-97].
3. The methane numbers of "IISc" and "Harboore" [100-130 MN] are greater than that of typical natural gas.
4. The difference in methane numbers amongst the producer gas compositions has been attributed to the roles of hydrogen and carbon dioxide acting as a knock propagator and knock suppressor, respectively.
5. Further, the effect of varying amounts of hydrogen and carbon dioxide in the producer gas composition on critical compression ratios was evaluated. It was found that a 1 % increase in CO_2 increased the compression ratio by 0.32 units and a 1 % increase in H_2 decreased the compression ratio by 0.14 units. Hence the relative impact of CO_2 on the critical compression ratio is over two times that of H_2.
6. The experimental methane numbers did not compare well to methane numbers obtained from the AVL model. The AVL model is based on empirical data. Thus, it could be modified by incorporating data from various producer gas compositions.

The key outcomes of the CHEMKIN modelling tests were:

1. Procedural validation tests for natural gas showed that the CHEMKIN method for methane number evaluation is very sensitive to the chemical mechanism used.

2. The methane number evaluation process was compared amongst four chemical mechanisms, namely GRImech 3.0, Pitz et al, Petersen et al and USC II, for one of the chosen compositions [“Gussing”]. USC II showed the closest result at 51.5 MN, compared to the experimental methane number of 57.2 MN.
3. But the USC II mechanism failed to give satisfactory results for the rest of the compositions.
4. Further work needs to be done to develop the CHEMKIN model for the evaluation of methane number of producer gas.

5.3 Future Work

The experience gained from this work has highlighted procedural aspects that could be improved upon. These suggestions are as follows:

- <u>Eliminate Determination of ‘Light Audible Knock’ by Human Ear</u>: The accuracy of determination of MN depends wholly on the accuracy of detection of knock. The method used here for detecting ‘slight audible knock’ was by the human ear. This determines the knock level at which a single methane number measurement is made. The knock meter is used to ensure that knock level is consistent for unknown fuel (producer gas in this case) and reference blend. Although this is an acceptable method, a quantifiable method would be preferred to the human ear. This could be done by measuring the in-cylinder pressure over multiple engine cycles. A set threshold amplitude at the characteristic knock frequency could be utilized by analyzing the pressure data with a fast Fourier transform and band-pass filter. This approach would establish consistency of knock level for different methane number measurements. It could also be implemented to maintain constant knock level from test fuel to reference blend. However, it is not clear how significant this improvement would be over the knock meter.

- Perform Additional Testing on Producer Gas Blends: The indirect approach considered by previous researchers is useful for statistical studies. The direct approach is time consuming; therefore it limits the number of tests conducted and requires more fuel. With additional resources the number of producer gas blends tested could be expanded. The above knock measurement modification that establishes knock level consistency between methane number measurements may improve the accuracy of the indirect technique, permitting more methane number measurements for a given test time. Additional methane number data, however it is collected, enables further development of models to estimate the methane number of producer gas compositions and provides engine manufacturers with needed data for producer gas engine design.
- Further Development of CHEMKIN Methane Number Model: The methane number model attempts to simulate the methane number measurement. Thus, if the model assumptions are accurate, large amounts of empirical data should not be necessary. This thesis documents the first attempt to evaluate methane number in this manner. One aspect of the model that future work could focus on is sensitivity analysis of the USC II chemical kinetic mechanism. Sensitivity analysis is a built-in feature of CHEMKIN and allows the user to identify critical reactions. The reaction constants for those reactions can then be modified to improve model-experiment comparison. Modification of the model to include multiple zones (e.g. burned and unburned) may also improve accuracy.

- Another way of simulating the ongoing combustion process in the engine cylinder would be to simulate the later half (after TBD) of the volume versus crank angle model based on the laminar flame speed of the fuel gas. This would then be a model of the propagating flame having a direct effect on the end gas. Hence auto ignition in such a model would refer to “end gas” auto ignition as required to identify knock.

References

[1] Perlack, R.D., Wright, L.L., Turhollow, A.F., Graham, R.L., Stokes, B.J., Erbach, D.C., "Biomass as feedstock for a bioenergy and bioproducts industry: The technical feasibility of a billion ton annual supply", A joint study sponsored by U.S. Department of Energy, U.S. Department of Agriculture, April 2005.

[2] Quaak, P., Knoef, H., Stassen, H., "Energy from Biomass – A review of Combustion and Gasification technologies", World Bank Technical Paper, 1999.

[3] Lettner, F., Timmerer, H., Haselbacher, P., "Biomass gasification- State of the art description", Graz University of Technology- Institute of Thermal Engineering, Austria, December 2007.

[4] Herdin, G.R., Henkel, W., Plohberger, D., "Experience with gas engines optimized for H2 rich fuels", 2003 Spring Technical Conference of the ASME Internal Combustion Engine Division, Salsburg, Austria, May 11-14, 2003.

[5] Hofbauer, H.,Veronik, G., Rauch, R., Vienna University of Technology, Austria; Mackinger,H., Fercher,E., Austrian Energy and E nvironment, Graz, Austria; "The FICFB Gasification process".

[6] Henriksen, U., Gobel, B., Ahrenfeldt, J., Jensen, T., Hindsgaul, C., Bentzen, J.B., Sorensen, L.H., "Status-2000 hours of operation with the Viking Gasifier",2nd World Conference on Biomass for energy,Industry and Climate Protection,10-14 May, 2004, Rome, Italy.

[7] Henriksen, U., Brandt, P., Larsen, E., "High Tar Reduction in a two stage gasification",Energy & Fuels, 2000.

[8] Dasappa, S., Sridhar, G., Sridhar, H.V., Paul, P.J., Subbukrishnan, D.N., Rajan, N.K.S., "Green Electricity from Biomass fuelled Producer Gas Engine", Indian Institute of Science, Bangalore, India.

[9] Teislev, B., "Harboore - Woodchips updraft Gasifier and 1500 KW Gas engines operating at 32% power efficiency in chip configuration", Babcock and Wilcox Volund R&D Centre.

[10] Wilson, B., "Field Sample Collection and Methane Number and Emissions testing of alternative gaseous fuels", Master's Thesis, Colorado State University, 2009.

[11] Hernandez, J.J., Serrano, C., Perez, J., "Prediction of the Autoignition Delay Time of Producer Gas from Biomass Gasification", Energy & Fuels, 2005.

[12] Hernandez, J.J., Serrano, C., Lapuerta, M., "Estimation of the Laminar Flame Speed of Producer Gas from Biomass Gasification", Energy & Fuels, 2005.

[13] Heywood, J.B., "Internal Combustion Engine Fundamentals", New York : McGraw-Hill, 1988.

[14] Leikar, M., Christoph, K., Rankl, M., Cartellieri, E., Pfeifer, U., "Evaluation of Antiknocking Property of Gaseous Fuels by means of Methane Number and its practical application to gas engines", ASME, 1972.

[15] Malenshek, M., Olsen, D.B., "Methane number testing of alternative gaseous fuels." 4, Fuel, Vol. 88, pp. 650-656.

[16] Waukesha Motor Company, "F-1 & F-2 Octane Rating Units Operation & Maintenance", Second Edition, 2003.

[17] Ryan, T,W., Callahan, T,J., King, S,R., "Engine Knock Rating of Natural Gases-Methane Number", Southwest Research Institute; published in ASME,Vol.115,p 769-776, October 1993.

[18] Kline, S.J., and McClintock, F.A., "Describing Uncertainties in single-sample experiments", Mech.Eng.(75),pp. 3-8, Jan 1953

[19] Kee, R. J. , Rupley, F. M. , Miller, J. A. , Coltrin, M. E. , Grcar, J. F. , Meeks, E. , Moffat, H. K. , Lutz, A. E. , Dixon-Lewis, G. , Smooke, M. D. , Warnatz, J., Evans, G. H. , Larson, R. S. , Mitchell, R. E. , Petzold, L. R. , Reynolds, W. C. , Caracotsios, M., Stewart, W. E. , Glarborg, P. , Wang, C. , McLellan, C. L., Adigun, O. , Houf, W. G. , Chou, C. P. , Miller, S. F. , Ho, P., Young, P. D. , Young, D. J. , Hodgson, D. W. , Petrova, M. V. , and Puduppakkam, K. V., CHEMKIN Release 4.1.1, Reaction Design, San Diego, CA (2007).

[20] Gregory, P. S., David, M. G., Michael, F., Nigel, W. M., Boris, E., Mikhail, G., C. Thomas, B .C., Ronald, K. H., Soonho Song, William, C. G., Jr., Vitali, V. L., and Zhiwei Qin, GRImech 3.0, http://www.me.berkeley.edu/gri_mech/

[21] Marinov, N. M., Pitz, W.J., Westbrook, C.K., Hori, M., and Matsunaga, N. "An Experimental and Kinetic Calculation of the Promotion Effect of Hydrocarbons on the NO-NO2 Conversion in a Flow Reactor", Proceedings of the Combustion Institute, Volume 27, pp. 389-396, 1998. (UCRL-JC-129372).

[22] Petersen L.E., Danielle M. K., Stefanie S., Gilles B., Henry J. C., John M. S., "Methane/Propane Oxidation at high pressures: Experimental and detailed chemical modelling", Proceedings of the Combustion Institute 31 (2007) 447-454

[23] Hai Wang, Xiaoqing You, Ameya V. J., Scott, G. D., Alexander Laskin, Fokion Egolfopoulos & Chung K. Law, USC Mech Version II. "High-Temperature Combustion Reaction Model of H2/CO/C_1-C_4 Compounds" http://ignis.usc.edu/USC_Mech_II.htm, May 2007.

Appendix I – Sample Calculations

Flow Rate calculations for composition “Harboore”:

The stoichiometric combustion of this gas takes place according to this equation:

$19.3H_2 + 22.8CO + 11.9CO_2 + 5.3CH_4 + 40.7\ N_2 + a_s\ (O_2 + 3.76\ N_2)$

$$\downarrow$$

$xCO_2 + yH_2O + (40.7 + as^* \ 3.76)\ N_2$

To find a_s:

Gas	Vol %	Mole Fraction of component in Wood Gas				
		Xi	#C	#H	#O	#N
H2	19.3	0.19	0	2	0	0
CO	22.8	0.23	1	0	1	0
CO2	11.9	0.12	1	0	2	0
CH4	5.3	0.05	1	4	0	0
N2	40.7	0.41	0	0	0	2
	100.00					

#C	#H	#O	#N
0.4	0.598	0.466	0.814

$\Sigma C := 0.4$

$\Sigma H := 0.598$

$\Sigma O := 0.466$

$\Sigma N := 0.814$

$\varphi := 1$ (Equivalence Ratio is1)

$$as := \frac{\left[\Sigma C + \left(\frac{\Sigma H}{4}\right) - \left(\frac{\Sigma O}{2}\right)\right]}{\varphi} \rightarrow 0.3165$$

$$AFRs := 4.76 \cdot as \cdot \frac{MolWt\ (air)}{MolWt\ (fuel)}$$

$$AFRs := 4.76 as \cdot \frac{28.85}{[(12.011 \cdot \Sigma C) + (1.008 \Sigma H) + (15.999 \Sigma O) + (14.008 \Sigma N)]}$$

$AFRs = 1.791$

Mass Flow rate of Intake Air-fuel (Ma)

$$Ma := 0.5 \cdot \eta_{vol} \cdot \rho(air) \cdot Vdisp \cdot RPS$$

where

$\eta_{vol} := 0.8$ Volumetric Efficiency of the Engine

$$\rho(air) = \blacksquare \cdot 0.996 \frac{kg}{m^3} \qquad \rho(air) \equiv \frac{P}{(R \cdot T)} = \blacksquare \cdot \frac{13.6 \cdot 1000 \cdot 9.81 \cdot 633 \cdot 0.001}{\left(\frac{8314}{28.84}\right) \cdot 294}$$

$$Vdisp := 6.11 \cdot 10^{-4} \quad m^3$$

$$RPS := \frac{900}{60}$$

$$Ma := 0.5 \cdot 0.8 \cdot 0.996 \cdot 6.11 \cdot 10^{-4} \cdot \left(\frac{900}{60}\right)$$

$$Ma = 3.651 \times 10^{-3} \quad \frac{kg}{sec}$$

Mass flow rate of the Fuel (Mf)

$$Mf := \frac{Ma}{(1 + AFRs)}$$

$$Mf = 1.308 \times 10^{-3} \quad \frac{kg}{sec}$$

Volumetric Flowrate of fuel (Vf)

$$Vf := \frac{(Mf \cdot 1000 \cdot 60)}{\rho fuel} \qquad \rho fuel := 1.005: \quad \frac{kg}{m^3} \text{ (At STP)}$$

To calculate ρ_{fuel} at STP (21deg C and 1 atm)

Gas	Density(kg/m3)	MW(kg/kmol)	Composition	density
H2	0.083527266	2.016	0.19	0.016121
CO	1.160515241	28.01	0.23	0.264597
CO2	1.823430052	44.01	0.12	0.216988
CH4	0.664696394	16.043	0.05	0.035229
C2H6	1.245865523	30.07		0
C3H8	1.827158948	44.1		0
N2	1.160639537	28.013	0.41	0.47238

Total density

1.005316 kg/m3

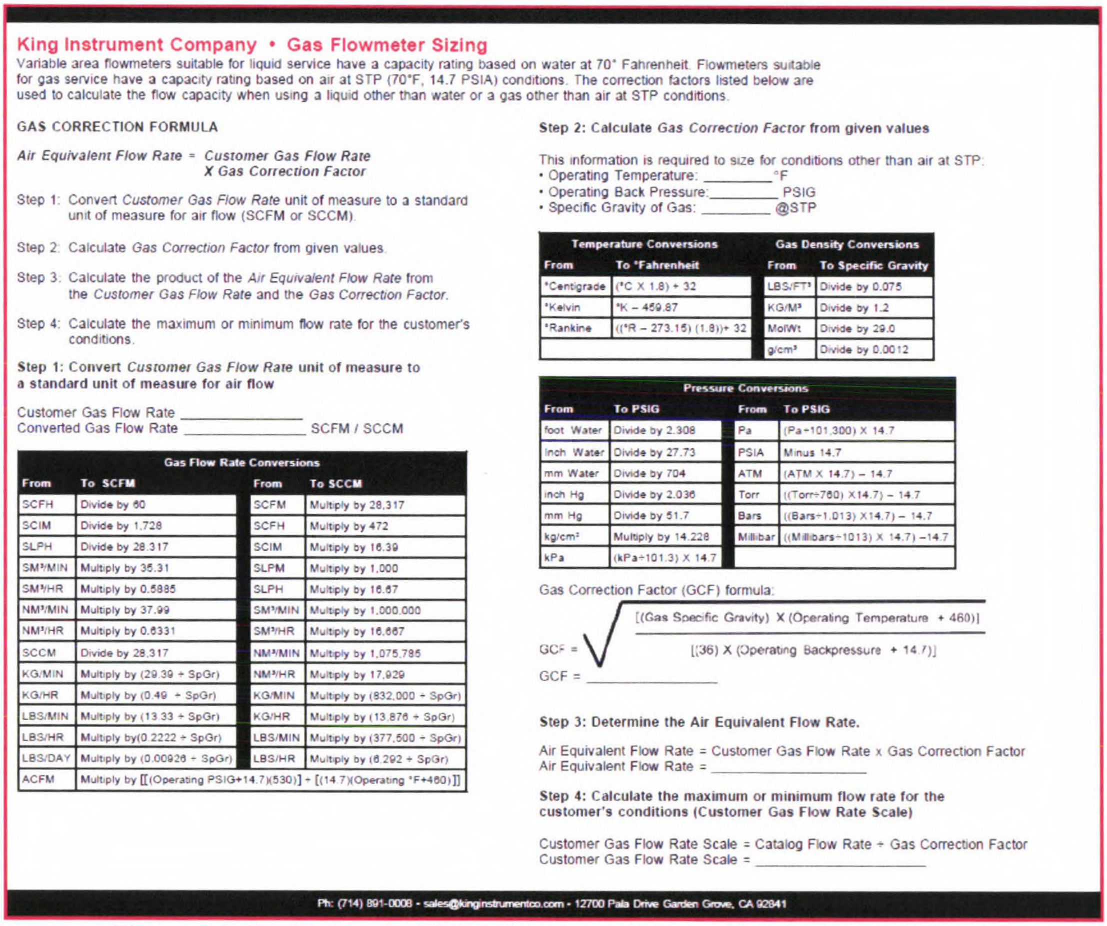
Vf = 78.076 SLPM

Volumetric Flowrate of N_2 (V_{N2}) :

$$VN2 := .40 \cdot Vf$$

VN2 = 31.23 SLPM

This gives volumetric flow of N_2 in SLPM. In order to set the flow rate on the rotameter, the air equivalent SCFH value is required. This was calculated using the gas flow meter sizing chart by King Instrument Company, whose flow meter was used. The sizing chart is attached as **Figure A.1**. Using this, the air equivalent flow rate of N_2 was found to be 64.12 SCFH.



King Instrument Company • Gas Flowmeter Sizing

Variable area flowmeters suitable for liquid service have a capacity rating based on water at 70° Fahrenheit. Flowmeters suitable for gas service have a capacity rating based on air at STP (70°F, 14.7 PSIA) conditions. The correction factors listed below are used to calculate the flow capacity when using a liquid other than water or a gas other than air at STP conditions.

GAS CORRECTION FORMULA

Air Equivalent Flow Rate = Customer Gas Flow Rate X Gas Correction Factor

Step 1: Convert *Customer Gas Flow Rate* unit of measure to a standard unit of measure for air flow (SCFM or SCCM).

Step 2: Calculate *Gas Correction Factor* from given values.

Step 3: Calculate the product of the *Air Equivalent Flow Rate* from the *Customer Gas Flow Rate* and the *Gas Correction Factor*.

Step 4: Calculate the maximum or minimum flow rate for the customer's conditions.

Step 1: Convert *Customer Gas Flow Rate* unit of measure to a standard unit of measure for air flow

Customer Gas Flow Rate ______________
Converted Gas Flow Rate ______________ SCFM / SCCM

Gas Flow Rate Conversions			
From	**To SCFM**	**From**	**To SCCM**
SCFH	Divide by 60	SCFM	Multiply by 28,317
SCIM	Divide by 1,728	SCFH	Multiply by 472
SLPH	Divide by 28.317	SCIM	Multiply by 16.39
SM³/MIN	Multiply by 35.31	SLPM	Multiply by 1,000
SM³/HR	Multiply by 0.5885	SLPH	Multiply by 16.67
NM³/MIN	Multiply by 37.99	SM³/MIN	Multiply by 1,000,000
NM³/HR	Multiply by 0.6331	SM³/HR	Multiply by 16,667
SCCM	Divide by 28,317	NM³/MIN	Multiply by 1,075,785
KG/MIN	Multiply by (29.39 ÷ SpGr)	NM³/HR	Multiply by 17,929
KG/HR	Multiply by (0.49 ÷ SpGr)	KG/MIN	Multiply by (832,000 ÷ SpGr)
LBS/MIN	Multiply by (13.33 ÷ SpGr)	KG/HR	Multiply by (13,876 ÷ SpGr)
LBS/HR	Multiply by(0.2222 ÷ SpGr)	LBS/MIN	Multiply by (377,500 ÷ SpGr)
LBS/DAY	Multiply by (0.00926 ÷ SpGr)	LBS/HR	Multiply by (6,292 ÷ SpGr)
ACFM	Multiply by [[(Operating PSIG+14.7)(530)] ÷ [(14.7)(Operating °F+460)]]		

Step 2: Calculate *Gas Correction Factor* from given values

This information is required to size for conditions other than air at STP:
- Operating Temperature: ________ °F
- Operating Back Pressure: ________ PSIG
- Specific Gravity of Gas: ________ @STP

Temperature Conversions		Gas Density Conversions	
From	**To °Fahrenheit**	**From**	**To Specific Gravity**
°Centigrade	(°C X 1.8) + 32	LBS/FT³	Divide by 0.075
°Kelvin	°K – 459.87	KG/M³	Divide by 1.2
°Rankine	((°R – 273.15) (1.8))+ 32	MolWt	Divide by 29.0
		g/cm³	Divide by 0.0012

Pressure Conversions			
From	**To PSIG**	**From**	**To PSIG**
foot Water	Divide by 2.308	Pa	(Pa÷101,300) X 14.7
Inch Water	Divide by 27.73	PSIA	Minus 14.7
mm Water	Divide by 704	ATM	(ATM X 14.7) – 14.7
inch Hg	Divide by 2.036	Torr	((Torr÷760) X14.7) – 14.7
mm Hg	Divide by 51.7	Bars	((Bars÷1.013) X14.7) – 14.7
kg/cm²	Multiply by 14.228	Millibar	((Millibars÷1013) X 14.7) –14.7
kPa	(kPa÷101.3) X 14.7		

Gas Correction Factor (GCF) formula:

$$GCF = \sqrt{\frac{[(\text{Gas Specific Gravity}) \times (\text{Operating Temperature} + 460)]}{[(36) \times (\text{Operating Backpressure} + 14.7)]}}$$

GCF = ______________

Step 3: Determine the Air Equivalent Flow Rate.

Air Equivalent Flow Rate = Customer Gas Flow Rate x Gas Correction Factor
Air Equivalent Flow Rate = ______________

Step 4: Calculate the maximum or minimum flow rate for the customer's conditions (Customer Gas Flow Rate Scale)

Customer Gas Flow Rate Scale = Catalog Flow Rate ÷ Gas Correction Factor
Customer Gas Flow Rate Scale = ______________

Ph: (714) 891-0008 • sales@kinginstrumentco.com • 12700 Pala Drive Garden Grove, CA 92841

Figure A.1 Gas Flowmeter Sizing Chart provided by King Instrument Company

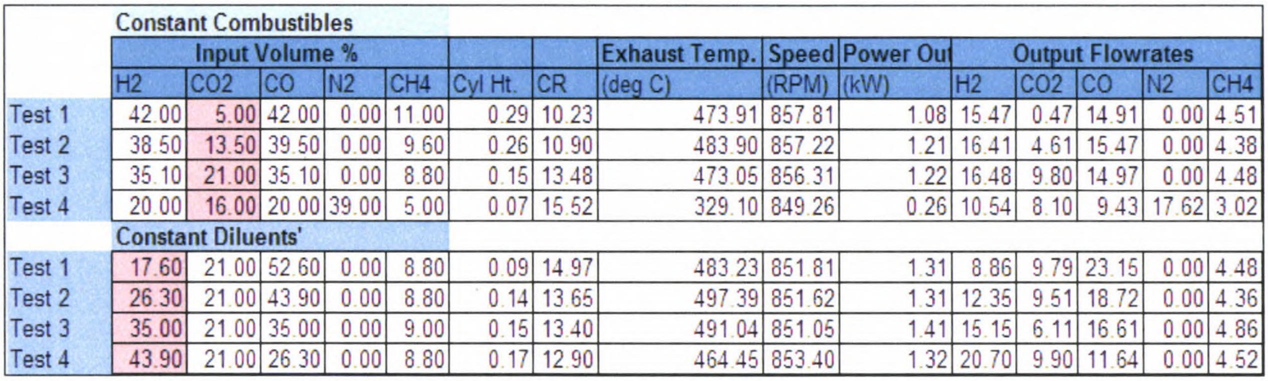
Appendix II- Test Data

Test gas composition and reference gas composition were both taken through the mass flow controller flow rate output availed on the VI. The consolidated data for all the tests is in **Table A.1** and **Table A.2**. Each of the data points are an average of data points collected over three minutes of testing.

Table A.1 Consolidated composition data for each test

		Input Volume %					Cyl Ht.	CR	Exhaust Temp.	Speed	Power Out	Output Flowrates				
		H2	CO2	CO	N2	CH4			(deg C)	(RPM)	(KW)	H2	CO2	CO	N2	CH4
Gussing	Comp 1	38	23	26	3	10	0.272	10.639	533.73	863.08	1.36	21.34	12.62	13.45	2.66	5.74
	Comp 2	38	23	26	3	10	0.277	10.54	531.84	862.23	1.40	21.13	12.35	13.32	2.68	5.71
	Comp 3	39	23	25	3	10	0.272	10.639	523.48	862.23	1.30	21.38	12.36	12.63	2.67	5.64
	MN 1	41	0	0	0	59	0.272	10.639	529.39	865.55	1.79	8.96	0.00	0.00	0.00	11.98
	MN 2	42.5	0	0	0	57.5	0.277	10.54	533.71	864.67	1.77	11.75	0.00	0.00	0.00	14.60
	MN 3	44	0	0	0	56	0.272	10.639	521.37	864.11	1.78	11.53	0.00	0.00	0.00	13.60
Viking	Comp 1	45	23	29	0	3	0.279	10.501	472.48	859.36	1.02	24.92	12.50	14.86	0.00	2.21
	Comp 2	45	23	29	0	3	0.279	10.501	479.73	860.58	1.01	24.66	12.40	14.69	0.00	2.19
	Comp 3	45	23	29	0	3	0.279	10.501	478.44	859.60	1.04	24.90	12.49	14.86	0.00	2.21
	MN 1	41.5	0	0	0	58.5	0.279	10.501	519.79	864.41	1.76	9.98	0.00	0.00	0.00	12.98
	MN 2	44.5	0	0	0	55.5	0.279	10.501	521.43	864.38	1.72	10.82	0.00	0.00	0.00	12.55
	MN 3	44.5	0	0	0	55.5	0.279	10.501	523.07	863.46	1.75	11.08	0.00	0.00	0.00	12.80
IISc-new	Comp 1	37	23.2	37	0	2.8	0.162	13.099	454.74	855.97	1.01	20.17	12.35	18.61	0.00	1.93
	Comp 2	37	23.2	37	0	2.8	0.162	13.099	451.00	854.99	1.02	19.93	12.20	18.38	0.00	2.01
	Comp 3	37	23.2	37	0	2.8	0.147	13.48	492.32	858.68	0.95	17.25	12.91	19.48	0.00	2.15
	MN 1	0	20	37	0	120	0.162	13.099	534.91	860.73	1.80	0.00	4.52	0.00	0.00	16.35
	MN 2	0	23	37	0	123	0.162	13.099	525.22	859.35	1.76	0.00	5.03	0.00	0.00	15.55
	MN 3	0	30	37	0	130	0.147	13.48	545.96	861.20	1.75	0.00	7.41	0.00	0.00	16.46
Harboore	Comp 1	32.5	20.2	38.4	0	8.9	0.203	12.12	487.26	859.05	1.15	16.02	10.36	18.57	0.00	4.89
	Comp 2	32.5	20.2	38.4	0	8.9	0.202	12.143	492.62	861.22	1.24	15.96	9.65	17.27	0.00	4.61
	Comp 3	32.5	20.2	38.4	0	8.9	0.201	12.166	489.02	859.28	1.23	16.20	9.80	17.54	0.00	4.67
	MN 1	0	4	0	0	104	0.203	12.12	520.35	863.71	1.88	0.00	0.87	0.00	0.00	17.00
	MN 2	0	5	0	0	105	0.202	12.143	524.07	865.07	1.86	0.00	0.95	0.00	0.00	14.91
	MN 3	0	5	0	0	105	0.201	12.166	525.10	864.68	1.95	0.00	1.10	0.00	0.00	17.04
CPC	Comp 1	42.3	4.1	48.3	0	5.3	0.293	10.23	476.68	858.71	1.08	19.49	1.98	20.80	0.00	2.94
	Comp 2	42.3	4.1	48.3	0	5.4	0.293	10.23	469.17	857.34	0.88	19.43	1.99	20.76	0.00	2.97
	Comp 3	42.3	4.1	48.3	0	5.3	0.293	10.23	464.10	854.53	1.03	19.76	1.99	20.81	0.00	2.95
	MN 1	44	0	0	0	56	0.293	10.23	534.01	862.54	1.76	11.89	0.00	0.00	0.00	14.11
	MN 2	40	0	0	0	60	0.293	10.23	525.58	860.12	1.72	10.65	0.00	0.00	0.00	14.99
	MN 3	37	0	0	0	63	0.293	10.23	511.87	859.18	1.79	9.8582	0	0	0	15.43

Table A.2 Constant Combustibles and Constant Diluents' Data



	Constant Combustibles														
	Input Volume %							Exhaust Temp.	Speed	Power Out	Output Flowrates				
	H2	CO2	CO	N2	CH4	Cyl Ht.	CR	(deg C)	(RPM)	(kW)	H2	CO2	CO	N2	CH4
Test 1	42.00	5.00	42.00	0.00	11.00	0.29	10.23	473.91	857.81	1.08	15.47	0.47	14.91	0.00	4.51
Test 2	38.50	13.50	39.50	0.00	9.60	0.26	10.90	483.90	857.22	1.21	16.41	4.61	15.47	0.00	4.38
Test 3	35.10	21.00	35.10	0.00	8.80	0.15	13.48	473.05	856.31	1.22	16.48	9.80	14.97	0.00	4.48
Test 4	20.00	16.00	20.00	39.00	5.00	0.07	15.52	329.10	849.26	0.26	10.54	8.10	9.43	17.62	3.02
	Constant Diluents'														
Test 1	17.60	21.00	52.60	0.00	8.80	0.09	14.97	483.23	851.81	1.31	8.86	9.79	23.15	0.00	4.48
Test 2	26.30	21.00	43.90	0.00	8.80	0.14	13.65	497.39	851.62	1.31	12.35	9.51	18.72	0.00	4.36
Test 3	35.00	21.00	35.00	0.00	9.00	0.15	13.40	491.04	851.05	1.41	15.15	6.11	16.61	0.00	4.86
Test 4	43.90	21.00	26.30	0.00	8.80	0.17	12.90	464.45	853.40	1.32	20.70	9.90	11.64	0.00	4.52

Appendix III- Results

Table A.3 Summary of Results

Test Gas Composition	Trial	H_2%	CO%	CH_4%	CO_2%	N_2%	Methane Number
Gussing		*40*	*24*	*10*	*23*	*3*	
	Trial 1	39.10	23.09	10.31	22.31	4.89	54.11
	Trial 2	38.23	24.10	10.29	22.61	4.76	57.20
	Trial 3	38.28	24.14	10.34	22.38	4.86	55.40
Viking		*30.5*	*19.6*	*1.6*	*15.4*	*33.3*	
	Trial 1	30.05	17.90	2.65	15.06	34.33	56.53
	Trial 2	29.41	17.52	2.61	14.79	35.67	53.71
	Trial 3	29.52	17.61	2.62	14.81	35.45	53.61
IISc.		*19.39*	*19.39*	*1.53*	*12.24*	*47.45*	
	Trial 1	17.87	20.17	2.23	13.37	46.36	131.04
	Trial 2	20.66	19.05	1.98	12.64	45.67	121.65
	Trial 3	20.52	18.92	2.07	12.56	45.92	124.45
Harboore		*19.3*	*22.8*	*5.3*	*11.9*	*40.7*	
	Trial 1	20.10	23.29	6.13	13.00	37.47	104.88
	Trial 2	20.63	22.33	5.95	12.48	38.61	105.98
	Trial 3	20.75	22.46	5.98	12.56	38.26	106.07
CPC		*18.78*	*21.02*	*2.24*	*1.42*	*56.53*	
	Trial 1	20.00	21.34	3.02	2.03	53.61	54.26
	Trial 2	19.95	21.32	3.05	2.04	53.63	58.46
	Trial 3	20.21	21.29	3.01	2.03	53.45	59.68

The co-relation between the heating value, adiabatic flame temperature and output power is evident from **Figures A.2, A.3** and **A.4**. Upon comparison of any of these quantities with the Methane Number, "Gussing" seems to give an impression that due to its higher heating value, the Methane Number is low. "IISc" gives an impression that its lower heating value is causing it to have a higher Methane Number. But in the case of the other three compositions no such trend is evident. They indeed have similar heating values which should have ideally given them all a similar Methane Number, but that was not the case. Hence, each individual gas and the associated chemical reactions seem to play a major role in determining its knocking tendency.

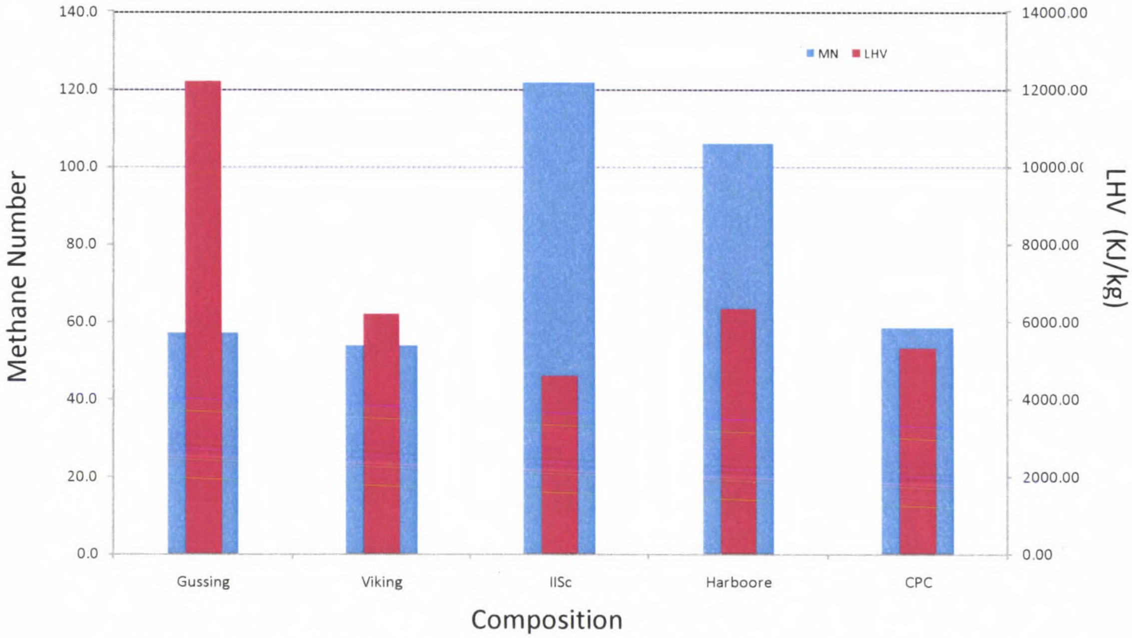


Figure A.2 Comparison of Methane Numbers of test gases with their heating value

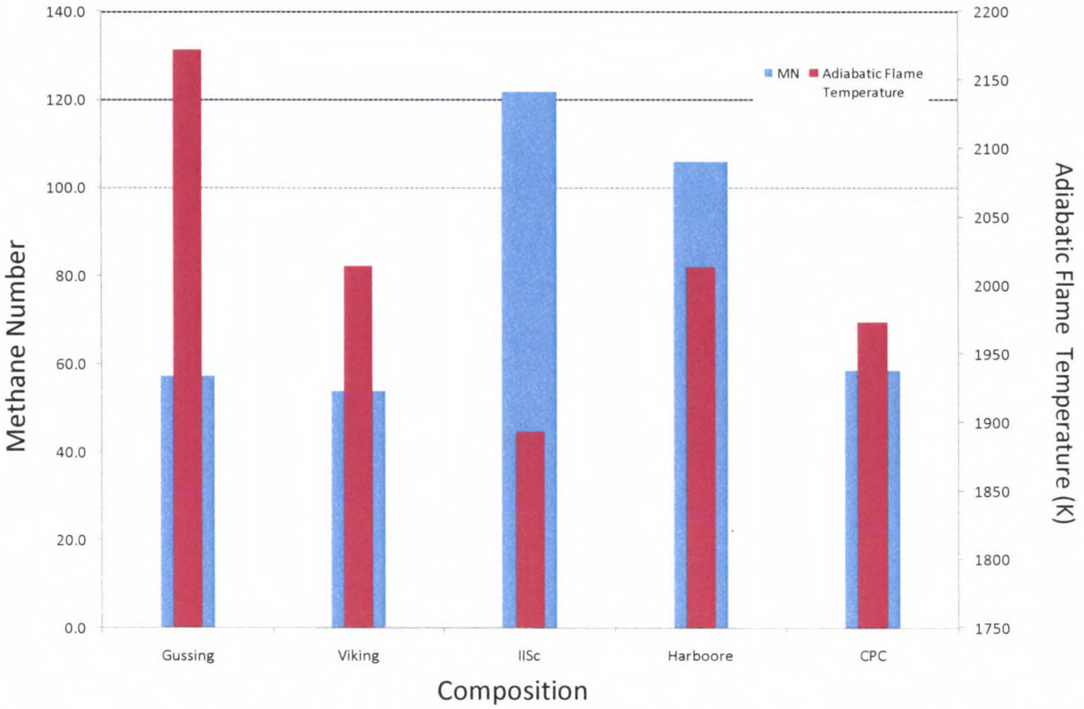


Figure A.3 Comparison of Methane Numbers of test gases with their adiabatic flame temperature

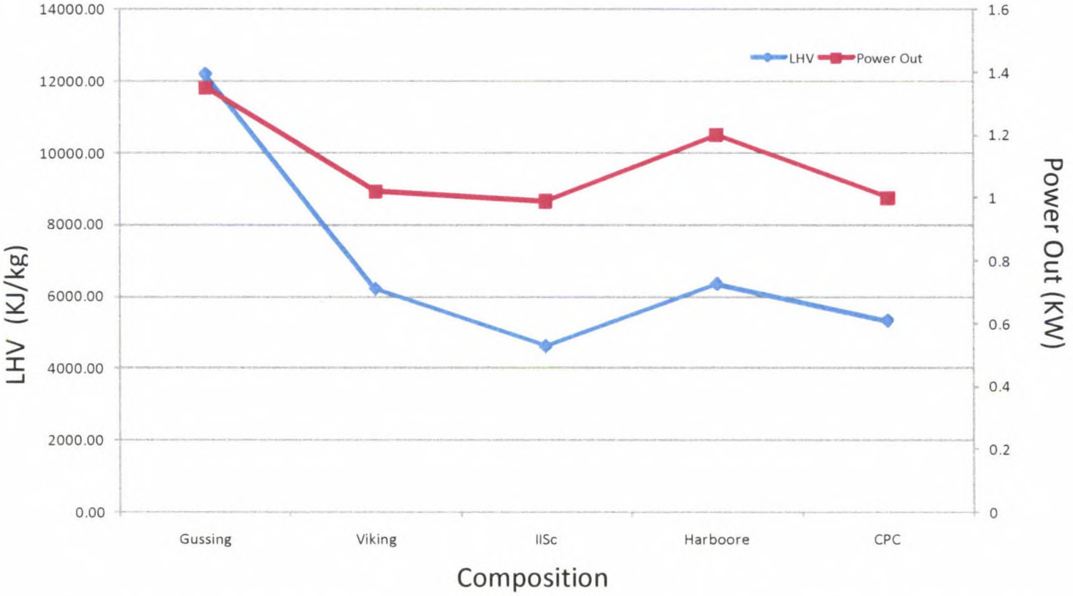


Figure A.4 Comparison of LHV and Output Power for each test gas composition

Appendix IV - Error Analysis

There are two cases elaborated here.
CASE1. When the reference gas blend is made of hydrogen and methane, Methane Number is defined as:

$$\mathrm{MN1}(\mathrm{CH4},\mathrm{H2}) := \mathrm{CH4}\cdot\frac{100}{\mathrm{CH4}+\mathrm{H2}}$$

Using the Kline and McClintock **[18]** method for individual uncertainties, we have the following overall equation to assess error in MN1 (given by δ MN1)

$$\delta\mathrm{MN1}(\mathrm{CH4},\mathrm{H2},\Delta\mathrm{CH4},\Delta\mathrm{H2}) := \left[\left[\left(\frac{d}{d\mathrm{CH4}}\mathrm{MN1}(\mathrm{CH4},\mathrm{H2})\right)\Delta\mathrm{CH4}\right]^2 + \left[\left(\frac{d}{d\mathrm{H2}}\mathrm{MN1}(\mathrm{CH4},\mathrm{H2})\right)\Delta\mathrm{H2}\right]^2\right]^{0.5}$$

$$\frac{d}{d\mathrm{CH4}}\mathrm{MN1}(\mathrm{CH4},\mathrm{H2}) \rightarrow \frac{100}{\mathrm{CH4}+\mathrm{H2}} - \frac{100\cdot\mathrm{CH4}}{(\mathrm{CH4}+\mathrm{H2})^2}$$

$$\frac{d}{d\mathrm{H2}}\mathrm{MN1}(\mathrm{CH4},\mathrm{H2}) \rightarrow -\frac{100\cdot\mathrm{CH4}}{(\mathrm{CH4}+\mathrm{H2})^2}$$

Δ CH4 is the sum of accuracy of CH4 flow controller and accuracy of calibration flow meter.

$$\Delta\mathrm{CH4} := \left[\frac{1.5}{100}(30) + \frac{1}{100}(60)\right] \rightarrow 1.05$$

Δ H2 is the sum of accuracy of H2 flow controller and accuracy of calibration flow meter.

$$\Delta\mathrm{H2} := \left[\frac{1.5}{100}(80) + \frac{1}{100}(60)\right] \rightarrow 1.8$$

The reference gas flow rates for Trial 2 of "Gussing" were found from Table A.3:

$\mathrm{CH4} := 11.98$ lpm

$\mathrm{H2} := 8.96$ lpm

$$\mathrm{MN1}(\mathrm{CH4},\mathrm{H2}) \rightarrow 57.202$$

$$\frac{d}{d\mathrm{CH4}}\mathrm{MN1}(\mathrm{CH4},\mathrm{H2}) \rightarrow 2.043$$

$$\frac{d}{d\ H2}MN1(CH4,H2) \rightarrow -2.731$$

$$\delta MN1\ (CH4\ ,H2\ ,\Delta CH4\ \ ,\Delta H2\ ) \rightarrow 5.364$$

Hence the value of MN for Trial 2 of "Gussing" composition can be given as: **57.202±5.364** MN units.

CASE 2: When the reference gas blend is made of carbon dioxide and methane, Methane Number is defined as:

$$MN2(CH4,CO2) := 100 + \frac{CO2\cdot 100}{CH4 + CO2}$$

Using the Kline and McClintock [18] method for individual uncertainties, we have the following overall equation to assess error in MN2(given by δ MN2)

$$\delta MN2(CH4,CO2,\Delta CH4,\Delta CO2) := \left[\left[\frac{d}{dCH4}(MN2(CH4,CO2)\cdot\Delta CH4)\right]^2 + \left[\frac{d}{dCO2}(MN2(CH4,CO2)\cdot\Delta CO2)\right]^2\right]^{0.5}$$

$$\frac{d}{dCH4}MN2(CH4,CO2) \rightarrow -\frac{100\cdot CO2}{(CH4 + CO2)^2}$$

$$\frac{d}{dCO2}MN2(CH4,CO2) \rightarrow \frac{100}{CH4 + CO2} - \frac{100\cdot CO2}{(CH4 + CO2)^2}$$

Δ CH4 is the sum of accuracy of CH4 flow controller and accuracy of calibration flowmeter.

$$\Delta CH4\ := \left[\frac{1.5}{100}(30) + \frac{1}{100}(60)\right] \rightarrow 1.05$$

Δ CO2 is the sum of accuracy of CO2 flow controller and accuracy of calibration flowmeter.

$$\Delta CO2\ := \left[\frac{1.5}{100}(15) + \frac{1}{100}(60)\right] \rightarrow 0.825$$

The reference gas flow rates of Trial 2 for "Harboore" are found from Table A.3:

$$CH4\ := 14.909\ \ lpm$$

$$CO2\ := 0.948\ \ lpm$$

$$MN2\ \ (CH4\ \ ,CO2\ ) = 105.978$$

$$\frac{d}{dCH4} MN2\,(CH4\,, CO2\,) \rightarrow -0.377$$

$$\frac{d}{dCO2} MN2\,(CH4\,, CO2\,) \rightarrow 5.929$$

$$\delta MN2\,(CH4, CO2, \Delta CH4\,, \Delta CO2\,) \rightarrow 4.908$$

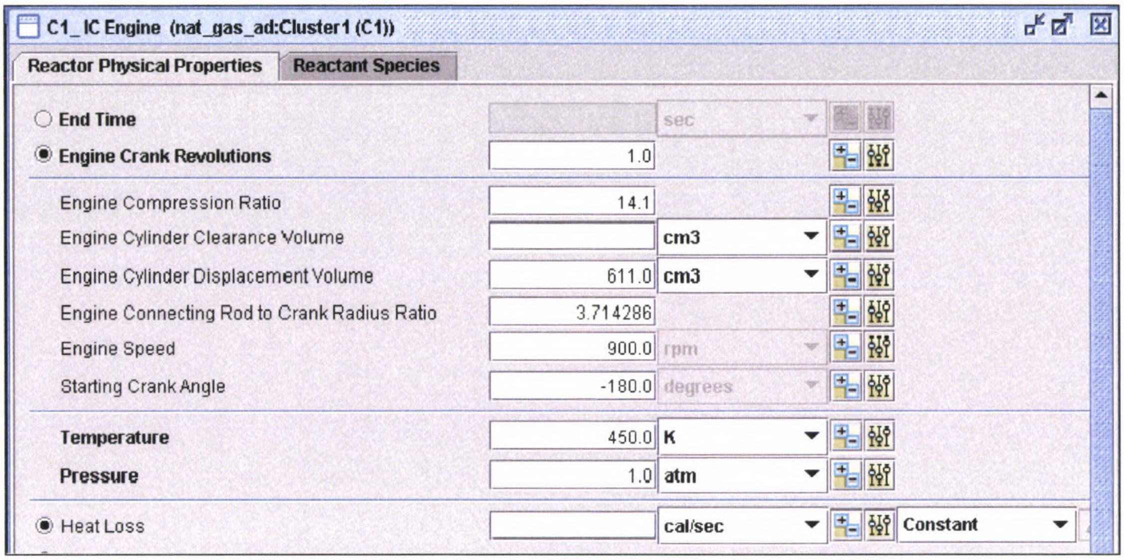
Hence the value of MN for Trial 2 of "Harboore" composition can be given as **105.978±4.908** MN units**.**

The errors for all the Trials of all test gases in summarized in Table A.4

Table A.4 Summary of errors for each of the test gases

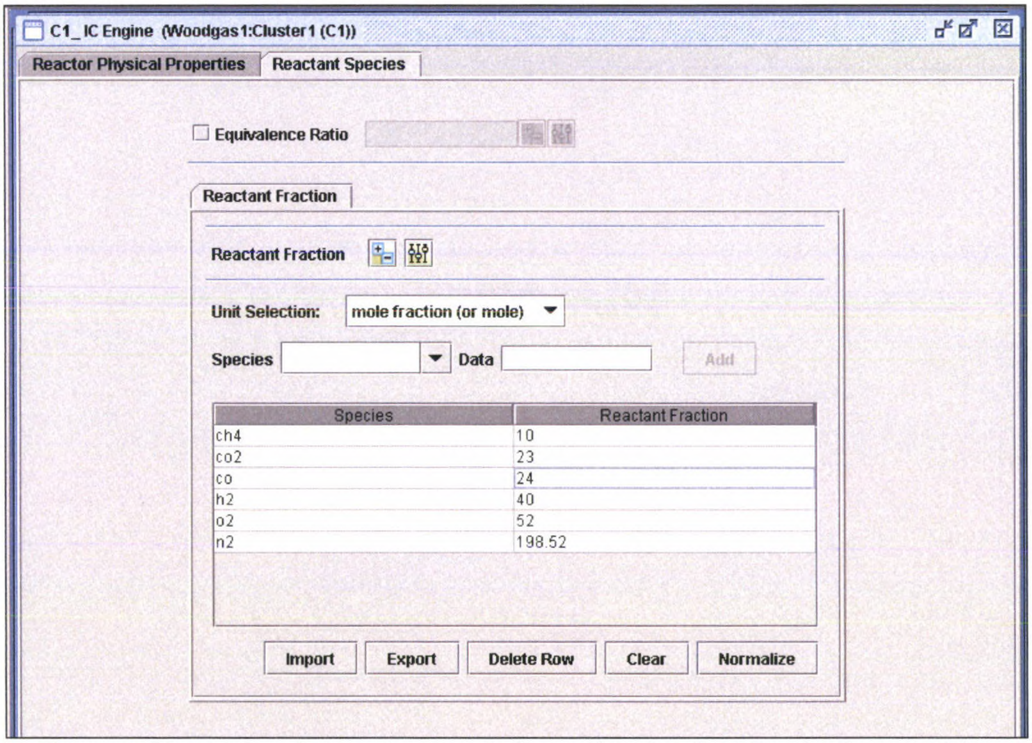
		Gussing			Viking			IISc			Harboore			CPC	
MN	54.11	57.20	55.40	56.53	53.71	53.61	131.04	121.65	124.45	104.87	105.98	106.07	54.26	58.46	59.68
CH4	13.60	11.98	14.60	12.98	12.55	12.80	16.46	16.35	15.55	16.99	14.91	17.04	14.11	14.99	15.43
H2/CO2	11.53	8.96	11.75	9.98	10.82	11.08	7.41	4.52	5.03	0.87	0.95	1.10	11.89	10.65	10.43
δMN	4.32	5.36	4.18	4.86	4.63	4.53	2.75	3.28	3.27	4.40	4.91	4.29	4.19	4.44	4.46

Appendix V – CHEMKIN data input



○ End Time		sec
● Engine Crank Revolutions	1.0	
Engine Compression Ratio	14.1	
Engine Cylinder Clearance Volume		cm3
Engine Cylinder Displacement Volume	611.0	cm3
Engine Connecting Rod to Crank Radius Ratio	3.714286	
Engine Speed	900.0	rpm
Starting Crank Angle	-180.0	degrees
Temperature	450.0	K
Pressure	1.0	atm
● Heat Loss		cal/sec Constant

Figure A.5 Input data for "reactor physical properties"



☐ Equivalence Ratio

Reactant Fraction

Unit Selection: mole fraction (or mole)

Species	Reactant Fraction
ch4	10
co2	23
co	24
h2	40
o2	52
n2	198.52

Figure A.6 Input data for reactant species' mole fraction for "Gussing" composition

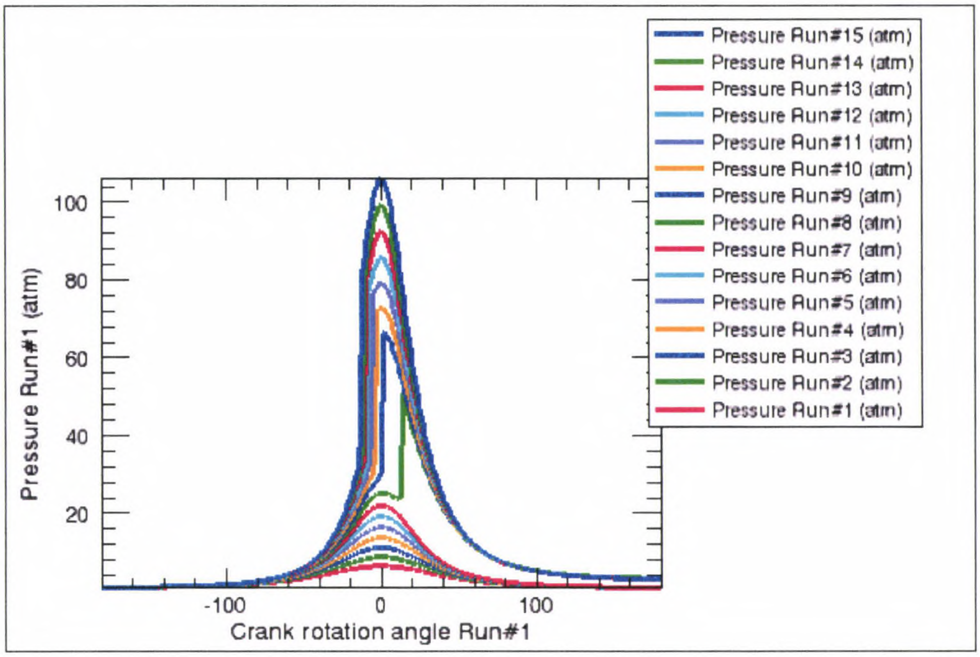


Figure A.7 Pressure Rise for varying compression ratios

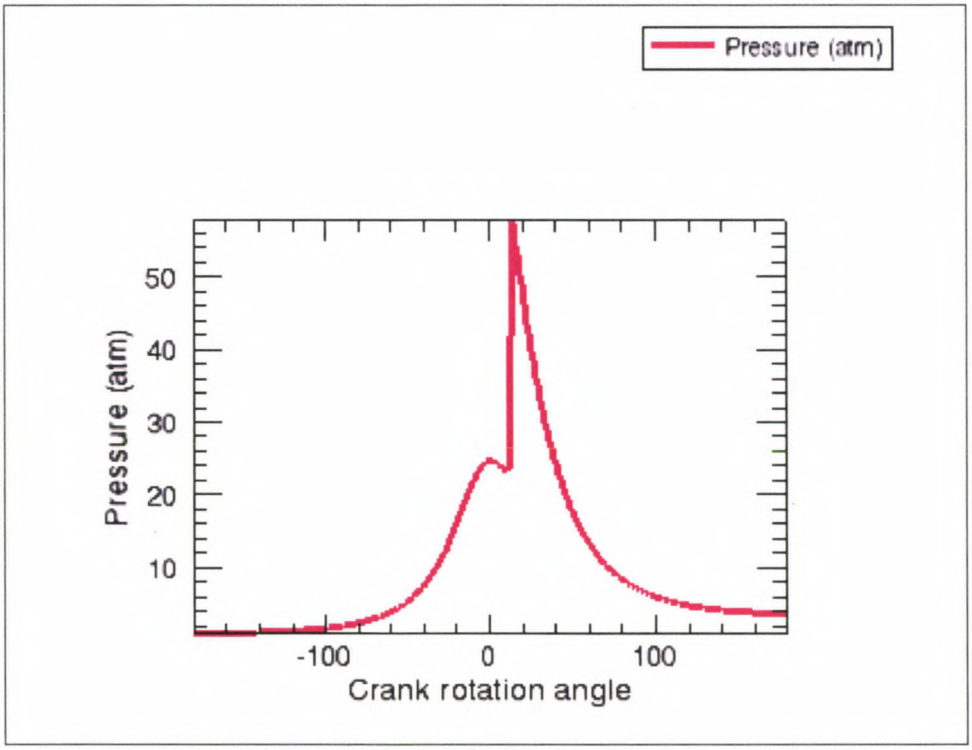


Figure A.8 Identification of Auto Ignition