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Combustion Analysis of Various Gaseous Fuels in Spark Ignition Engine Using MATLAB Simulation

by
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ABSTRACT

MATLAB, an extremely potent programming tool that can simulate a variety of scenarios based on the demands and inputs provided, was used for the simulation. The performance of each fuel in a spark ignition engine can be compared when the output of each fuel is evaluated under the same operating conditions, such as equivalency ratio, rpm, compression ratio, and spark timing. This effort is also a tiny step toward computer simulation for determining whether Hydrogen, Syngas, Natural gas can be used as the fuel for spark ignition engines. In this project, hydrogen and other fuels are used to simulate a spark-ignition engine. The purpose of this simulation is to do a thermodynamic analysis of the engine while taking into account various parameters using hydrogen, and to compare the results with those obtained using gasoline, biogas, and hydrogen mixtures, syngas and natural gas.

The simulation's results are useful for describing all of the fundamental physical processes taking place in the combustion chamber and for determining engine power and emission under various operating situations. Increasing the CR ratio from 9:1 to 10:1, maximum pressure was increased up to 15% and NOx emission was increased to 10% for each gas. Similarly, other aspect such as Spark ignition showed a change up to 12%-15% increment in pressure and NOx emission when spark timing was increased by 5 degree. Increment in rpm showed an increase of 15%-20% when rpm was increased by 1000. Increment in equivalence ratio by 0.1 increases the pressure by 10%-15% while NOx emission was increased up to 20% for each gas.

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LIST OF ABBREVIATIONS

IC	Internal Combustion
SI	Spark Ignition
H_2	Hydrogen
mJ	Milli joule
m/s	Meter per second
mm	Millimeter
kg/m3	Kilogram per Cubic Meter
MJ/kg	Mega joule per Kilogram
NTP	Normal Temperature and Pressure
MFB	Mass Fraction Burnt
NOx	Oxide of Nitrogen
O_2	Oxygen
IMEP	Indicated Mean Effective Pressure
BTDC	Before Top Dead Centre
CR	Compression Ratio
RPM	Revolution Per Minute
ppm	Parts Per Million
KPa	Kilo Pascal
A/F	Air/Fuel
ATDC	After Top Dead Centre
C_p	Specific Heat at Constant Pressure
R	Gas Constant
SA	Spark Advance

CHAPTER 1 INTRODUCTION

1.1 Background

Excessive consumption of fossils fuels has been today's generation biggest problem and it needs to be sort out soon. For this, alternative fuel source and energy is a thrust for researchers. These evolving problems have inspired researchers to come up with greener alternative fuels that can more or less replace the use of fossil fuels. The massive increase in the world population, the rapid increase in technological development and the standard of living in developed countries over the last decade have created a problematic situation in the area of energy supply. In today's energy scenario, energy demand is steadily increasing. IC engine needs new alternative source of energy like Hydrogen, Syngas or Natural gas. The rise in oil prices and environmental pollution are encouraging the development of competitive alternative energy sources (V. Kumar et al., 2015). As a result of numerous studies that have been conducted and are still being conducted, it has been determined that hydrogen can be a superior alternative fuel because it is readily available and even helps reduce pollution (K. Shivaprasad et al., 2018)

The vast quest for alternative fuels has been prompted by environmental concerns and the depletion of fossil fuel stocks. Therefore, it is crucial to take every action possible to protect our ecosystem. We could replace gasoline with alternative fuels like Hydrogen, syngas or Natural gas as well. Natural gas, biogas, air gas, and hydrogen gas are the fuels of choice for many engines that are often produced and it can be used in a modified engine either compression or spark ignition for better use.

Reverend W. Cecil made the first attempt to create a hydrogen engine in 1820. On a piece of paper titled "On the Application of Hydrogen Gas to Produce Moving Power in Machinery," A concept of vacuum is used to run the engine, whereby propelling of piston is done by atmospheric pressure to fight vacuum and generate power. The vacuum is produced when the hydrogen-air mixture is burned, allowing it to expand and subsequently low.60 years later, N. A. Otto is said to have employed synthetic gas with a hydrogen content of more than 50% when working on the Combustion Engine in the 1860s and 1870s. Otto also used another source of fuel i.e., gasoline, which he found was dangerous to use, leading him to switch back to using gaseous fuels (L. Walter, 2001) (Sandeep, K. J., 2021)

Although there are several studies and developments in hydrogen fuel cells, it will take a long time for them to be developed at prices that are cheap and for the shift from existing gasoline engines to hydrogen fuel cells (Sandeep, K. J., 2021). Therefore, using hydrogen in the internal combustion spark ignition engine seems to be the better alternative for running cars in that transitional phase or even further, as hydrogen can be easily produced using various methods like electrolysis of water, coal gasification, or using the steam reforming of natural gas (K. V. Shivaprasad et al., 2018)

Specific heat ratio of Hydrogen is found to be more in comparison with gasoline because its molecular structure is simpler than that of gasoline. Due to its wide spectrum of flammability and rapid flame, hydrogen maintains lower emissions and greater thermal efficiency than gasoline. Because the temperature during auto ignition is so great, spark ignition engines are the best candidates. Since, the auto ignition temperature of Hydrogen is more than that of gasoline, it may operate with a lean mixture while still providing quick ignition. The fact that hydrogen burns in spark ignition engines without producing any carbon dioxide, smoke, or hydrocarbons is another benefit of hydrogen as a fuel over gasoline (Wallner et al., 2009)

Recent years have seen the development of computer programs that can model the internal combustion engine's thermodynamic cycle. As a function of the engine design parameters, it aids in predicting engine performance and efficiency as well as helping to comprehend the observed behavior of the engine. We can forecast how different parameters in these alternative fuels will affect them by utilizing MATLAB. The user can also adjust the model using this program to the required engine test conditions listed in the software library.

1.2 Objectives

The main objective is to analyze the combustion effect of Hydrogen, Biogas, syngas and natural gas as a fuel in spark ignition engines.

The specific objectives are listed below:

- To develop a program to simulate the combustion of hydrogen and its mixture with gasoline and biogas in internal combustion spark ignition engine using MATLAB

- To study the feasibility of replacing standard fuels like gasoline with alternative fuels like hydrogen, biogas, syngas and Natural gas

1.3 Limitations

The limitations of this project were:

- The study of combustion parameters is restricted to the following variables: mass fraction, heat release, pressure, crank angle, equivalence ratio, and burn fraction
- The output of the MATLAB software is used to plot various curves and perform analyses on them
- The economy and policy have not been taken into consideration
- Only NOx production is covered in the emission research
- Can provide the option of running on gasoline and mixed fuel

CHAPTER 2 LITERATURE REVIEW

This section describes the existing works on the field of alternative fuels which also helps to analyze the observed value with the past and to predict the future. The main theme of this research is to study the properties of alternative source of combustible fuels such as Hydrogen, Syngas, Biogas and Natural gas in spark ignition engine.
This research work is about the Numerical Modeling, MATLAB coding, and performance analysis of various gases fuels mainly consisting of hydrogen, biogas, syngas and natural. Still the current practice in the world shows very limited development in the field of alternative fuels because of its complex combustion process. The study primarily focuses on using simulation in MATLAB to find the optimum alternative fuels for spark ignition engines with various operating conditions. Given that gasoline is the current standard operating fuel for engines, the study is mainly focused on comparing the various parameters of Hydrogen, Biogas, syngas and natural gas with those of gasoline.

Here, various fuel properties were studied. Different thermodynamic equations were studied which could be simulated in MATLAB. Also, various parameters' feasibility in MATLAB was studied. MATLAB is a numerical tool used for solving various higher order functions, computing graph. MATLAB was used to obtain solution and plots for different engine parameters. MATLAB was used to compute values under different conditions and equations. Also, it was used to plot results obtained from the calculation. The obtained results, solutions, charts, figures, etc. were documented for comparison and selecting suitable fuels in spark ignition engine, suggest proper methods to decrease knocking.

Hydrogen, Syngas, Biogas, Natural gas and LPG are promising alternatives to conventional gaseous fuels for spark ignition engines. Each of them is advantageous in its own way and is appropriate for particular uses. The commonly available petroleum-based fuels are natural gas and LPG. Syngas, Hydrogen gas, and Biogas are renewable forms of fuel energy which are in gaseous state. In addition to stationary power generation, CNG is extensively used in the industrial sector. In rural areas without significant infrastructure for the provision of electricity and petroleum goods, syngas can be utilized for transportation, stand-alone power generation, and irrigation.

Due to its gaseous condition and low impurity content, natural gas promotes clean combustion when employed in spark ignition engines. The temperature at which it self-ignites is 540 °C. Natural gas is compressed and it is converted into compressed natural gas. In a hard container, it is kept and distributed under pressure of 200–248bar (Ferguson et al., 2015). Air/fuel mixture in case of natural gas is more properly mixed than gasoline because natural gas has a higher molar mass than gasoline. A homogenous air-fuel mixture requires more time to atomize and vaporize liquid fuels (Shamekhi A et al., 2022) (T. Iskandar Mohamad et al., 2009) (AL., M. M. Tahir et al., 2015).A sensor was used to compare the data between Gasoline and natural gas during combustion in spark ignition engine which showed that gasoline has more than 18% more power than natural gas (Boroomand et al., 2013) (M. Muñoz et al., 2000) There was a 40–50% reduction in electricity. The low energy density of syngas is responsible for 30% of the power loss, with pressure drops in intake valves and pipelines accounting for the remaining 40%. Spark ignition engines must be slightly modified in order to run on producer gas (AL., C. Ji et al., 2012). A petrol engine's performance under lean conditions is observed to be affected by the addition of syngas. The test was conducted with a MAP sensor reading of 62.5 KPa and 1800 revolutions per minute. Adding 2.5% Syngas showed a better response at cylinder peak pressure and it also improved the thermal efficiency of the spark ignition engine (Grab-Rogalinski et al., 2009). The emission of NOx and CO was increased as well. Multiple misfiring was also observed with the addition of syngas (V. Jithin et al., 2021). It was investigated how well SI engines running on 100% producer gas performed under various load circumstances.

2.1 Properties of gases

2.1.1 Hydrogen Gas

Since hydrogen is more flammable than other types of gasoline, gasoline fuel could be replaced with hydrogen or partly adding hydrogen in gasoline in spark ignition engine. Utilizing hydrogen has the ability to operate in lean mixes, which is a big benefit. Hydrogen has a very low energy of ignition. Gasoline required more energy to ignite than Hydrogen. This hydrogen engine makes it possible for the ignition to quickly ignite the lean mixture. Compared to other fuels, hydrogen has a much shorter quenching distance. As a result, hydrogen flames pass quite near the cylinder wall.

Therefore, understanding hydrogen flame is more challenging than understanding gasoline flame. A significantly high auto-ignition temperature exists for hydrogen. The important result of compressing a hydrogen-air mixture is this. When hydrogen is present in stoichiometric proportions, it burns quickly. So, starting from relatively close cycles, hydrogen engines can approach thermodynamically optimal engines. The diffusivity of hydrogen is extremely high. There are two key advantages to this significantly greater airborne spreading capacity compared to gasoline (A. CERNAT, C. Pana, N. Negurescu, G. Lazaroiu, C. Nutu, and D. Fuiorescu, 2020)

Reaction between hydrogen and oxygen

$2H_2+O_2 \longrightarrow 2H_2O$

Reaction between hydrogen, oxygen and nitrogen forms Nitrogen oxides

$2H_2+O_2 + N_2 \longrightarrow 2H_2O+NO_x$

Nitrogen oxides formation is dependent on various factors:

- Spark Ignition timing
- RPM of engine
- Various CR
- Mixture of air and fuel and its proportions

2.1.2 Synthetic Gas (Syngas)

Because of its clean combustion and minimal greenhouse gas emissions, syngas is often said to be a best replacement for gasoline. The feedstock and the manufacturing technique are major determinants of syngas composition. Syngas' extensive compositional variation makes it difficult to create devices like burners and combustion chambers. The most dependable and energy-efficient conversion technology is gasification, which also has advantages for both upstream and downstream flexibility. In gasification process, carbon bonds are broken and hydrogen is added to the gaseous product. The created gas is known as syngas. Synthetic gas is formed from the combination of carbon monoxide and Hydrogen in different proportions. The quality of the syngas is influenced by the gasifying agent. During the process, the main gasifiers used are air, steam, and oxygen. Syngas with a medium calorific value is one that is created using either oxygen or steam as the gasifying agent. The heating value of this substance, which is also known as "syngas," is 10-28 MJ/Nm3. Syngas is referred to as lower calorific value gas and is produced by using air as a gasifier. It also goes by the moniker "producer gas" and has a 4 to 7

MJ/Nm3 heating value. These fuels both have low syngas energy densities and 8–12 psi SI engine compression ratios. Producer gas's laminar velocity of burning is 30% more than that of methane gas. With this feature, the ignition time of the engine used to create gas fuel-based engines must advance less. Because to greater dilution, the presence of inert (CO, and N) in the raw gas may decrease the pre-flame reactions that cause knocking. Less than one mole of product is produced per mole of reactant in producer gas. Increasing the hydrogen content of syngas makes it more ignitable and reduces the first stage's ignition delay as a result.

2.1.3 Natural Gas

Light Hydrocarbons such as propane, butane, ethane, pentane and methane are the main composition element of natural gas. The secondary elements are Nitrogen, hydrogen sulfide, CO2, and helium. Natural gas's composition is never consistent; however, methane (which normally makes up at least 90% of the gas) is its main constituent. The most flammable gas is methane and it burns quickly as well. There isn't much air pollution made by it. Natural gas is a safe fossil fuel if compared to other fuel sources because it is neither poisonous nor corrosive.

Liquid LNG and compressed CNG are the two main types of natural gas. LNG is not used as it is more expensive. LNG has a high-octane rating as well (Thring, R. H., 1983). LNG vehicles release 80% lower emissions than gasoline-powered vehicles, namely CO and NOx (Wojtyniak et al., 2005). The price of the vehicle increases to $4000 as it needs a new compressor and compressed tank.

2.2 Internal Combustion Engines

Any engine that burns fuel inside is referred to as an internal combustion engine. Gas-powered internal combustion engines are the most prevalent. Additionally, there are others that operate on hydrocarbons like propane, ethanol, ethane, Hydrogen and the most common type is Diesel. Engines are designed in such a way that one type of fuel must be used and the air/fuel mixture should be varied for desirable and proper combustion. An internal combustion engine is a type of combustion engine where fluid is the fuel which is combustible and air. An illustration of an internal combustion engine is a gas turbine, Compressed ignition engine (Diesel), Spark ignition engine (Petrol).

2.2.1 Spark Ignition Engine

The most often used reciprocating engines are spark ignition engines. Numerous road cars and some heavier vehicles have engines of this type. These types of engines are mainly used in small segment automobiles with light load capacity. They are used in cars, bikes, lawn movers, and chainsaws and sometimes used for power generation as well. Spark ignition engines are either two stroke of four stroke but mainly four stroke engines are used in automobiles. MPFI or carburetor system is applied on spark ignition engine. A spark plug is used for ignition as there is no auto ignition in spark ignition engine.

Air/fuel premix mixture is formed and then it is supplied inside the engine for proper combustion in case of spark ignition engines. To perform this mixing, numerous mechanical and electrical methods have been devised. Following compression, an electrical spark ignites the fuel mixture. A pre-ignition chamber exists in certain more sophisticated engines, where a fuel-rich mixture is ignited first before spreading into the main cylinder. In MPFI engine, an ECM controls all the injection and air supply from various sensors installed in intake and exhaust side of the manifold.

2.2.2 Combustion in SI Engine

There are three main categories that can be used to categorize the combustion process in SI engines: (1) Ignition, (2) Flame generation and propagation, and (3) Flame halt. In general, the first 6% of the air-fuel mixture is consumed during flame growth (other sources cite the first 10%). Although the combustion process begins and ignition happens during the flame development phase, there is lower rise of pressure and less work is formed. By creating turbulence, swirl, and squish inside the cylinder, the flame front's spread is significantly accelerated. Knock is prevented or nearly avoided when the proper fuel and operating conditions are used. The two different types of combustion are normal combustion and aberrant combustion.

2.2.3 Thermodynamics of combustion process

Unburned and Burned Mixture States

Volume of the engine’s which is caused by the motion of the piston ultimately changes the gas’s pressure, temperature and density. The pressure inside the chamber increases as a result from chemical energy that has been released from the combustible fuel and the density decreases by one forth. Burned and unburned gas composition is calculated from the mass conversation equation mentioned below.

$$\frac{V}{m} = \int_{0}^{xb} Vb\,dx + \int_{xb}^{1} Vy\,dx \qquad (2.1)$$

Conservation of energy:

$$\frac{U0-W-Q}{m} = \int_{0}^{Xb} ub\,dx + \int_{xb}^{1} uy\,dx \qquad (2.2)$$

Where,

W= Work done

Q= Heat energy

V= Volume of cylinder inside combustion chamber

m= Mass of cylinder contents

U0= Internal energy

u= Specific heat

θ= Rate of heat transfer

The work and heat transfer rate is calculated by the equations mentioned below:

$$w = \int_{V0}^{V} PdV' \qquad (2.3)$$

$$\mathrm{Q} = \int_{Q0}^{Q} \frac{Q}{360N}\,d\theta \qquad (2.4)$$

2.2.4 Abnormal Combustion

In IC engine, normal combustion plays a vital role in engine's performance. Abnormal combustion is essential to study as well as it plays an essential role in life of an engine. There are two vital aspects of abnormal combustion. They are as follows:

- Knock
- Surface ignition

2.2.5 Knock

Knocking is an unusual metal noise that comes from the engine because of pre ignition of left over exhaust gas inside the engine during compression stroke. Due to the noise produced when a portion of the fuel-air combination automatically ignites before the approaching flame, it was given the term "Knock." It moves forward of the flame as it spreads over the combustion chamber at a speed of around 15 to 30 m/s. Fast chemical reactions occur when there is anomalous combustion, which causes auto ignition before there is regular combustion.

Some of the vital effects of knocking are as follow:

- Unusual metal clicking noise.
- Low power and degrading efficiency.
- Deposition of soot particles and clogged up catalytic converter.
- Overheating of vehicle.
- Excessive wear and tear of engine components like head, bore, piston rings and pistons.

2.2.6 Surface Tension

There are various causes that lead to the occurrence of surface tension. It is the process of auto ignition of air/fuel mixture inside the engine as well. If there are any hot spots that has been triggered inside the combustion chamber because of some soot particles that has been left over during exhaust stroke, pre ignition occurs easily in this case. Pre ignition can also occur if the spark plugs are overheated or the valves are overheated as well. Carbon deposits are primarily to blame for surface igniting. Surface ignition can happen either before or after typical ignition, depending on how the spark plug ignites the charge (post ignition). Either a single flame or several flames may be produced. Pre ignition causes uncontrolled combustion to be most obvious and has the worst effects. Knock could also be brought on by surface ignition.

2.2.7 Wild Ping

The knocking surface ignition variation known as "wild ping" causes short bursts of loud cracking sounds. In case of wild ping, soot particles or carbon deposits particles plays a vital role. If there is more carbon deposits or soot particles that has high temperature, wild ping is most likely to occur. Wild ping will disappear if there is no carbon deposits or any soot particles. Most likely, burning loose deposit particles in the combustion chamber cause wild ping to occur.

2.2.8 Rumble

In high compression ratio engines, rumble is characterized by a small frequency noise which is produced as same as wild ping. It occurs due to surface based soot particles combustion as well. Engine vibration is caused by a quick rise in pressure to a high value. Together, rumble and knock are possible.

2.2.9 Emission in SI Engine

Various gases such as NOx, CO, CO2, and hydrocarbons along with Sulphur and its oxides are formed in the exhaust of the vehicle if there is abnormal combustion, fuel that is not burned completely and formation of hydrocarbons or any residual gases that has been formed during the exhaust stroke. The main exhaust emissions of SI engines include hydrocarbons, NO, CO, CO2, polycyclic aromatic hydrocarbons (PAH), and particulate matter. The amount of these gases released mostly depends on the fuel-to-air ration, kind of fuel utilized for combustion, flame turbulence, and timing of ignition. The emission of HC, CO, and NO2 for various fuel/air equivalency ratios is depicted in the below image:

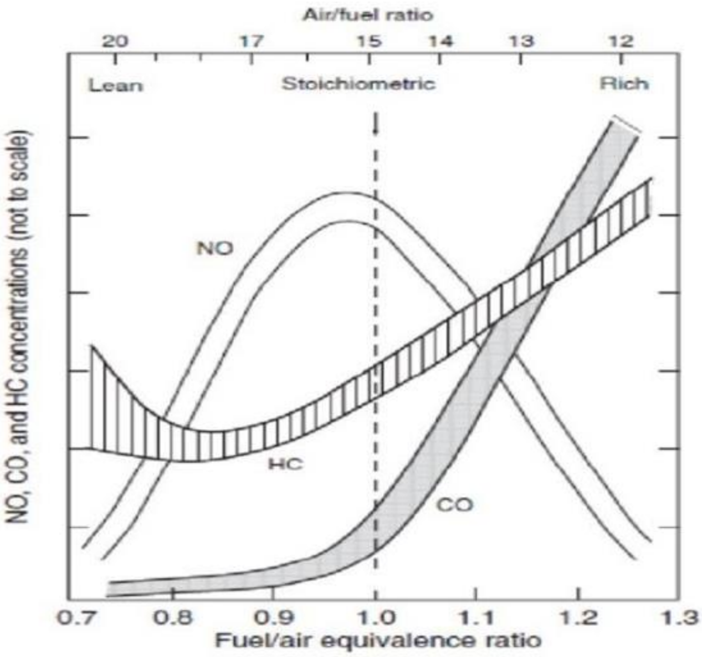

Figure 2.1 Emission of HC, CO and NOx for different fuel/air equivalence ratio.
(Source: Adapted from Heywood J.B, 2000)

CHAPTER 3 RESEARCH METHODOLOGY

A simulation based on mathematical modeling was obtained from the 4 strokes that take place in an IC engine. In an engine based mathematical simulation, combustion modeling plays a significant role. Mathematical equations were inserted in the simulation and then performance analysis was done on spark ignition engine of Hydrogen, Syngas and Natural gas and the results were compared with gasoline as well. Adequate literature review was done with the help of various sources such as internet, books and with the help of supervisor. MATLAB code was then developed for numerical simulation of various gases. Graphs were generated using the MATLAB simulation. Results obtained were compared with the conventional spark ignition engine and findings and conclusions were stated that supports the use of hydrogen or other gas with other fuel for the reduction of use of the fossil fuel. The below flow chart describes the work flow that will be followed while carrying out this research.

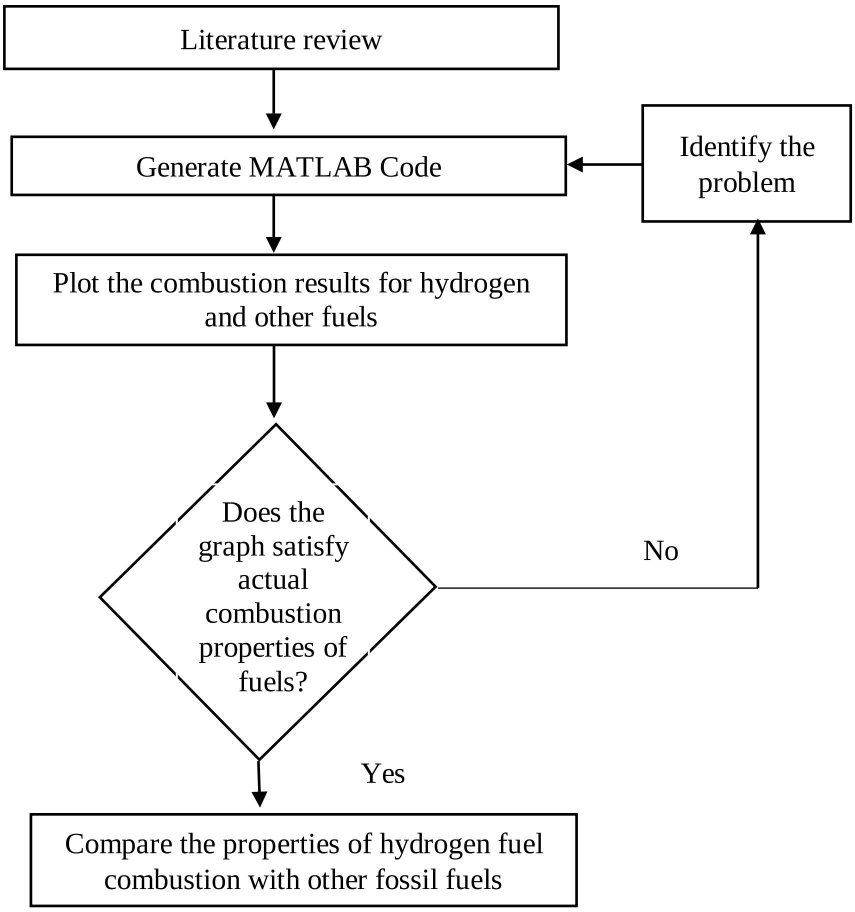

Figure 3.1 Schematic Flow diagram

3.1 MATLAB Simulation of S.I Engines

Various equations were developed for varying Compression ratio, RPM, Spark advance and equivalence ratio. Modeling of mathematical equations divides the combustion chamber into various zones of burned and unburned gases air/fuel mixture. There are various MATLAB program developed which replicates zone of combustion inside IC engine and thermodynamic activities in a real model based simulation. (Thring, R. H., 1983) (Ferguson et al., 2015)

3.1.1 Engine Specification for Simulation

The above engine specifications were used for simulation.

Table 3.1 Engine specification for Syngas and Natural gas (J. MA et al., 2003)

Specification of engine	Single Cylinder, SI, 4 stroke
Diameter of Bore(a)	0.0925 m
Length of Stroke(b)	0.1143 m
Length of connecting rod(l)	0.2286 m
Compression ratio(CR)	8:1-11:1
Engine Speed (RPM)	1500-4500

3.1.2 Air, Fuel, and Combustion Products Data

The curve fits constants ranges from a1 to a5 and there are 10 rows in one matrix. The constants ranging from a1 to a5 are the values of curve fits constant. There is a program called air data and fuel data in MATLAB simulation which provides the values of this curve fits constant for each simulation. These constants can be plotted using the curve-fit coefficients for equation 3.1 and equation 3.2 respectively for Hydrogen, syngas and Natural gas respectively.

$$\frac{C_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \quad (3.1)$$

$$\frac{C_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5\frac{1}{T^2} \quad (3.2)$$

where,

$\boldsymbol{C_p}$= specific heat at constant pressure

$\boldsymbol{R}$ =Gas constant

$\boldsymbol{T}$ = Temperature

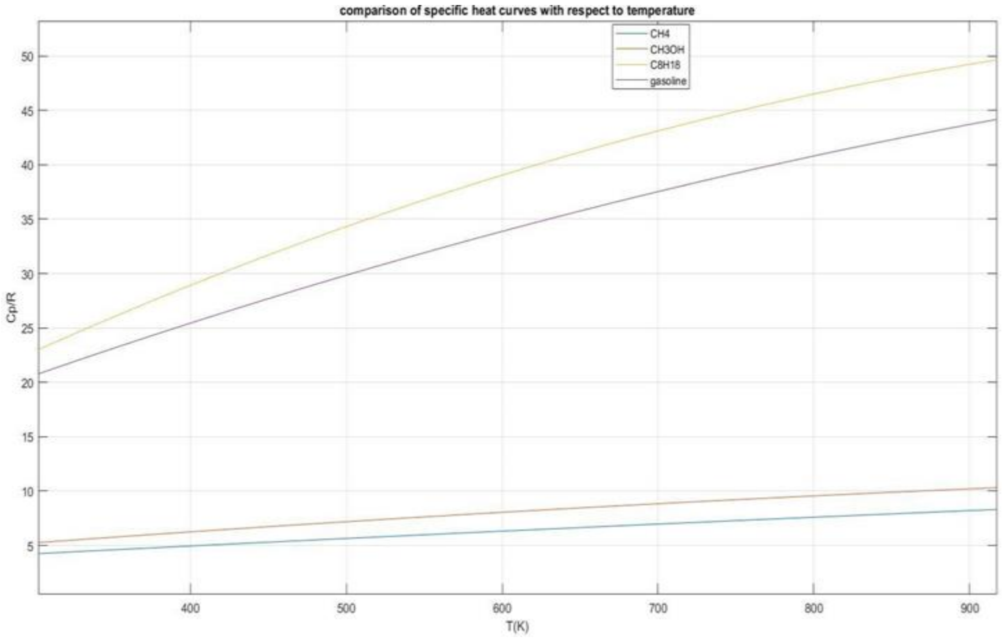

Figure 2.2 Specific heat curves comparison for hydrogen and other fuels using coefficients

3.1.2 Calculation of fuel-air-residual gases mole fraction

A program called FARG determines the range coefficients for the curve using reference from air data and fuel data program. FARG operates for low temperature ranging from 300k to 1000k. To determine the actual mole fraction it is required to study the actual moles of combustion gases taking part inside the combustion chamber. There is trace number of unburnt gases remaining when exhaust stokes completes. These left-over gases react with the new air/fuel mixture and new combustion process takes place.

The species mole fraction for carbon dioxide, nitrogen, hydrogen, carbon monoxide and water is given by the equation

$$\boldsymbol{yi} = (1 - y_r)y'_i + y_r y''_i, \quad i = 0 \ to \ 6 \qquad (3.3)$$

Where

$\boldsymbol{y_r}$ = residual mole fraction

$$\boldsymbol{y'_i} = \text{reactant mole fraction} = \frac{n_i}{n_{fa}} \qquad (3.4)$$

$\boldsymbol{y''_i}$ = product mole fraction = $\frac{n_i}{n_r}$

The values for y'_i and y''_i can be determined from the Appendix Table A5.

FARG program determines the mole fraction of the actual gases taking part inside the combustion chamber and it requires certain parameters such as pressure, fuel type, equivalence ratio and mass fraction of residual gases. The product equilibrium mole fractions resulting from the combustion of the listed fuels at 500 K, 100 kPa, ϕ=0.8, and f=0.05 are listed in Appendix table T6.

3.1.3 Calculation of Equilibrium Combustion Products Mole Fractions

At elevated temperatures (600-3500K) typical of combustion processes, the equilibrium state of the combustion products can be determined provided the mixture is not too rich ($0.3 \leq \Phi \leq 4$). A computer program, ecpH2.m (detailed in Appendix A.4), is designed to calculate the properties of equilibrium combustion products for different fuel-air mixtures. For this program, ten product mole fractions are computed for equilibrium combustion of the fuel-air mixture with inputs specified such as temperature (T) in Kelvin, pressure (P) in kPa, fuel-air equivalence ratio (ϕ), and fuel id. The species included in the product mixture are CO_2, H_2O, N_2, O_2, CO, H_2, H, O, OH, and NO. The product equilibrium mole fractions resulting from the combustion of the listed fuels at 5000 kPa, 3000 K, 0.8 ϕ are calculated and provided in Table A4.

3.1.4 Homogeneous Two Zone Combustion Cycle

A program Homogenous H2.m computes the heat and work of the system, heat loss from the system, mass loss from the system, and concentration of Nitrogen oxide, temperatures of burned and unburned fractions as well. Following are the equations which the simulation is performed in the program.

$$\frac{d\boldsymbol{H_1}}{d\boldsymbol{\theta}} = \frac{Cm}{\omega}[(1 - x^2)h_u + x^2 h_b] \tag{3.5}$$

Where,

$\boldsymbol{H_1}$ = burned fraction

$\boldsymbol{m}$ = Combustible gas's mass

$\boldsymbol{C}$ = blow by coefficient

$\boldsymbol{\omega}$ = engine frequency (rad/s)

$\boldsymbol{x}$ = mass fraction burned

$\boldsymbol{h_u}$ = Heat transfer coefficient (Unburned gas)

$\boldsymbol{h_b}$ = Heat transfer coefficient (Burned gas)

$$\frac{\boldsymbol{dP}}{\boldsymbol{d\theta}} = \frac{A + B + C}{D + E} \tag{3.6}$$

where

$\boldsymbol{P}$ = Pressure of the gas (kPa)

$\boldsymbol{A} = \frac{1}{m}(\frac{dV}{d\theta} + \frac{VC}{\omega})$

$\boldsymbol{V}$ = Volume of the cylinder (m^3)

$\boldsymbol{B} = \frac{hA_c}{\omega m}[\frac{1}{c_{pb}}\frac{\partial v_b}{\partial T_b}x^{\frac{1}{2}}(T_b - T_w) + \frac{1}{c_{pu}}\frac{\partial v_u}{\partial T_u} - (1 - x^2)(T_u - T_w)]$

$\boldsymbol{A_c}$ = Cylinder Area (m^2)

$\boldsymbol{c_{pb}}$ = Constant pressure specific heat (Burned gas)

$\boldsymbol{c_{pu}}$ = Constant pressure specific heat (Unburned gas)

$\boldsymbol{v_b}$ = specific volume at unburned zone (m^3/kg)

$\boldsymbol{T_b}$ = Temperature of the combustible gas (Burned)

$\boldsymbol{T_w}$ = Temperature of cylinder wall (K)

$\boldsymbol{v_u}$ = Unburned zone's specific volume (m^3/kg)

$\boldsymbol{T_u}$ = Temperature of the combustible gas (Unburned)

$\boldsymbol{C} = -(v_b - v_u)\frac{dx}{d\theta} - \frac{\partial v_b}{\partial T_b} - \frac{h_u - h_b}{c_{pb}}[\frac{dx}{d\theta} - \frac{(x - x^2)C}{\omega}]$

$\boldsymbol{D} = x[\frac{T_b}{c_{pb}}(\frac{\partial v_b}{\partial T_b})^2 + \frac{\partial v_b}{\partial P}]$

$\boldsymbol{E} = (1 - x)[\frac{T_u}{c_{pu}}(\frac{\partial v_u}{\partial T_u})^2 + \frac{\partial v_u}{\partial P}]$

$$\frac{\mathbf{dT_b}}{\mathbf{d\theta}} = \frac{-hA_C(T_b - T_w)}{\omega m c_{pb} x^{1/2}} + \frac{T_b}{c_{pb}}\frac{\partial v_b}{\partial T_b}\frac{A + B + C}{D + E} + \frac{h_u - h_b}{x c_{pb}}[\frac{dx}{d\theta} - (x - x^2)\frac{C}{\omega}] \tag{3.7}$$

where

$\boldsymbol{T_b}$ = Temperature of the burned gas (K)

$\boldsymbol{h}$ = convection heat transfer coefficient (W/m^2K)

$$\frac{\boldsymbol{dT_u}}{\boldsymbol{d\theta}} = \frac{-hA_C(1 - x^{1/2})(T_u - T_{W})}{\omega m c_{pu}(1 - x)} + \frac{T_u}{c_{pu}}\frac{\partial v_u}{\partial T_u}\frac{A + B + C}{D + E} \tag{3.8}$$

Where,

$\boldsymbol{T_u}$ = Temperature of the unburned gas (K)

The graphs obtained after running the HomogenousH2.m program are mentioned below:

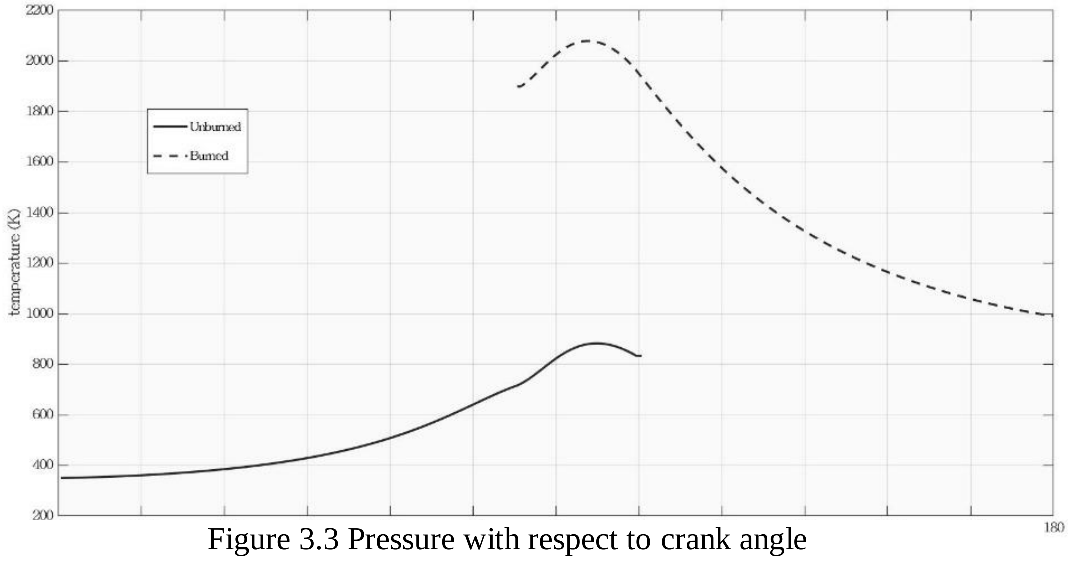

Figure 3.3 Pressure with respect to crank angle

The work and heat transfer loss is plotted in Figure 7 as a function of crank angle for the optimum case of θs = −15◦ by solving the equations 3.9 and 3.10 respectively.

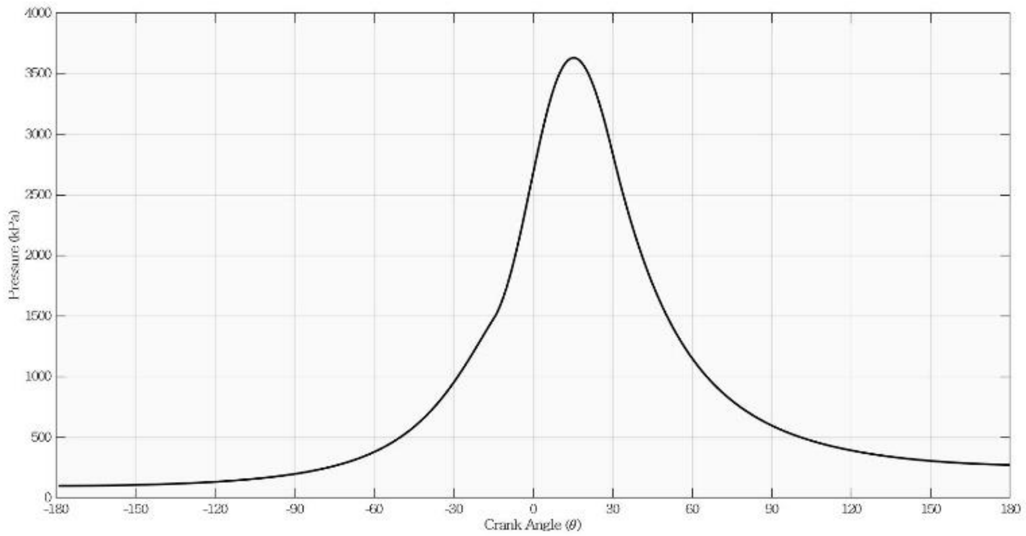

Figure 3.4 Temperature vs crank angle of burned and unburned gas

$$\frac{\boldsymbol{dW}}{\boldsymbol{d\theta}} = P\frac{dV}{d\theta} \tag{3.9}$$

where $\boldsymbol{W}$ = Work (J)

$$\frac{\boldsymbol{dQ_1}}{\boldsymbol{d\theta}} = \frac{hA_c}{\omega}[x^{1/2}(T_b - T_{u)} + (1 - x^{1/2})(T_u - T_{w)}] \tag{3.10}$$

where $\boldsymbol{Q_1}$= Heat transfer (J)

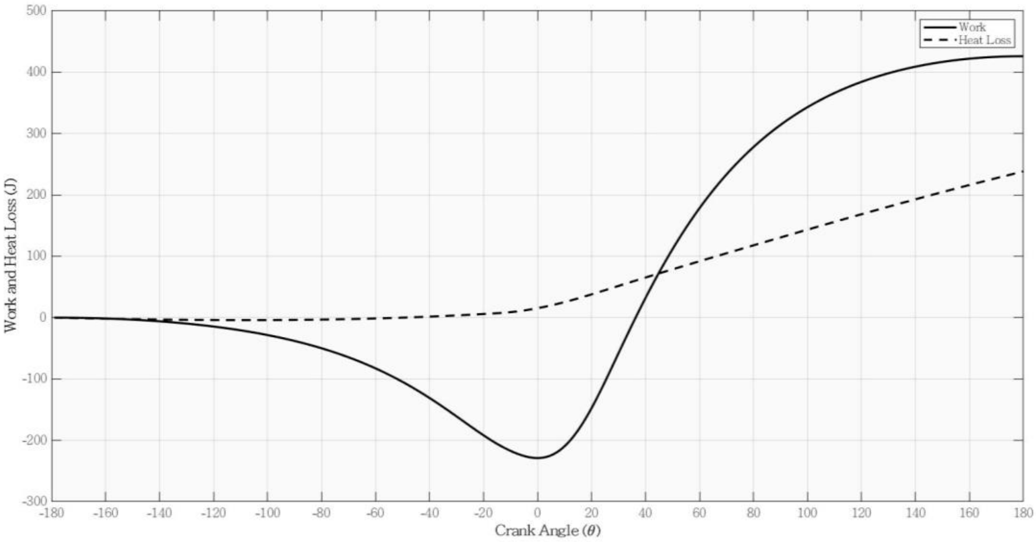

Figure 3.5 Heat and work loss with respect to crank angle

3.2 Calculation for Hydrogen composition

From law of stoichiometric, we can compute the mole required for hydrogen and oxygen to have complete combustion which is mentioned below:

$2H_2 + O_2 = 2H_2O$

From this equation, we can see that, 2 moles of hydrogen react with one mole of oxygen for complete combustion. This is theoretical approach. But we do know that air contains 70% nitrogen. We need to mention that and do our calculation on the basis of this approach.

We know that,

Number of moles of nitrogen in air on the basis of percentage is 3.76 moles. Thus, total number of moles of air has 4.76 moles of nitrogen. We know that oxygen weighs

32gm and nitrogen weighs 3.76*28 i.e., 105gm. Total weight of air now becomes 137gm. We also know that weight of hydrogen is 4gm.

Using law of reciprocal,

Air to fuel ratio for hydrogen and air is:

Air to fuel ratio based on mass: = $\frac{\text{Wt.of air}}{\text{Wt.of Hydrogen}}$ = $\frac{137.33}{4}$ = 34.33:1 (Gasoline is 14.7:1)

3.3 Calculation for Syngas composition

For the calculation of C, H, O and N we only consider the combustible gases present in the syngas. Since the software demands for the atoms and compounds that take part in the combustion only so gases taken into account were Carbon monoxide, Hydrogen and Methane only.

We have taken two different compositions for Syngas by varying the composition of Hydrogen, Carbon monoxide and Methane.

Table 3.1 Composition of syngas

Gas	Syngas A	Syngas B
H_2	11	17
CO	24	21
CH_4	3	1
CO_2	9	13
N_2	53	48

For Syngas (A),

The total percentage of CO, H2 and CH4 for Syngas (A) is

= (24+11+3) %

= 38%

Now, the proportion of these gases in the total combustible mass would be,

CO = $\frac{24}{38}$ = 0.632

H_2 = $\frac{11}{38}$ = 0.29

CH_4 = $\frac{3}{38}$ = 0.079

Calculating the atom-based proportion we get, Carbon (C) = (0.632+0.079) = 0.71

Hydrogen (H) = (2*0.29+4*0.079) = 0.896

Oxygen (O) = 0.632

The general chemical formula for Syngas (A) on above calculation becomes,

$C_{0.79}H_{0.896}O_{0.632}$

Carbon balance

$C_{0.79}H_{0.896}O_{0.632} + O_2 = 0.71CO_2 + aH_2O$

Hydrogen balance

$C_{0.79}H_{0.896}O_{0.632} + O_2 = 0.71CO_2 + 0.448H_2O$

Oxygen balance

$C_{0.79}H_{0.896}O_{0.632} + 0.618O_2 = 0.71CO_2 + 0.448H_2O$

(1 mol) (0.618 mol) (0.71 mol) (0.448 mol)

Therefore, 1 mole of syngas needs 0.618 mole of oxygen for complete combustion under combustion contains 0.71 mole of carbon dioxide and 0.448mole of water fuel respectively. A mole of air has 0.21 mole of Oxygen

So, 0.618 mole of Oxygen is contained in = $\frac{0.618}{0.21}$mole of air

= 2.94 mole of air

Then stoichiometric Air to fuel (A/F) ratio will be 2.94:1. This data is required as input during MATLAB simulation.

For Syngas (B),

The total percentage of CO, H2 and CH4 for Syngas (B) is

= (21+17+1)

= 39%

Now, the proportion of these gases in the total combustible mass would be,

CO = $\frac{21}{39}$ = 0.632

$H_2 = \frac{17}{39}$ = 0.44

$CH_4 = \frac{1}{39}$ = 0.03

Calculating the atom-based proportion we get, Carbon (C) = (0.54+0.03) = 0.57

Hydrogen (H) = (2*0.44+4*0.03) = 1 Oxygen (O) = 0.54

The general chemical formula for Syngas (A) on above calculation becomes, C0.57HO0.54

Carbon balance

$C_{0.57}HO_{0.54} + O_2 = 0.57CO_2 + aH2O$

Hydrogen balance

$C_{0.57}HO_{0.54}$+ O_2 = 0.57CO_2 + 0.5H_2O

Oxygen balance

$C_{0.57}HO_{0.54}$ + 0.55O_2 = 0.57CO_2 + 0.5H_2O

(1 mol) (0.55 mol) (0.57 mol) (0.5 mol)

Therefore, 1 mole of syngas needs 0.55 mole of oxygen for complete combustion under combustion contains 0.57 mole of carbon dioxide and 0.5 mole of water fuel respectively. A mole of air has 0.21 mole of Oxygen

So, 0.618 mole of Oxygen is contained in = $\frac{0.55}{0.21}$ mole of air

= 2.62 mole of air

Then stoichiometric Air to fuel (A/F) ratio will be 2.62:1. This data is required as input during MATLAB simulation.

3.4 Calculation for Natural Gas

For the calculation of C, H, O and N atoms, the gas taken into account for Natural gas was methane since it only takes part in combustion.

Table 3.2 Actual Composition of natural gas

Gas	Composition (%)
Butane (C_4H_{10})	1
Propane (C_3H_8)	1
Ethane(C_2H_6)	3
Methane (CH_4)	95

The total percentage of methane (CH4) is 95% Calculating the atom-based proportion we get, Carbon(C) = 0.95

Hydrogen (H) = 3.8

The general formula for natural gas from above calculation becomes,

$C_{0.95}H_{3.8}$

Carbon balance

$C_{0.95}H_{3.8}$ + O_2 = 0.95CO_2 + a H_2O

Hydrogen balance

$C_{0.95}H_{3.8}$ + O2 = 0.95CO_2 + 1.9H2O

Oxygen balance

$C_{0.95}H_{3.8}$ +1.9 O_2 = 0.95CO_2 + 1.9H_2O

Therefore, 1 mole of natural gas needs 1.9 mole of oxygen for complete combustion under combustion contains 0.95 mole of carbon dioxide and 1.9 mole of water per fuel respectively.

1 mole of air has 0.21 mole of Oxygen.

So, 1.9 mole of Oxygen is contained in = 1.9

0.21 mole of air.

=9.047 mole of air.

Then stoichiometric Air to Fuel (A/F) ratio for Natural Gas will be 9.047:1. This will be used as input data during MATLAB simulation.

CHAPTER 4 RESULTS AND DISCUSSION

The simulation was performed for the hydrogen gas, syngas and Natural gas under various operating condition on the basis of different parameters. The plot obtained from the simulation along with the emission is discussed below.

4.1 Comparison plots for Hydrogen:

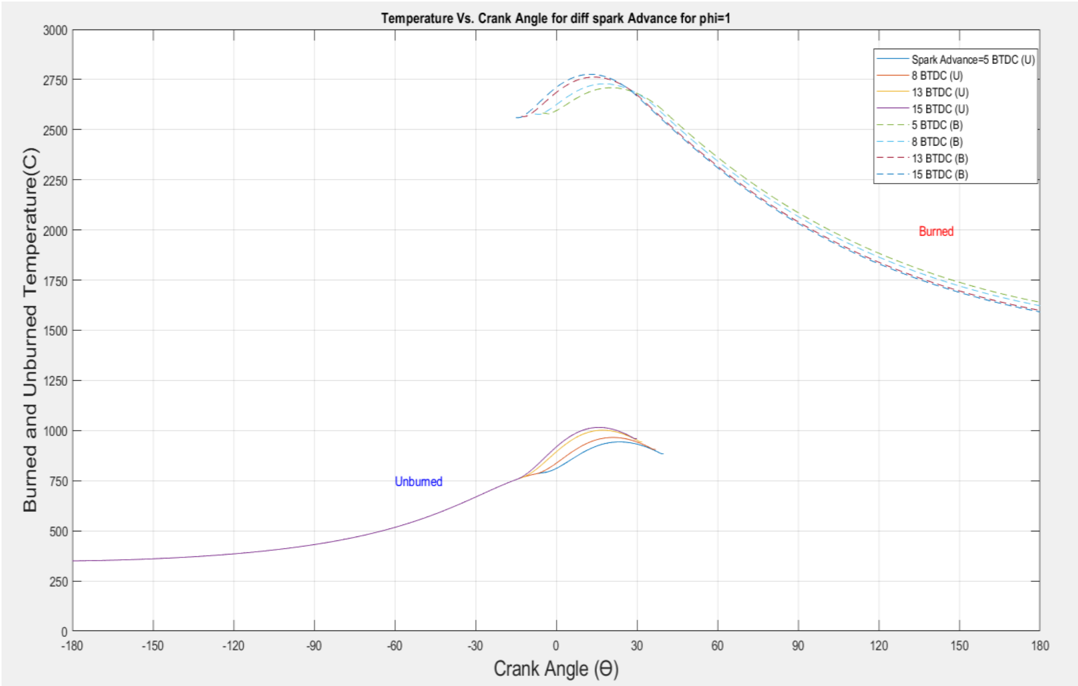

Figure 4.1 Variation of Burned and Unburned Hydrogen Gas Temperature vs. Crank Angle

Figure 4.1 describes the relation between temperature changes with respect to crank angle. It shows how the temperature of burned and unburned gas changes with the changes in crank angle. Crank angle determines when the next cycle firing is supposed to take place. As we can observe that temperature of burned gas is higher than that of unburned gas. From the figure we can observe that the temperature profile of unburned gas rises from -15 degree to +30 degree. This is because of the compression stroke inside the combustion chamber. This process increases the heat transfer rate as well, thus increasing the temperature of the burned and unburned gas. For burned gas, the temperature profiles rise from -20 degree to +35 degree. This is also because of the compression stroke inside the combustion chamber. The adiabatic flame temperature for unburned gas is 950K and it increases up to 1050k. Similarly, for unburned gas, the adiabatic flame temperature for burned gas is 2550k and it increases up to 2760k. From the graph, if we increase the spark advance of the combustion process involved for burned and unburned gas, the temperature profile also increases respectively and vice versa.

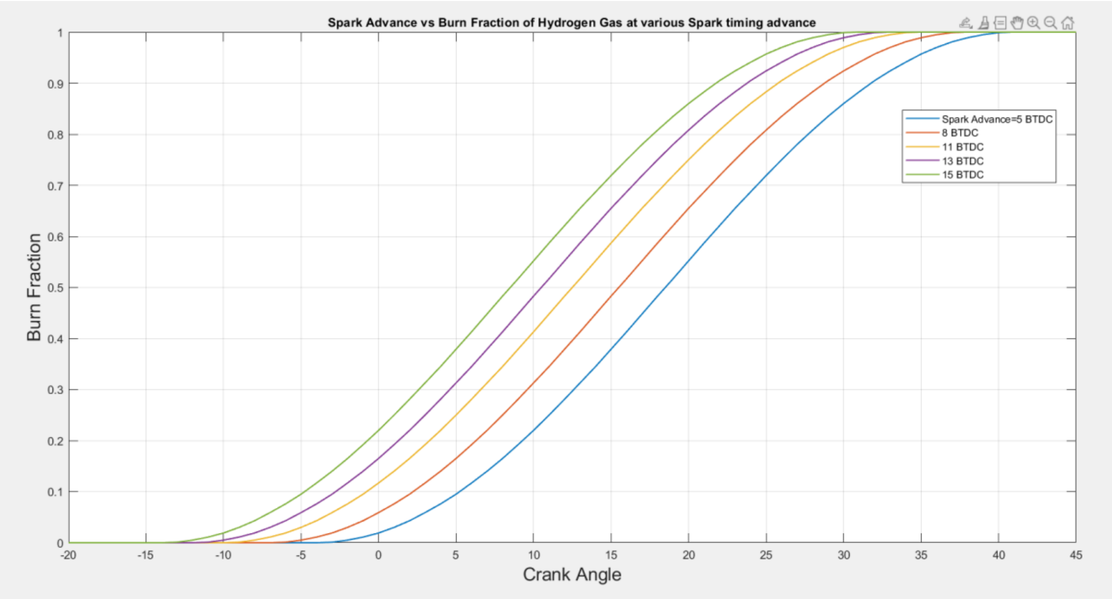

Figure 4.2 Burn Fraction versus Crank angle of Hydrogen gas

Figure 4.2 shows the variation in mass fraction burned in a spark ignition for the hydrogen on the basis of crank angle. From this graph, the mass fraction burned at 15° BTDC, 13° BTDC, and 11° BTDC shows a kind of fast burn. The crank angle for one BTDC differs approximately -2° over the duration of the 10%-90% burn fraction from other BTDC. The burn fraction at 8° BTDC is slower burn as compared to the others.

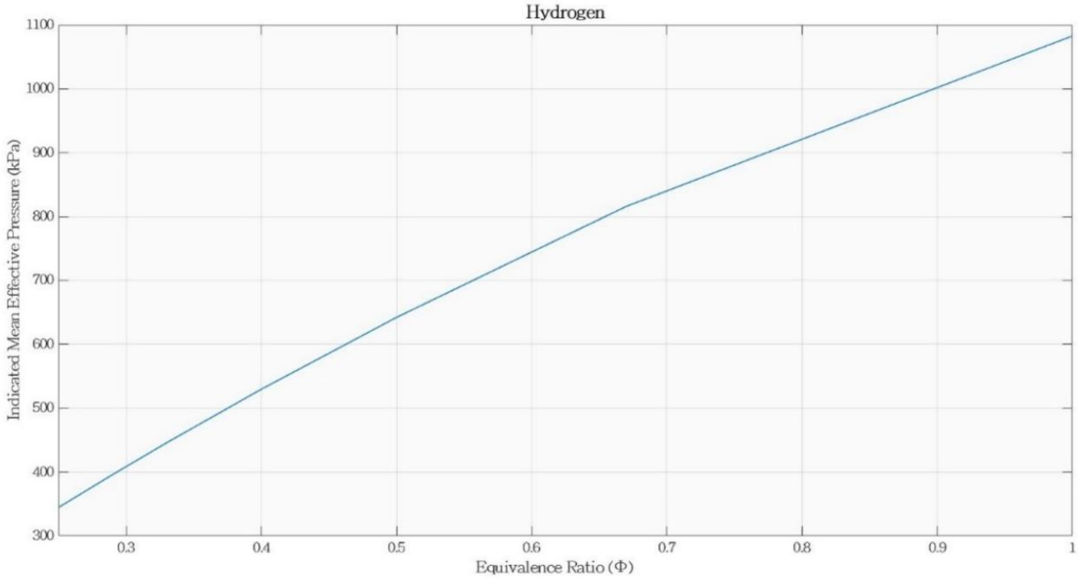

Figure 4.3 Variation of Indicated Mean Effective Pressure with respect to Equivalence Ratio

Figure 4.3 shows the variation of pressure with respect to equivalance ratio for hydrogen gas. It can be seen from the graph that, if equivalance ratio is increased, the pressure inside the chamber also increases and vice versa. At lean conditions, the maximum indicated pressure is about 350 Kpa while at rich condition the pressure is about 1090 Kpa.

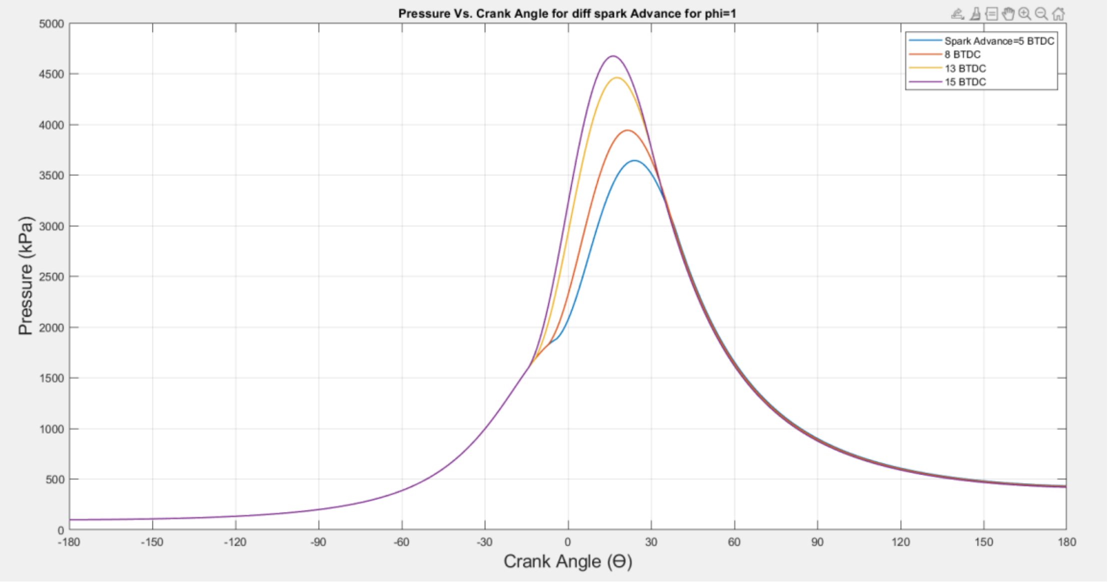

Figure 4.4 Pressure vs crank angle when spark advanced at different positions

Figure 4.4 shows the pressure in hydrogen with respect to crank angle at various spark ignition timing. The cylinder pressure from this thermodynamics model shows that it is the peak pressure about 4700 KPa at 15° BTDC and the peak pressure about 3600 KPa at 15 BTDC and the cylinder pressure from this thermodynamics model shows that it is the peak cylinder pressure about 3850 KPa & 3600 KPa at 13° BTDC & 8° BTDC. From this, it can be said that if crank angle increases, the effective pressure also increase and vice versa and for all BTDC it remains the same until it reaches around -30 ° to 0 °. After that, it reaches its BTDC maximum pressure and falls. After a 30-degree crank angle, pressure decreases the same for all BTDC.

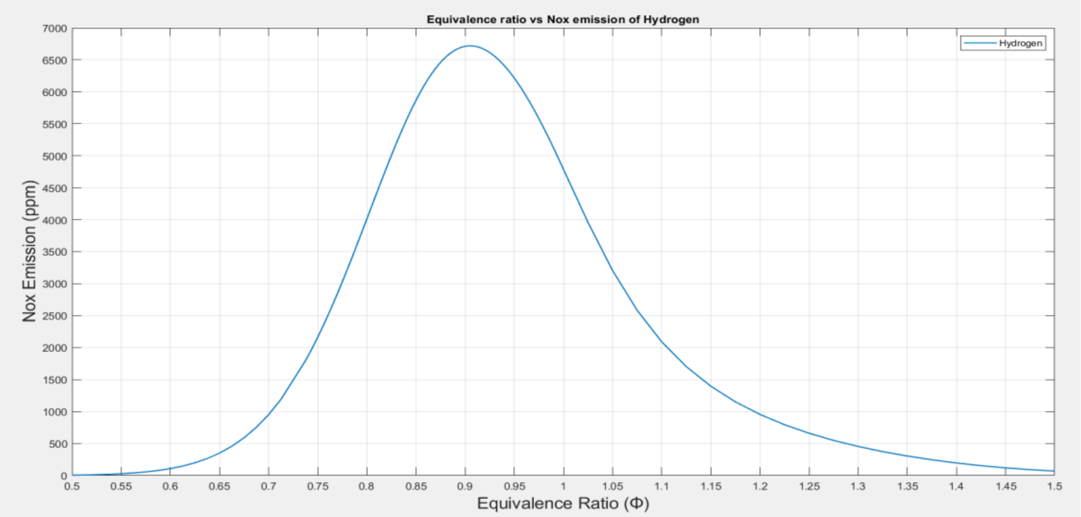

Figure 4.5 Nox Emission vs Equivalence ratio of Hydrogen at CR 8:1& 1500 RPM

Figure 4.5 shows the Nox emission in ppm of hydrogen gas with respect to Equivalence ratio. From the graph, it is seen that as the mixture changes form lean to rich, Nox emission also changes from high to low. Nox emission is higher in lean mixture. Nox emission is higher at equivalence ratio of 0.9. The maximum emission of Nox at this point is 6650 ppm.

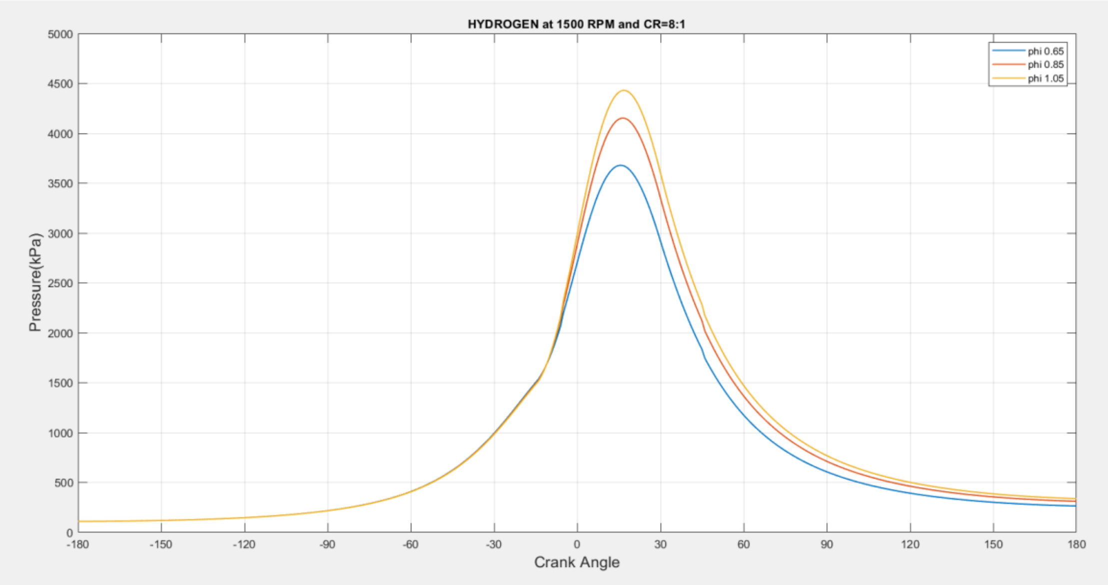

Figure 4.6 Pressure vs Crank angle of Hydrogen at CR 8:1 & 1500 RPM

Figure 4.6 represents the relation between pressures with crank angle for Hydrogen gas at compression ratio of 8:1 and speed of 1500RPM at different equivalence ratios. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at phi 0.65, 0.85 and 1.05 was found to 3600kpa, 4100kpa and 4300kpa respectively (M. M. Noor et al., 2014)

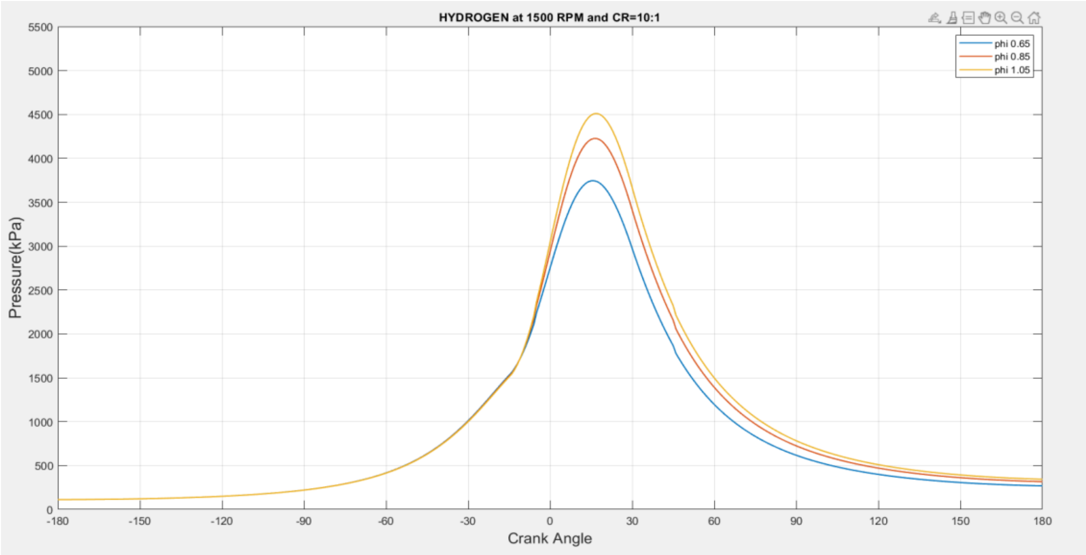

Figure 4.7 Pressure vs Crank angle of Hydrogen at CR 10:1 &1500 RPM

Figure 4.7 represents the relation between pressures with crank angle for Hydrogen gas at compression ratio of 10:1 and speed of 1500RPM at different equivalence ratios. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at phi 0.65, 0.85 and 1.05 was found to 3800kpa, 4350kpa and 4550kpa respectively. It is seen that at higher compression ratio, the pressure inside the chamber also increases keeping rpm and equivalence ratios constant (M. M. Noor et al., 2014).

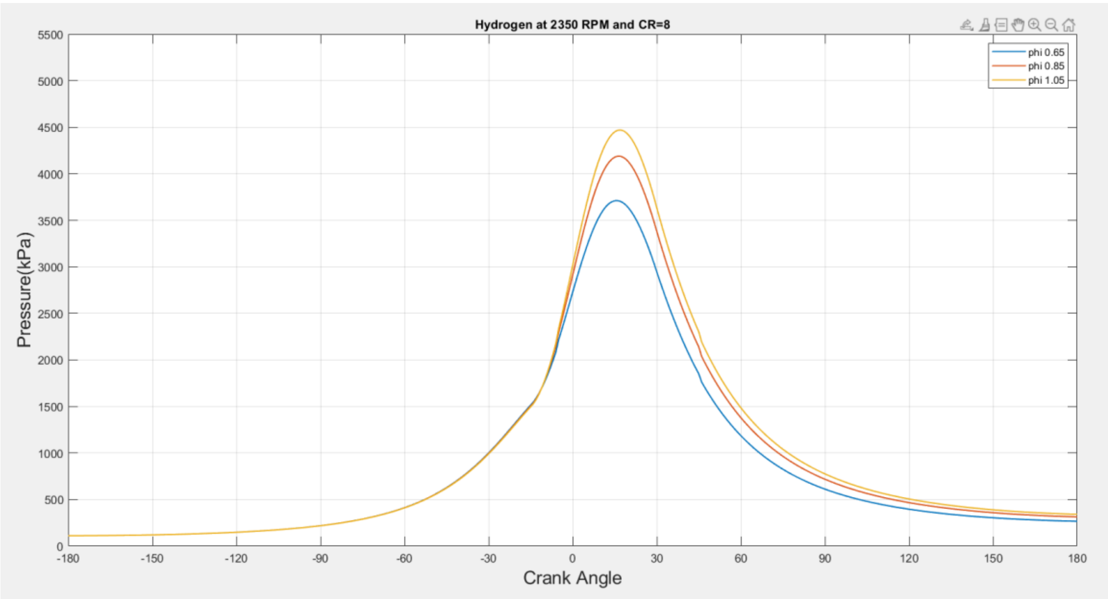

Figure 4.8 Pressure vs Crank angle of Hydrogen at CR 8:1 and 2350 RPM

Figure 4.8 represents the relation between pressures with crank angle for Hydrogen gas at compression ratio of 8:1 and speed of 2350RPM at different equivalence ratios. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at phi 0.65, 0.85 and 1.05 was found to 3800kpa, 4350kpa and 4550kpa respectively. It is seen that at higher compression ratio, the pressure inside the chamber also increases keeping rpm and equivalence ratios constant.

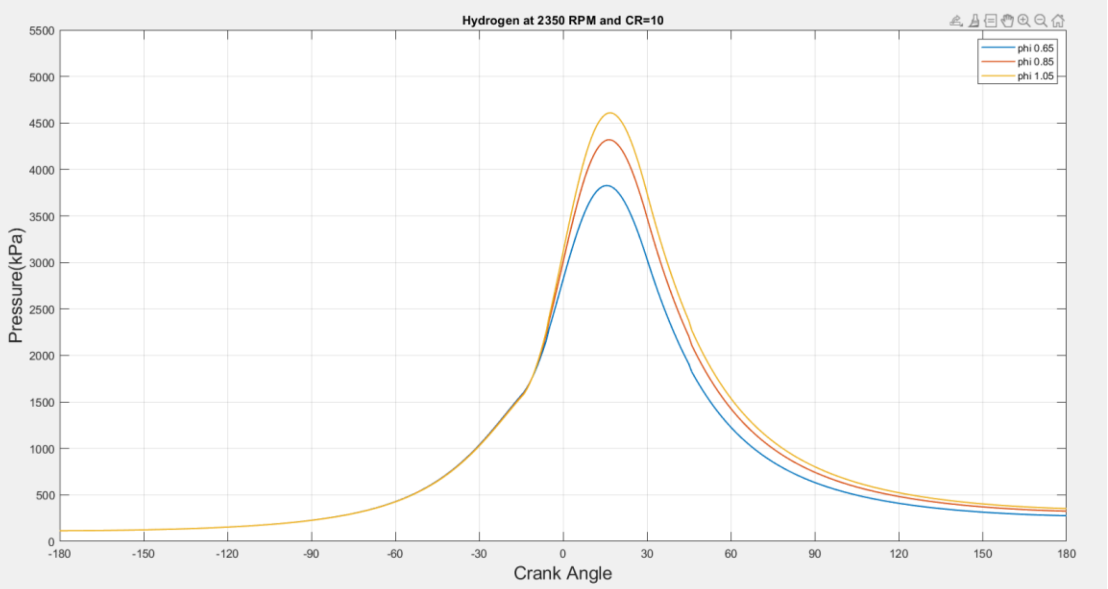

Figure 4.9 Pressure vs crank angle of Hydrogen at CR=10:1 and 2350 RPM

Figure 4.9 represents the relation between pressures with crank angle for Hydrogen gas at compression ratio of 10:1 and speed of 2350RPM at different equivalence ratios. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at phi 0.65, 0.85 and 1.05 was found to 3800kpa, 4450kpa and 4650kpa respectively. It is seen that at higher compression ratio, the pressure inside the chamber also increases keeping rpm and equivalence ratios constant. It can be seen that increasing the compression ratio has more effect on pressure than increasing the rpm.

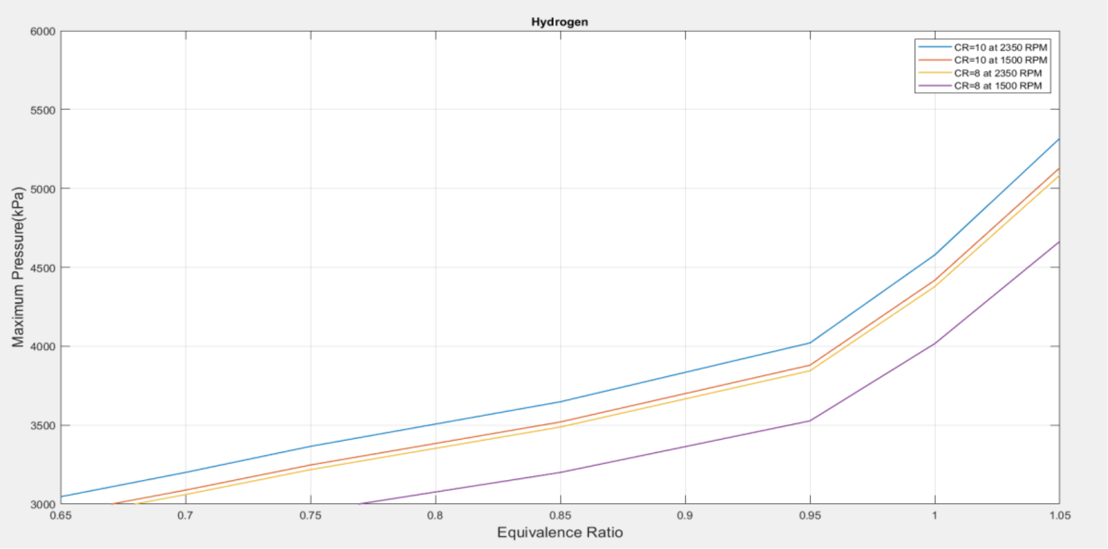

Figure 4.10 Maximum pressure vs equivalence ratio at various CR and RPM

Figure 4.10 represents the relation between maximum pressure with equivalence ratio for Hydrogen gas at various compression ratio of 8:1, 10:1 and speed of 1500RPM, 2350RPM. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at CR 10:1 and speed of 2350RPM was found to be 5400kpa. It is seen that at higher compression ratio and higher RPM, the pressure inside the chamber also increases. The maximum pressure is lower for Hydrogen at CR 8:1 and speed of 1500 rpm. The maximum pressure at this point is 4200kpa. Although, at various compression ratio and different speed, the maximum pressure of Hydrogen at CR 8:1 and 10:1 at 1500rpm and 2350rpm was found to be close i.e. 5200kpa and 5225kpa respectively (Raine et al., 2008).

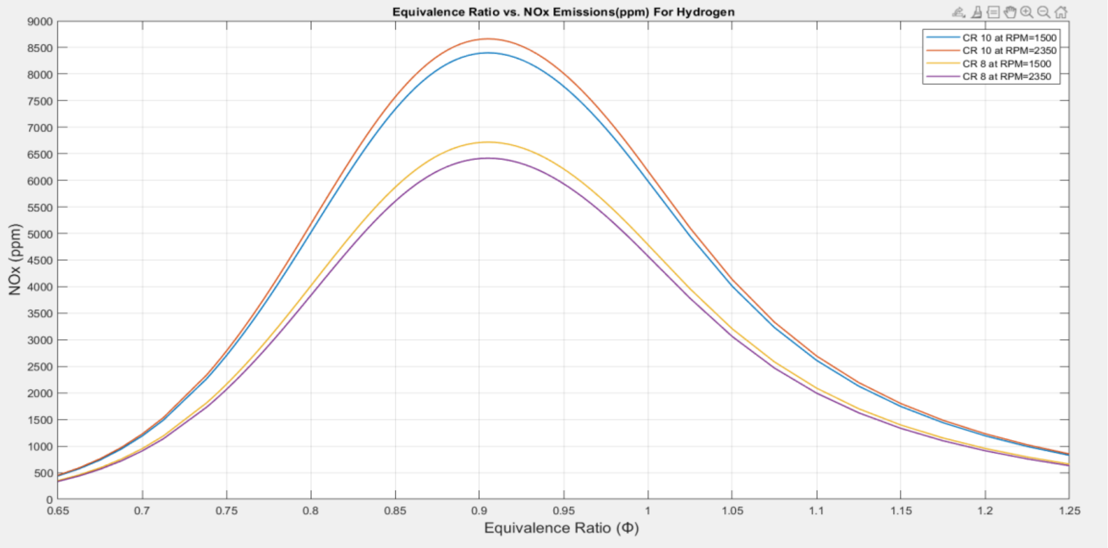

Figure 4.11 Nox Emission vs Equivalence ratio at various CR and RPM

Figure 4.11 represents the relation between Nox emission with equivalence ratio for Hydrogen gas at various compression ratio of 8:1, 10:1 and speed of 1500RPM, 2350RPM. It can be found that at lean mixtures, Nox emission is higher than at rich mixtures. The maximum emission of NOx at CR 10:1 and speed of 2350RPM was found to be 8600ppm. It is seen that at higher compression ratio and higher RPM, NOx emission also increases. NOx emission is lower for Hydrogen at CR 8:1 and speed of 1500 rpm. Maximum emission at this point is 6200ppm. Although, at various compression ratio and different speed, the maximum pressure of Hydrogen at CR 8:1 and 10:1 at 1500rpm and 2350rpm was found to be 6600ppm and 8400ppm respectively (A. Hull et al., 2006)

4.2 Comparison plots for Syngas:

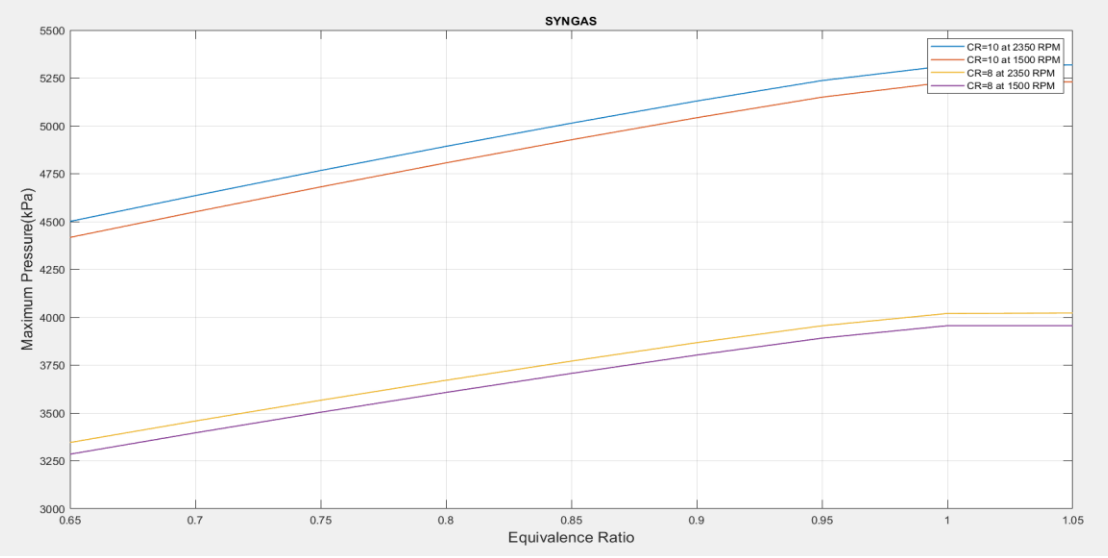

Figure 4.12 Maximum Pressure versus Equivalence Ratio for Syngas at various CR and RPM

The graph represents a relation between Maximum pressure and equivalence ratio for Syngas at different CR & RPM. At an equivalence ratio of 0.65, the pressure is about 4500 KPa for CR 10 & RPM 2350 however 4400 KPa for CR 10 and 1500 RPM. From this, we conclude that the greater the RPM the greater the pressure generated during combustion. As the equivalence ratio increases, maximum pressure also increases. At an equivalence ratio of 0.65, the pressure is about 3450 KPa for CR 8 & RPM 2350 however 3300 KPa for CR 10 and 1500 RPM. From this, we conclude that the greater the CR the greater the pressure generated during combustion (M. M. Noor et al., 2014)

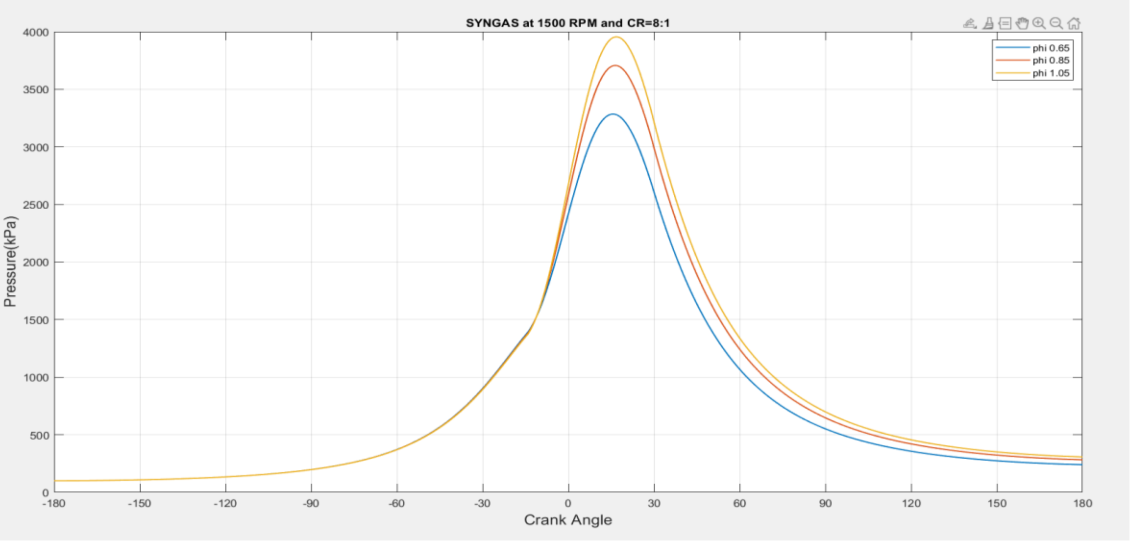

Figure 4.13 Pressure versus crank angle for Syngas at CR 8:1 and 1500 RPM

Figure 4.13 represents the relation between pressures with crank angle for Syngas gas at compression ratio of 8:1 and speed of 1500RPM at different equivalence ratios. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at phi 0.65, 0.85 and 1.05 was found to 3200kpa, 3700kpa and 3950kpa respectively.

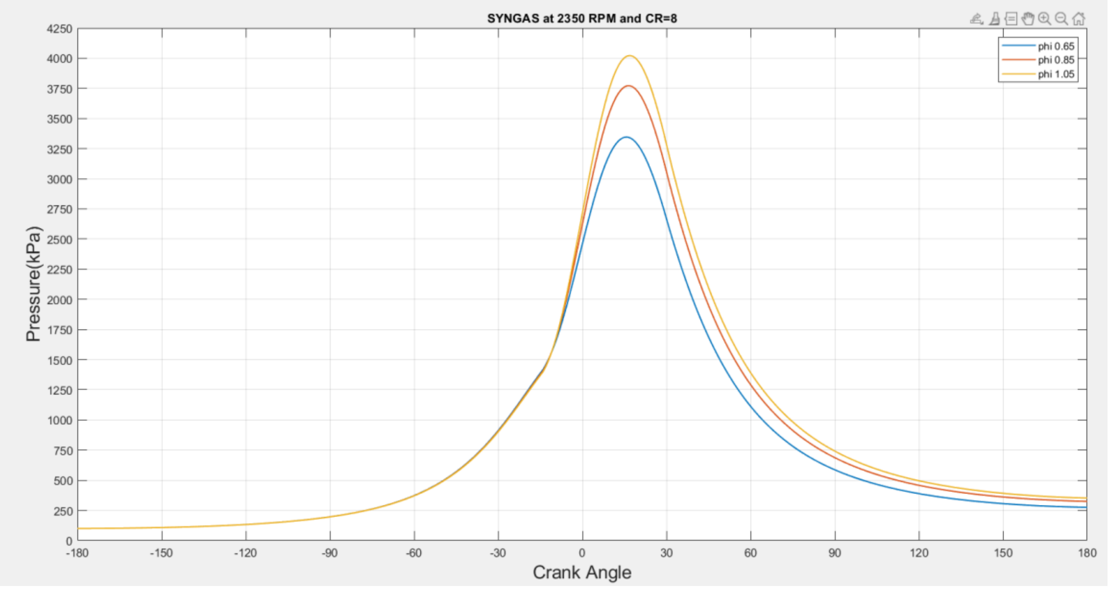

Figure 4.14 Pressure versus crank angle for Syngas at CR 8:1 and 2350 RPM

The graph between Maximum pressure and equivalence ratio for Syngas at CR 8:1& 2350 RPM is shown in the figure 4.14. At an equivalence ratio of 0.65, the pressure is about 3300 KPa for CR 8 & RPM 2350. At an equivalence ratio of 0.85, the pressure is about 3750 KPa for CR 8 & RPM 2350. At an equivalence ratio of 1.05, the pressure is about 4000 KPa for CR 8 & RPM 2350. From this, we conclude that the greater the equivalence ratio, the greater the pressure generated during combustion (M. M. Noor et al., 2014).

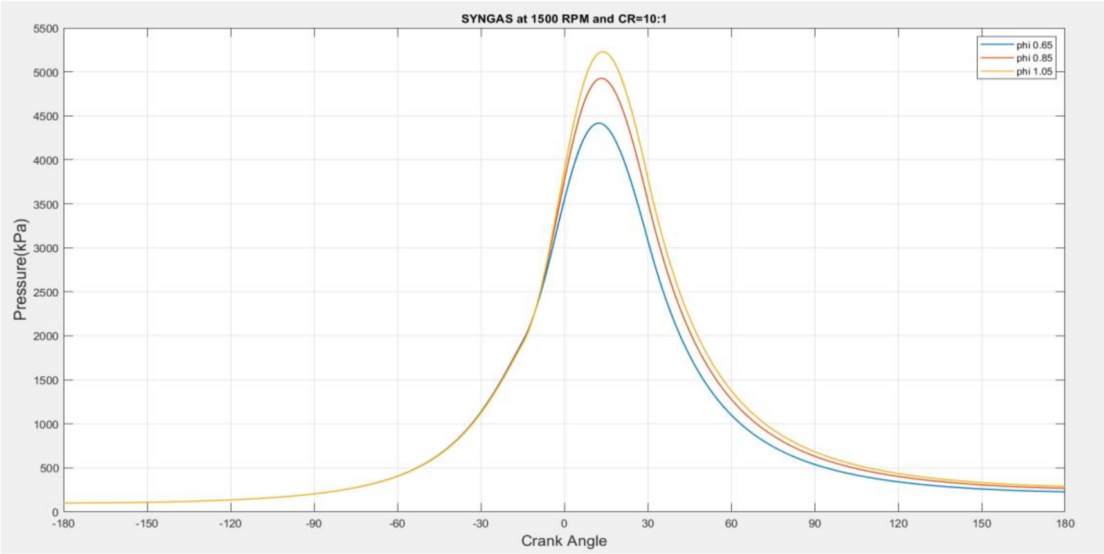

Figure 4.15 Pressure vs Crank angle of Syngas at CR 10:1 AND 1500 RPM

The graph between pressure and equivalence ratio for Syngas at different CR 10:1 & 1500 RPM is shown in the figure 4.15. At an equivalence ratio of 0.65, the pressure is about 4400 KPa. At an equivalence ratio of 0.85, the pressure is about 4750 KPa. At an equivalence ratio of 1.05, the pressure is about 5300 KPa. From this, we conclude that the greater the equivalence ratio, the greater the pressure generated during combustion. Also, increasing the CR, pressure inside the cumustion chamber increases as well (M. M. Noor et al., 2014).

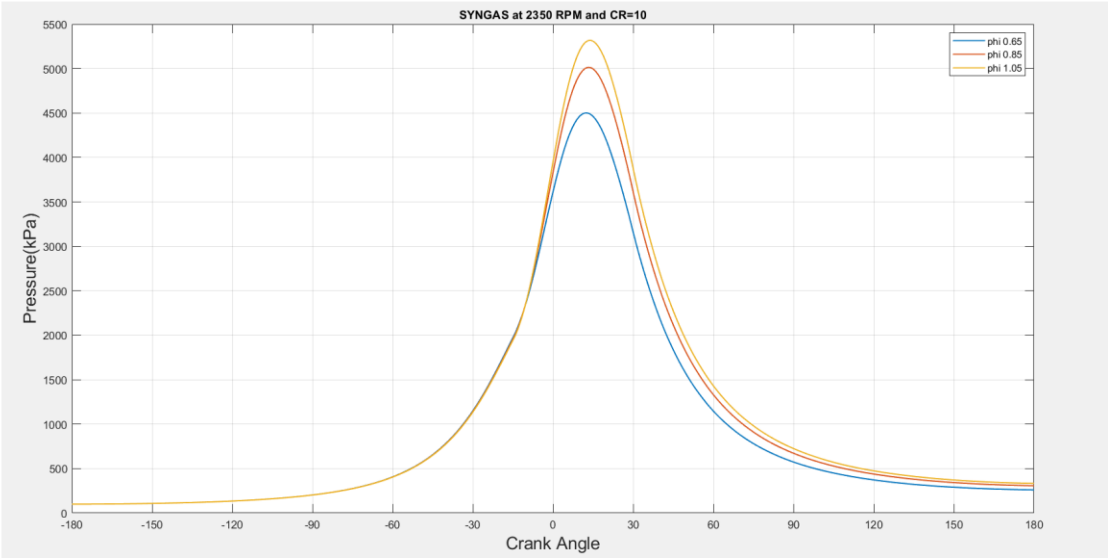

Figure 4.16 Pressure vs Crank angle of Syngas at CR 10:1 and 2350 RPM

Figure 4.16 represents the relation between pressures with crank angle for Syngas gas at compression ratio of 10:1 and speed of 2350RPM at different equivalence ratios. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at phi 0.65, 0.85 and 1.05 was found to 4500kpa, 5000kpa and 5350kpa respectively. It is seen that at higher compression ratio, the pressure inside the chamber also increases keeping rpm constant (M. M. Noor et al., 2014).

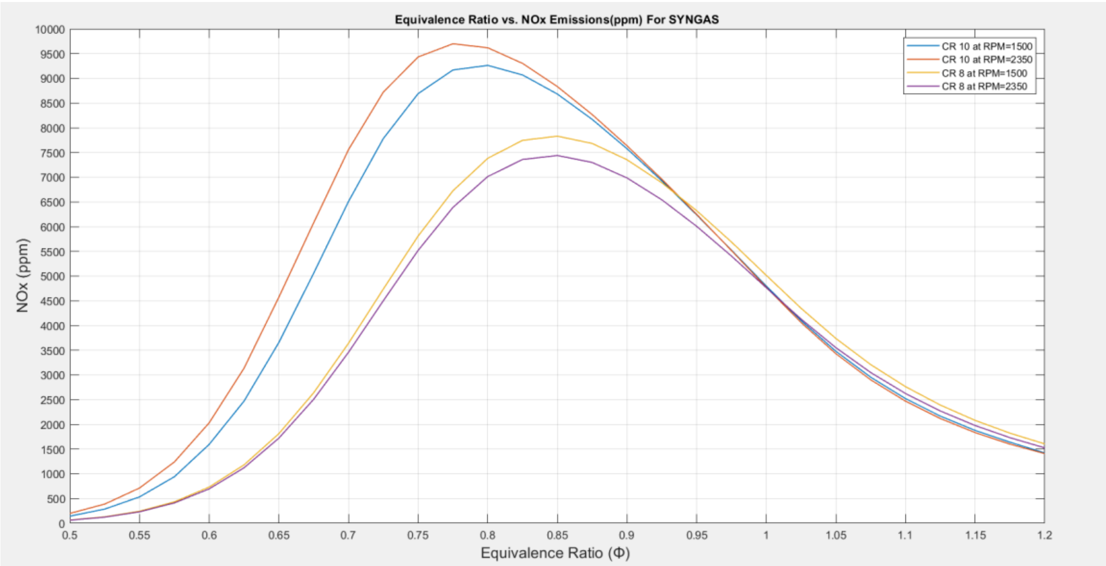

Figure 4.17 Nox vs Equivalence ratio of Syngas at various CR and RPM

Figure 4.17 represents the relation between Nox emission with equivalence ratio for Syngas at various compression ratio of 8:1, 10:1 and speed of 1500RPM, 2350RPM. It can be found that at lean mixtures, Nox emission is higher than at rich mixtures. The maximum emission of NOx at CR 10:1 and speed of 2350RPM was found to be 9600ppm. It is seen that at higher compression ratio and higher RPM, NOx emission also increases. NOx emission is lower for Syngas at CR 8:1 and speed of 1500 rpm. Maximum emission at this point is 7450ppm. Although, at various compression ratio and different speed, the maximum pressure of Hydrogen at CR 8:1 and 10:1 at 1500rpm and 2350rpm was found to be 9200ppm and 7800ppm respectively (A. Hull et al., 2006).

4.3 Comparison plots for Natural gas:

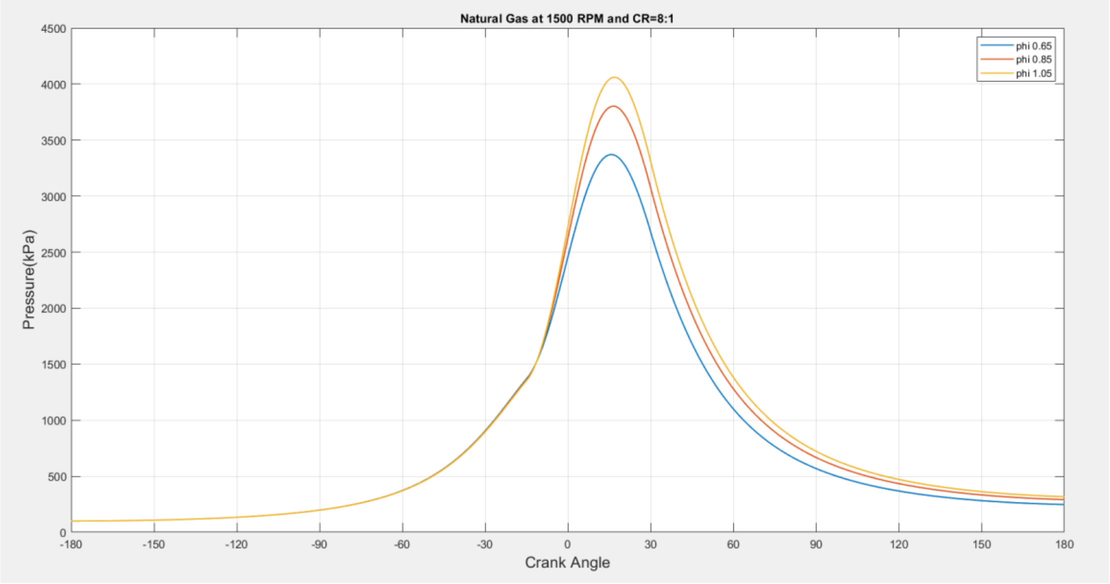

Figure 4.18 Pressure versus Crank Angle of Natural Gas at 1500RPM and CR 8:1 and different equivalence ratio

Figure 4.18 represents the relation between pressures with crank angle for Natural gas at compression ratio of 8:1 and speed of 1500RPM at different equivalence ratios. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at phi 0.65, 0.85 and 1.05 was found to 3300kpa, 3700kpa and 4100kpa respectively.

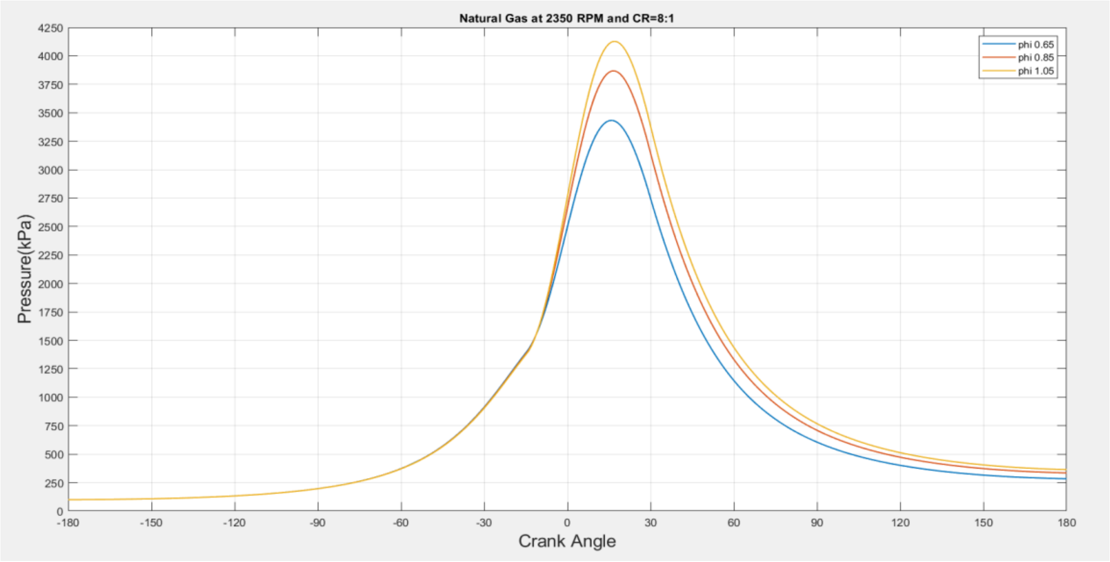

Figure 4.19 Pressure versus Crank Angle of Natural Gas at 2350RPM, CR 8:1 and different equivalence ratio

The graph between Maximum pressure and equivalence ratio for Syngas at CR 8:1& 2350 RPM is shown in the figure 4.19. At an equivalence ratio of 0.65, the pressure is about 3350 KPa for CR 8 & RPM 2350. At an equivalence ratio of 0.85, the pressure is about 3800 KPa for CR 8 & RPM 2350. At an equivalence ratio of 1.05, the pressure is about 4200 KPa for CR 8 & RPM 2350. From this, we conclude that the greater the equivalence ratio, the greater the pressure generated during combustion (M. M. Noor et al.,2014).

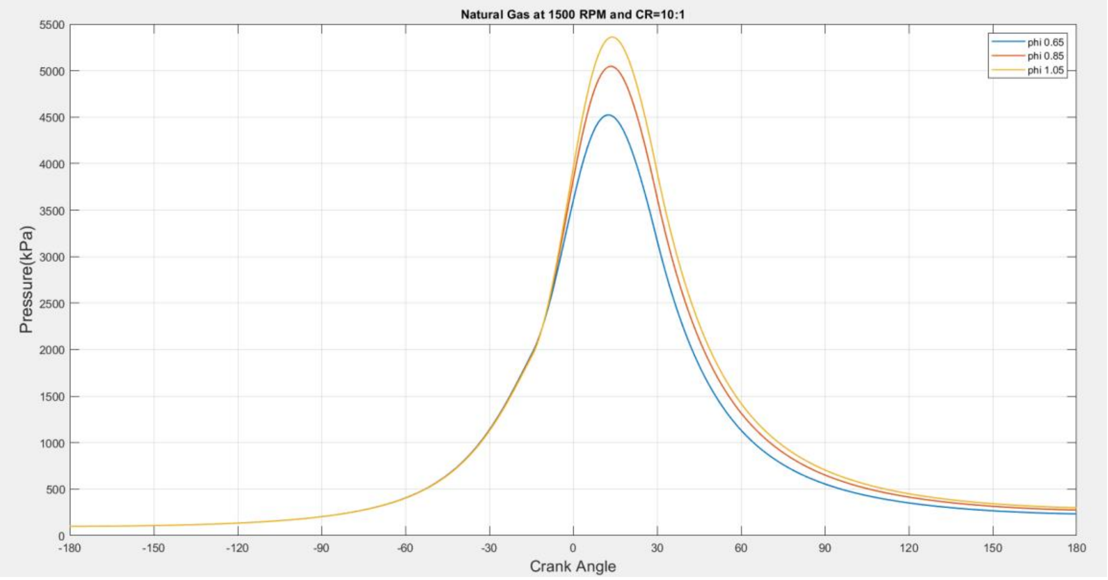

Figure 4.20 Pressure versus Crank Angle of Natural Gas at 1500RPM, CR 10:1 and different equivalence ratio

The graph between pressure and equivalence ratio for Natural gas at CR 10:1 & 1500 RPM is shown in the figure 4.20. At an equivalence ratio of 0.65, the pressure is about 4500 KPa. At an equivalence ratio of 0.85, the pressure is about 5100 KPa. At an equivalence ratio of 1.05, the pressure is about 5400 KPa. From this, we conclude that the greater the equivalence ratio, the greater the pressure generated during combustion. Also, increasing the CR, pressure inside the cumustion chamber increases as well.

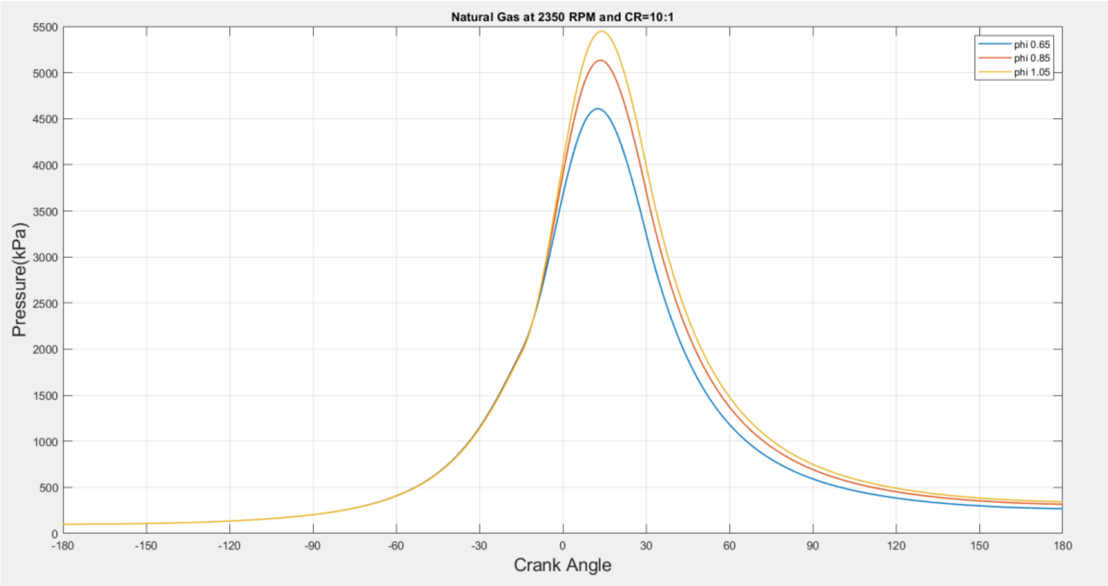

Figure 4.21 Pressure versus Crank Angle of Natural Gas at 2350RPM, CR 10:1 and different equivalence ratio

Figure 4.21 represents the relation between pressures with crank angle for Natural gas at compression ratio of 10:1 and speed of 2350RPM at different equivalence ratios. It can be found that at lean mixtures, the pressure inside the chamber is lower and at rich mixtures, the pressure inside the chamber is higher. The maximum pressure inside the combustion chamber at phi 0.65, 0.85 and 1.05 was found to 4600kpa, 5200kpa and 5450kpa respectively. It is seen that at higher compression ratio, the pressure inside the chamber also increases keeping rpm constant. From these figures, we studied that the pressure gradually increases from the beginning and increases rapidly after the -60° crank angle and reaches the maximum pressure at the 15° crank angle. After 15 ° the pressure decreases. When the equivalence ratio increases the pressure is also increased. The increase in pressure is the same for all equivalence ratios for a beginning. After -15 °, the greater the equivalent ratio, the greater the pressure. From these graphs, we also concluded that the greater the value of RPM & CR, the greater the pressure generated during the combustion (M. M. Noor et al., 2014) (Raine et al., 2008).

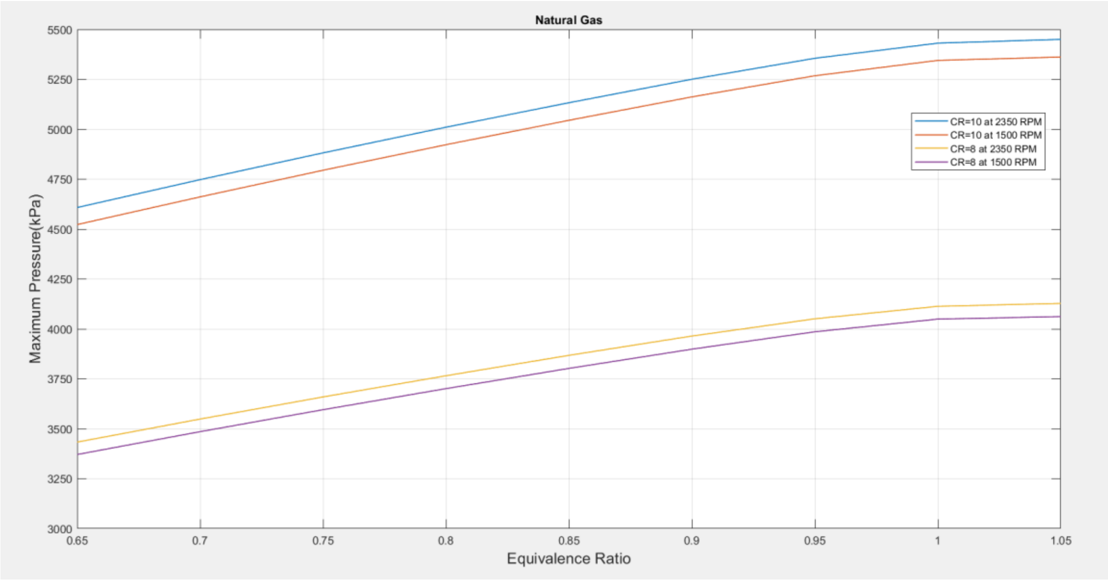

Figure 4.22 Maximum pressure vs Equivalence ratio at various CR and RPM

The graph represents a relation between Maximum pressure and equivalence ratio for Natural gas at different CR & RPM. At an equivalence ratio of 0.65, the pressure is about 4600 KPa for CR 10 & RPM 2350 however 4550 KPa for CR 10 and 1500 RPM. From this, we conclude that the greater the RPM the greater the pressure generated during combustion. As the equivalence ratio increases, maximum pressure also increases. At an equivalence ratio of 0.65, the pressure is about 3475 KPa for CR 8 & RPM 2350 however 3350 KPa for CR 10 and 1500 RPM. From this, we conclude that the greater the CR the greater the pressure generated during combustion.

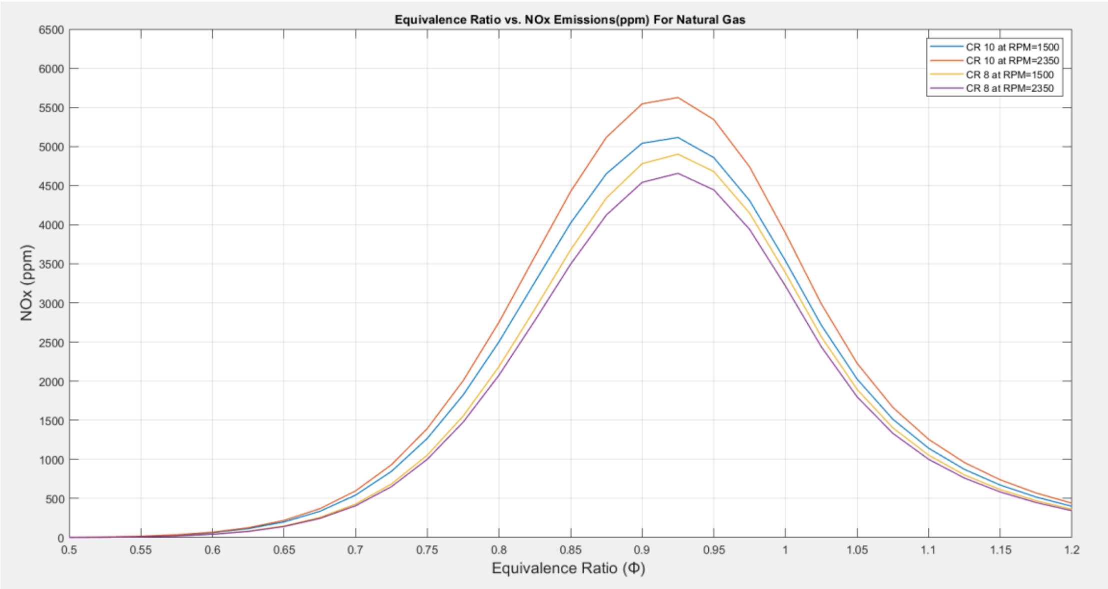

Figure 4.23 Nox Emission vs Equivalence ratio at various CR and RPM

Figure 4.23 represents the relation between Nox emission with equivalence ratio for Natural gas at various compression ratio of 8:1, 10:1 and speed of 1500RPM, 2350RPM. It can be found that at lean mixtures, Nox emission is higher than at rich mixtures. The maximum emission of NOx at CR 10:1 and speed of 2350RPM was found to be 5600ppm. It is seen that at higher compression ratio and higher RPM, NOx emission also increases. NOx emission is lower for Natural gas at CR 8:1 and speed of 1500 rpm. Maximum emission at this point is 4600ppm. Although, at various compression ratio and different speed, the maximum pressure of Hydrogen at CR 8:1 and 10:1 at 1500rpm and 2350rpm was found to be 4800ppm and 5100ppm respectively (A. Hull et al., 2006).

4.4 Comparison plots of various gases with respect to Gasoline:

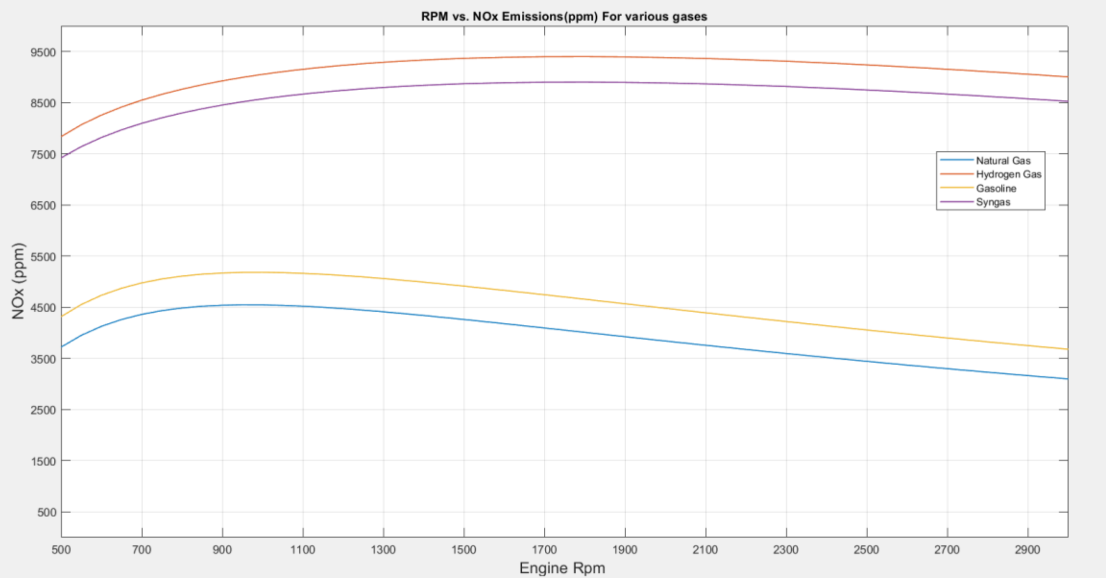

Figure 4.24 Nox vs Engine RPM of various gases at CR 8:1

The above graph represents the relation between NOx emissions in ppm with engine rpm of Natural gas, hydrogen gas, Gasoline and Syngas at CR 8:1 and Equivalence ratio of 0.8. It is found that NOx emission is high for Hydrogen and it is least for Natural gas. Hydrogen and Syngas has the most Nox emission at 1500 to 1700rpm. Gasoline and Syngas has the least NOx emission from 1300 to 3000rpm 4800 and 4500 respectively. The peak emission for Hydrogen gas occurs at 1700rpm and its value is about 9500ppm. Similarly, for Syngas the peak emission occurs at 1700rpm and its value is about 8500ppm. From this, we conclude that Hydrogen and Syngas shows similar properties for NOx emission from 500 rpm to 3000rpm. Hydrogen has more NoX emission than Syngas, Gasoline and Natural gas. NOx emission is however constant from 1700 to 3000 rpm for Hydrogen and Syngas while NOx emission is gradually decreasing from 1700 to 3000rpm in case of Gasoline and Natural gas (M. M. Noor et al., 2014).

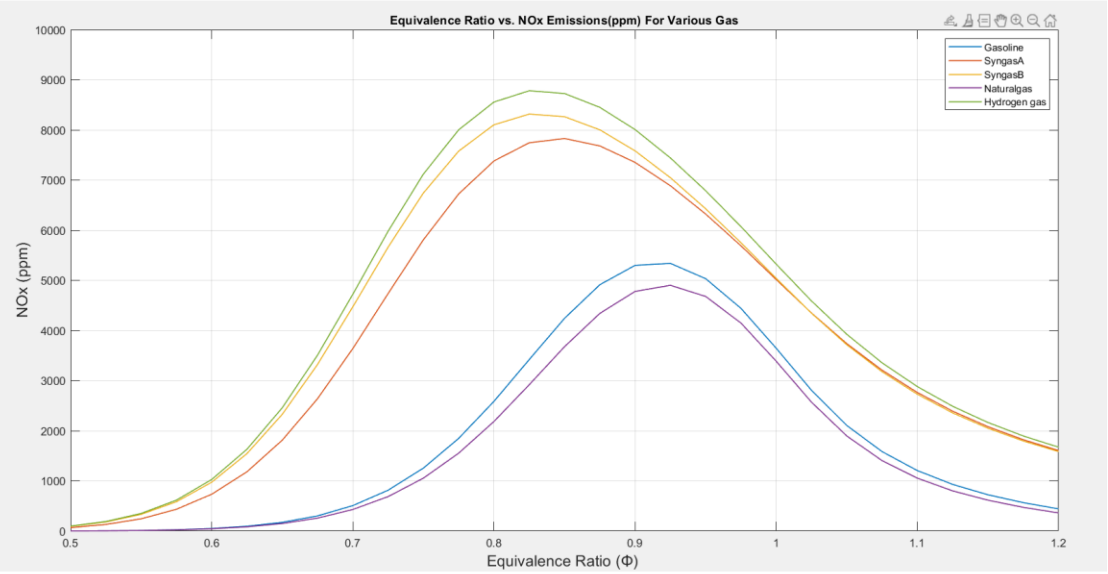

Figure 4.25 Nox Emission vs Equivalence ratio of various gases at CR 8:1

Figure 4.25 represents the relation between NOx emission with equivalence ratio for Hydrogen, Syngas, Natural gas and gasoline at compression ratio of 8:1 and speed of 1500RPM. It can be found that at lean mixtures, NOx emission is higher at lean mixtures than at rich mixtures for all gases. However, it can be seen that gasoline and natural gas has maximum NOx emission from equivalence ratio of 0.8 to 1 i.e. 5100ppm and 4900ppm respectively, while Syngas and Hydrogen gas has maximum NOx emission from equivalence ratio form 0.6 to 0.9 i.e. 8100ppm and 8900ppm respectively. It can be seen that for gasoline and natural gas, Maximum NOx emission takes place during lean mixture. For Hydrogen and Syngas, NOx emission takes place during leaner mixture than Gasoline and Natural gas (A. Hull et al., 2006).

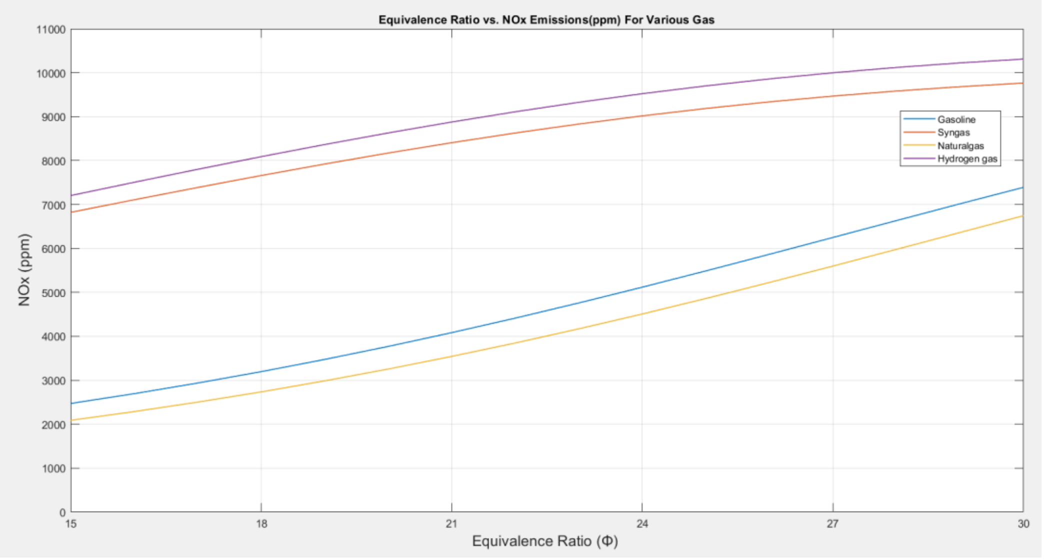

Figure 4.26 Nox vs Equivalence ratio of various gases at CR 8:1

Figure 4.26 represents the relation between NOx emission with equivalence ratio for Hydrogen, Syngas, Natural gas and gasoline at compression ratio of 8:1 and speed of 1500RPM. It can be found that at various mixtures, NOx emission is higher at rich mixtures than at lean mixtures for all gases. However, it can be seen that gasoline and natural gas has maximum NOx emission from equivalence ratio of 30 i.e. 7300ppm and 6800ppm respectively, while Syngas and Hydrogen gas has maximum NOx emission from equivalence ratio form 15 to 30 i.e. 9900ppm and 10200ppm respectively. For Hydrogen, Syngas, Natural gas and Gasoline maximum NOx emission takes place during rich mixture (A. Hull et al., 2006).

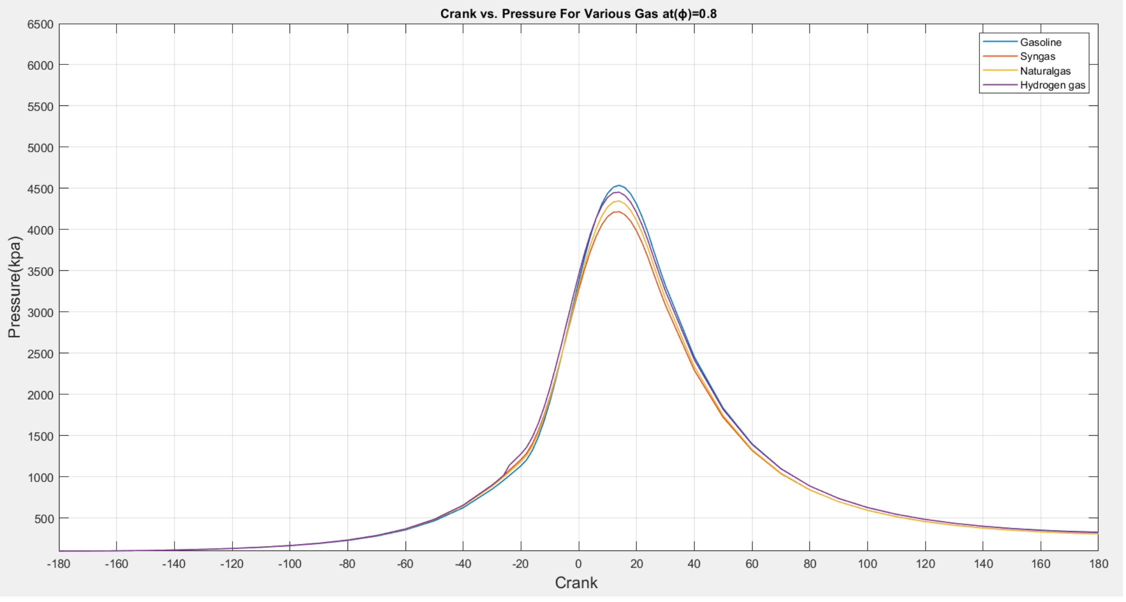

Figure 4.27 Pressure vs Crank angle of various gases at phi=0.8

Figure 4.27 shows cylinder peak pressure for gasoline, syngas, natural gas and Hydrogen at compression ratio 8:1, spark timing 20° BTDC, 1500 rpm and at equivalence ratio 0.8 with respect to crank angle. The peak cylinder pressure for Gasoline is found to be 4500 kpa, while for syngas it is found to be 4200 kpa and for natural gas it is found to be 4300 kpa. The cylinder pressure for Hydrogen is found to be 4400kpa.The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas. This is because of highercalorific value of the gasoline and almost all the component of the fuel are regarded as combustible which produces much heat and as a result pressure increases. Natural gas has higher peak pressure than that of syngas since it has higher calorific value than syngasand contains higher quantity of burning fuel while syngas contains higher concentration of non-combustible gases in the fuel and it has lower calorific value (Raine et al., 2008) (A. Hull et al., 2006)

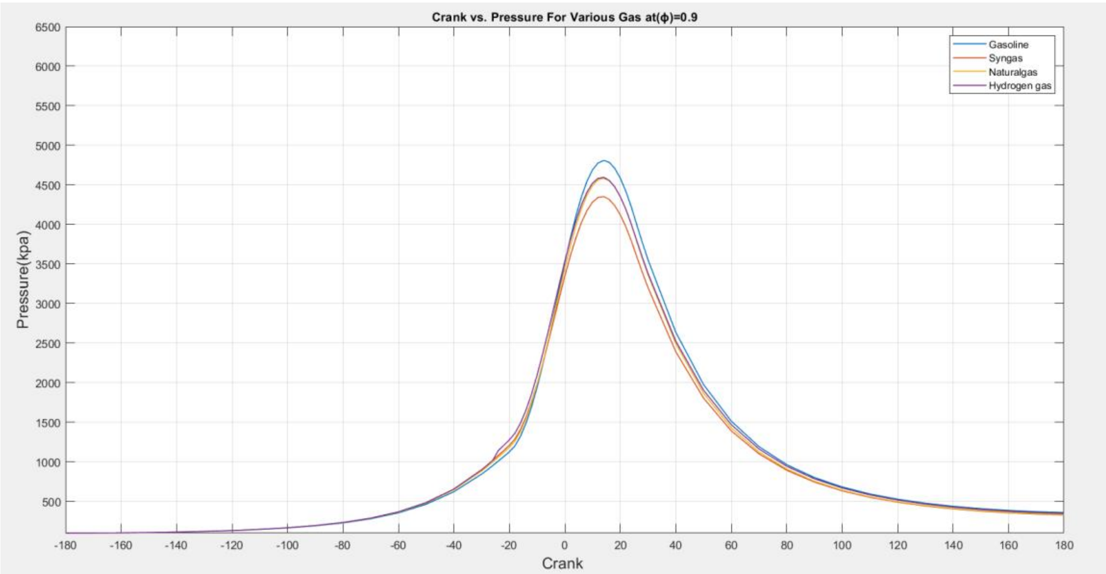

Figure 4.28 Pressure vs Crank angle of various gases at phi=0.9

Figure 4.28 shows cylinder peak pressure for gasoline, syngas, natural gas and Hydrogen at compression ratio 8:1, spark timing 20° BTDC, 1500 rpm and at equivalence ratio 0.9 with respect to crank angle. The peak cylinder pressure for Gasoline and Hydrogen is found to be 4800 kpa and 4600 respectively, while for syngas it is found to be 4200 kpa and for natural gas it is found to be 4600 kpa. The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas.

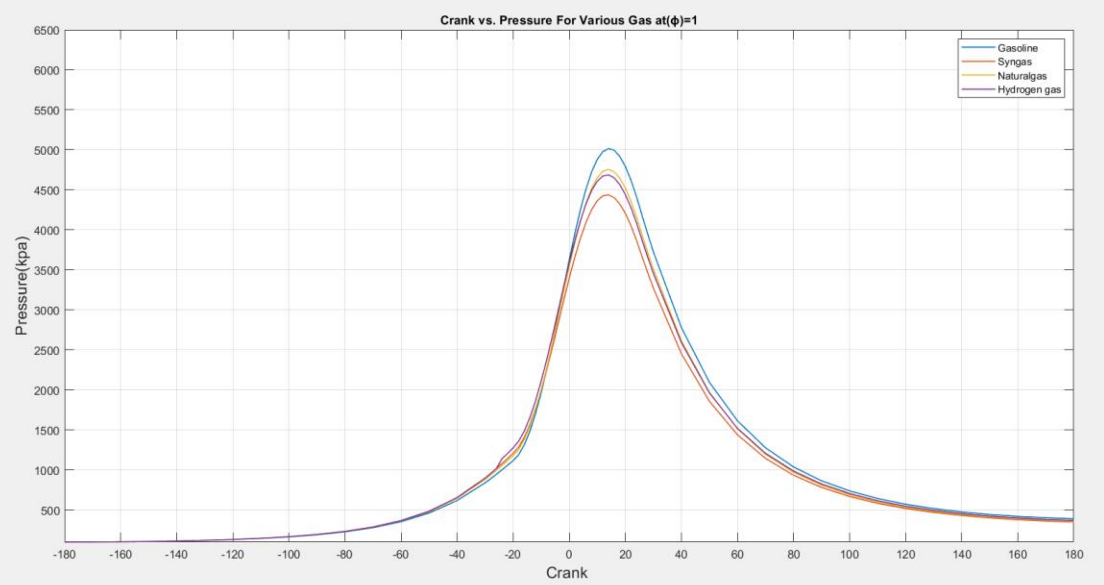

Figure 4.29 Pressure vs Crank angle of various gases at phi=1

Figure 4.29 shows cylinder peak pressure for gasoline, syngas, natural gas and Hydrogen at compression ratio 8:1, spark timing 20° BTDC, 1500 rpm and at equivalence ratio 1 with respect to crankangle. The peak cylinder pressure for Gasoline and Hydrogen is found to be 4800kpa and 4600kpa respectively, while for syngas it is found to be 4400kpa and for natural gas it is found to be 4700kpa. The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas (A. Hull et al., 2006).

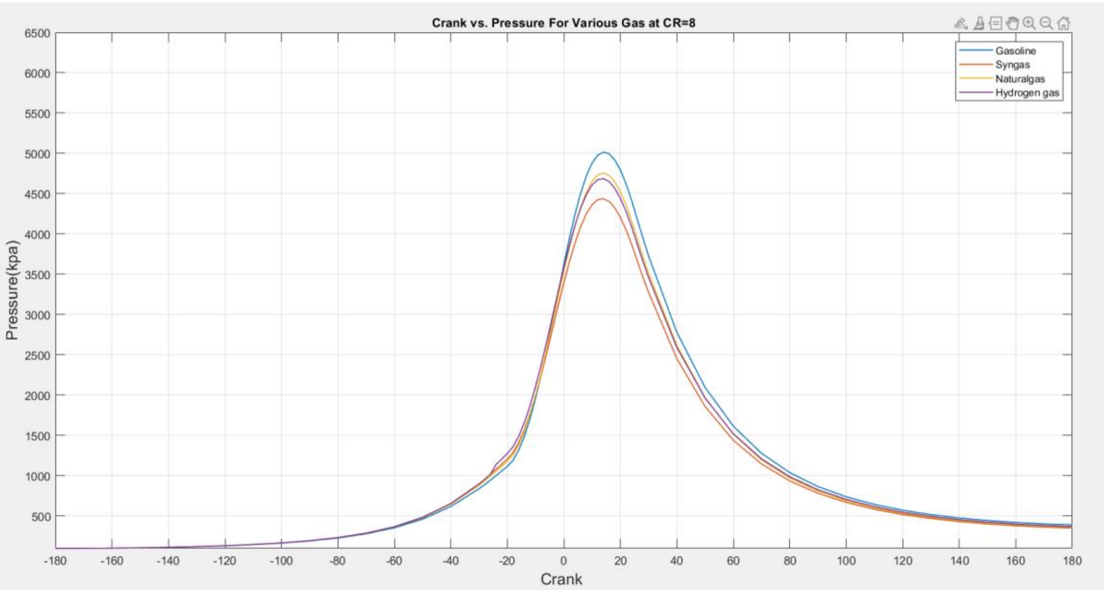

Figure 4.30 Pressure vs Crank angle of various gases at CR=8:1

Figure 4.30 shows cylinder peak pressure for gasoline, syngas, natural gas and

Hydrogen at compression ratio 8:1, spark timing 20° BTDC, 1500 rpm and at equivalence ratio 1 with respect to crankangle. The peak cylinder pressure for Gasoline and Hydrogen is found to be 5000kpa and 4600kpa respectively, while for syngas it is found to be 4400kpa and for natural gas it is found to be 4700kpa. The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas.

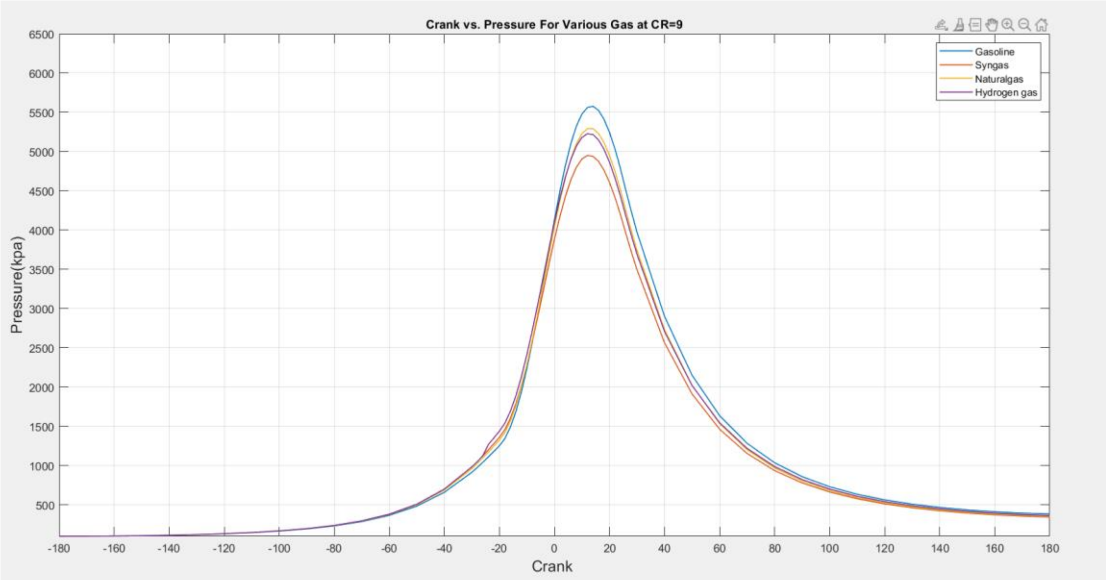

Figure 4.31 Pressure vs Crank angle of various gases at CR=9:1

Figure 4.31 shows cylinder peak pressure for gasoline, syngas, natural gas and Hydrogen at compression ratio 8:1, spark timing 20° BTDC, 1500 rpm and at equivalence ratio 1 with respect to crankangle. The peak cylinder pressure for Gasoline and Hydrogen is found to be 5600kpa and 5200kpa respectively, while for syngas it is found to be 4800kpa and for natural gas it is found to be 5300kpa. The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas (A. Hull et al., 2006).

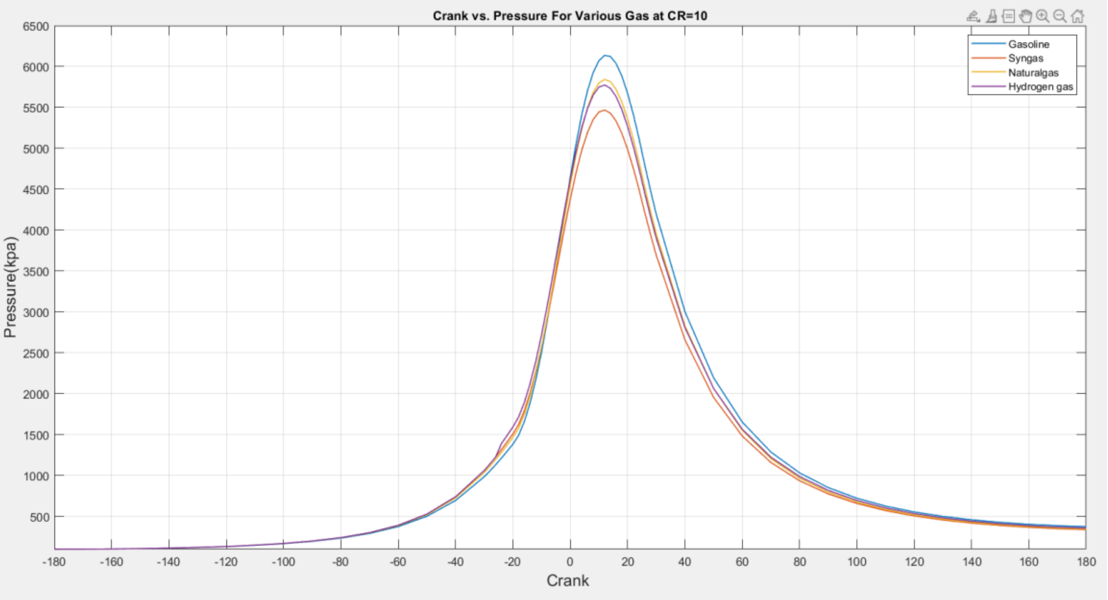

Figure 4.32 Pressure vs Crank angle of various gases at CR= 10:1

Figure 4.32 shows cylinder peak pressure for gasoline, syngas, natural gas and Hydrogen at compression ratio 10:1, spark timing 20° BTDC, 1500 rpm and at equivalence ratio 1 with respect to crankangle. The peak cylinder pressure for Gasoline and Hydrogen is found to be 6200kpa and 5700kpa respectively, while for syngas it is found to be 5800kpa and for natural gas it is found to be 5600kpa. The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas (A. Hull et al., 2006).

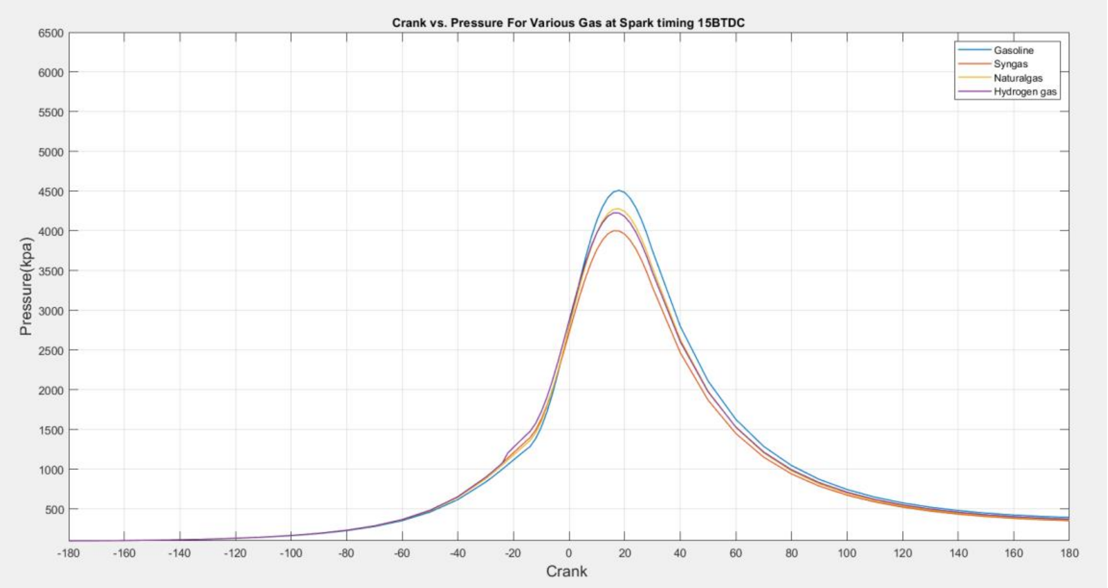

Figure 4.33 Pressure vs Crank angle for various gas at Spark timing 15BTDC

Figure 4.33 shows cylinder peak pressure for gasoline, syngas, natural gas and Hydrogen at compression ratio 8:1, spark timing 15° BTDC, 1500 rpm and at equivalence ratio 1 with respect to crankangle. The peak cylinder pressure for Gasoline and Hydrogen is found to be 4500kpa and 4200kpa respectively, while for syngas, it is found to be 4000kpa and for natural gas it is found to be 4300kpa. The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas. Decreasing the spark timing angle from 20 degree to 15 degree reduces the cylinder peak pressure.

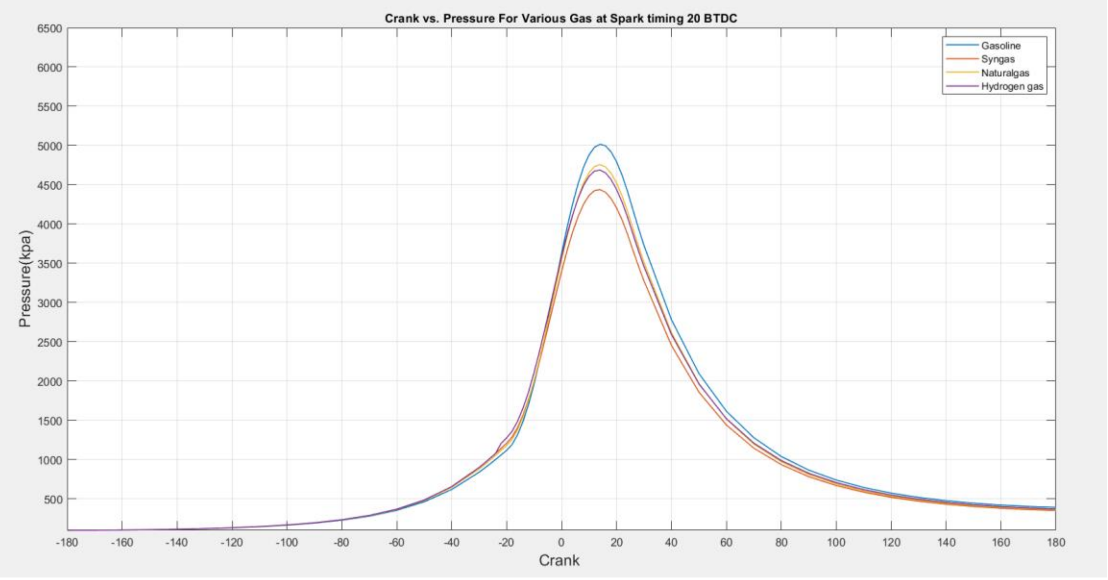

Figure 4.34 Pressure vs Crank angle for various gas at Spark timing 20BTDC

Figure 4.34 shows cylinder peak pressure for gasoline, syngas, natural gas and Hydrogen at compression ratio 8:1, spark timing 20° BTDC, 1500 rpm and at equivalence ratio 1 with respect to crankangle. The peak cylinder pressure for Gasoline and Hydrogen is found to be 5000kpa and 4700kpa respectively, while for syngas, it is found to be 4400kpa and for natural gas it is found to be 4750kpa. The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas. Increasing the spark timing angle from 15 degree to 20 degree increases the cylinder peak pressure.

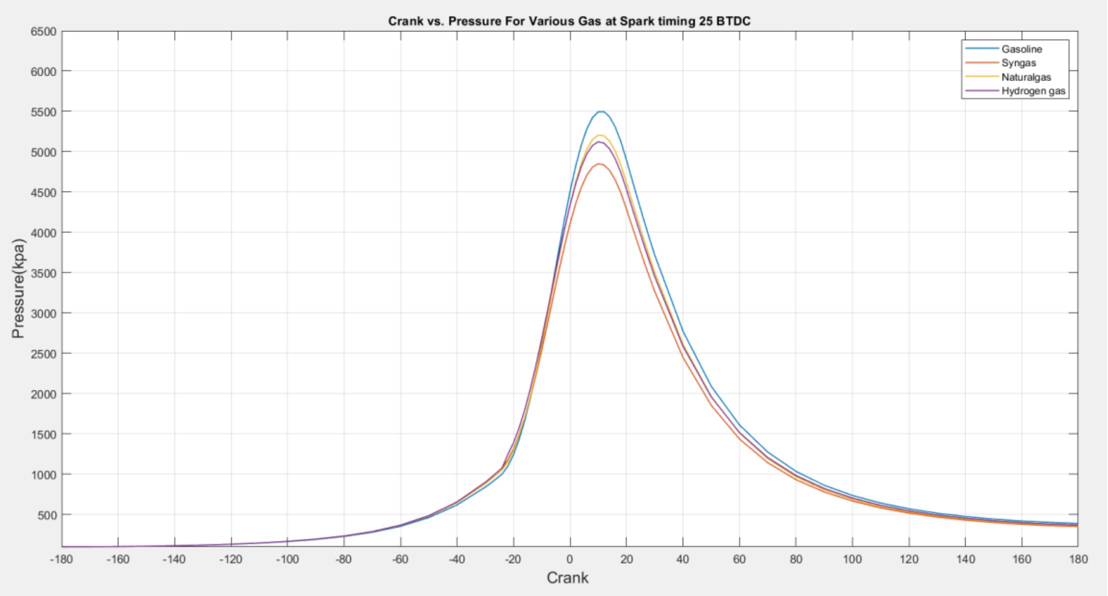

Figure 4.35 Pressure vs Crank angle for various gases at Spark timing 25BTDC

Figure 4.35 shows cylinder peak pressure for gasoline, syngas, natural gas and Hydrogen at compression ratio 8:1, spark timing 25° BTDC, 1500 rpm and at equivalence ratio 1 with respect to crankangle. The peak cylinder pressure for Gasoline and Hydrogen is found to be 5500kpa and 5200kpa respectively, while for syngas, it is found to be 4800kpa and for natural gas it is found to be 5250kpa. The cylinder peak pressure occurs at 18-20 degree before top dead center for all fuel but the peak pressure of gasoline is higher in comparison than that of natural gas, syngas and Hydrogen gas. Increasing the spark timing angle from 20 degree to 25 degree increases the cylinder peak pressure.

CHAPTER 5 CONCLUSION AND RECOMMENDATIONS

5.1 Conclusions:

The research for the final is "Study of Combustion of Various Gaseous Fuels in SparkIgnition Engine". A certain composition of syngas fuel and natural gas were taken for which a simulation was done varying different parameters as spark timing, compression ratio and equivalence ratios. The results were then plotted and compared with gasoline. The major findings of the thesis are summarized below:

- Syngas has low specific heat capacity so it needs less heat energy than natural gas and gasoline fuel to ignite. And natural gas requires less heat energy than gasoline to ignite.
- Hydrogen is highly flammable and requires least heat energy to ignite. With increase of hydrogen composition, the fuel will be more flammable.
- For same input data Gasoline has higher peak pressure than Hydrogen, natural gas and syngas,and syngas has lower peak pressure than Hydrogen, gasoline and natural gas.
- Higher calorific value and higher concentration of combustible gases helps to increase peak pressure more. So, gasoline has higher peak pressure than Hydrogen, syngas andnatural gas with same input.
- Peak pressure of Hydrogen, gasoline, natural gas and syngas keeps on increasing with increase of compression ratio, equivalence ratio (ϕ) and advanced spark timing.
- Hydrogen and Syngas can be run in both lean and rich condition which helps to reduce fuel consumption which is not possible for gasoline and natural since gasoline and natural gas can run only at stoichiometric air-fuel ratio.
- With increase of engine speed, NOx emission at first increase and later it decreases. NOx emission is found to be higher at lean operating point ($\phi<1$) than at rich operating point ($\phi>1$) since at lean operating point there is enough availability of oxygen.
- With increase of spark advanced and compression ratio the temperature of unburned gas rises high, this might lead to knock. So, spark timing shouldn't be too early and compression ratio shouldn't be too high.

5.2 Recommendation

Future works could include the following for attainment of more information about thesefuels:

- Experimental analysis of fuels should be compared with MATLAB simulation.
- Further analysis on brake power, brake torque might be helpful for obtaining more insights on fuels.
- Analysis on the varying composition of Hydrogen, syngas and natural gas might provide a better result which can be utilized as an alternative fuel for a spark ignition engine.
- Further studies on various spark engine simulation software might be helpful for obtaining error minimized outputs.

REFRENCES

A. Cernat, C. Pana, N. Negurescu, G. Lazaroiu, C. Nutu, and D. Fuiorescu. 2020. Hydrogen—an alternative fuel for automotive diesel engines used in transportation. *Sustain*. 12(22), pp.1–21.

A. Hull, I. Golubkov, B. Kronberg, T. Marandzheva, and J. Van Stam. 2006. An alternative fuel for spark ignition engines. *Int. J. Engine Res*. 7(3), pp.203-214.

Boroomand, B. Yadollahi and M. 2013. The effect of combustion chamber geometry on injection and mixture preparation in a CNG direct injection SI engine. *Fuel*. 45(3), pp.52-62.

C. Ji et. 2012. Improving the performance of a spark-ignited gasoline engine with the addition of syngas produced by onboard ethanol steaming reforming. I*nt. J. Hydrogen Energy*. 37(9), pp.7860-7868.

Ferguson, Colin R., and Allan T. Kirkpatrick. 2015. Internal combustion engines: applied thermosciences. *John Wiley & Sons.*

Ferguson, Colin R., and Allan T. Kirkpatrick. 2015. nternal combustion engines : applied thermosciences. *John Wiley & Sons.*

Grab-rogalinski, S. Szwaja and K. 2009. Hydrogen combustion in a compression ignition diesel engine. *Int. J. Hydrogen Energy.* 34(10), pp.4413–4421.

J. Ma, Y. Su, Y. Zhou, and Z. Zhang. 2003. Simulation and prediction on the performance of a vehicle's hydrogen engine. *Int. J. Hydrogen Energy*. 28(1), pp.77–83.

K. Shivaprasad, R. Rajesh, W. Anteneh Wogasso, B. Nigatu, and F. Addisu. 2018. Usage of Hydrogen as a Fuel in Spark Ignition Engine. *IOP Conference Series: Materials Science and Engineering.*

K. V. Shivaprasad, R. Rajesh, W. Anteneh Wogasso, B. Nigatu, and F. Addisu. 2018. Usage of Hydrogen as a Fuel in Spark Ignition Engine. *IOP Conference Series: Materials Science and Engineering.*

M. M. Noor, A. P. Wandel, and T. Yusaf. 2014. Air fuel ratio study for mixture of biogas and hydrogen on mild combustion. *Int. J. Automot. Mech. Eng*. 10(1), pp.2144-2154.

M. M. Tahir et. 2015. Performance Analysis of A Spark Ignition Engine Using Compressed Natural Gas (CNG) as Fuel. *Energy Procedia.* 68(2), pp.355-362.

M. Muñoz, F. Moreno, J. Morea-Roy, J. Ruiz, and J. Arauzo. 2000. Low heating value gas on spark ignition engines. *Biomass and Bioenergy.* 18(5), pp.431-439.

Raine, N. N. Mustafi and R. R. 2008. Application of a spark ignition engine simulation tool for alternative fuels. *Gas Turbines Power.* 130(1), pp.1-6.

Sandeep, K. J. 2021. Use of Hydrogen in IC Engines Study on Performance. *Emission and Fuel Injection System*. 10(3), pp.1014-1023.

Shamekhi A., Khatib zadeh N. 2022. A Comprehensive Comparative Investigation Of Compressed Natural Gas As An Alternative Fuel In A Bi-Fuel Spark Ignition Engine. 2(3), pp.1-4.

T. Iskandar Mohamad, H. Heoy Geok, S. Abdullah, Y. Ali, A. Shamsudeen, and E. Adril. 2009. Experimental Investigation of Performance and Emission of a Sequential Port Injection Natural Gas Engine Cite this paper Experimental Investigation of Performance nd Emission of a Sequential Port Injection Natural Gas Engine. 1(2), pp.4-12.

Thring, R. H. 1983. Alternative Fuels for Spark-Ignition Engines.

Thring, R. H. 1983. Alternative Fuels for Spark-Ignition Engines. SAE J. Automot. Eng. 91(12), pp.30-33.

V. Jithin, G. K. S. Raghuram, T. V. Keshavamurthy, R. K. Velamati, C. Prathap, and R. J. Varghese. 2021. A review on fundamental combustion characteristics of syngas mixtures and feasibility in combustion devices. *Renewable and Sustainable Energy Reviews*. 146.

V. Kumar, D. Gupta, and N. Kumar. 2015. Hydrogen Use in Internal Combustion Engine: a Review. *Int. J. Adv. Cult. Technoly.* 3(2), pp.87-99.

Wallner, S. Verhelst and T. 2009. Hydrogen-fueled internal combustion engines. *Progress in energy and combustion science*. 35(6), pp.490-527.

Walter, L. 2001. Hydrogen Use in Internal Combustion Engines. *Hydrogen Fuel Cell* , pp.1-23.

Wojtyniak, A. Kowalewicz and M. 2005. Alternative fuels and their application to combustion engines. 219(1), pp.103-125.

APPENDIX A: Computed Data

Table A.1 Low-Temperature (T<1000 K) Combustion Products

Species	$\boldsymbol{n_i}$	$\boldsymbol{\phi \leq 1}$	$\boldsymbol{\phi > 1}$
CO_2	n_1	a	$a - n_5$
H_2O	n_2	$\frac{b}{2}$	$\frac{b}{2} - d_1 + n_5$
N_2	n_3	$\frac{d}{2} + \frac{3.76\, a_s}{\phi}$	$\frac{d}{2} + \frac{3.76\, a_s}{\phi}$
O_2	n_4	$a_s(\frac{1}{\phi} - 1)$	$\frac{d}{2} + \frac{3.76\, a_s}{\phi}$
CO	n_5	0	$\frac{d}{2} + \frac{3.76\, a_s}{\phi}$
H_2	n_6	0	$d_1 - n_5$

where,

$$\boldsymbol{a_s} = \mathrm{a} + \frac{b}{4} - \frac{c}{2}$$

$$\boldsymbol{d_1} = 2a_s(1 - \frac{1}{\phi})$$

$$\mathbf{t} = \frac{T}{1000}$$

$$\ln \boldsymbol{K} = 2.743 - \frac{1.761}{t} - \frac{1.611}{t^2} + \frac{0.2803}{t^3}$$

$$\boldsymbol{a_1} = 1 - \mathrm{K}$$

$$\boldsymbol{b_1} = \frac{b}{2} + aK - d_1(1 - \mathrm{K})$$

$$\boldsymbol{c_1} = -\mathrm{a}d_1K$$

$$\boldsymbol{n_5} = \frac{(-b_1 + \sqrt{{b_1}^2 - 4\boldsymbol{a_1 c_1}})}{2\boldsymbol{a_1}}$$

Table A.2 Mole fractions of fuel-air-residual mixture

Mole Fractions of	**Pure gasoline**	**Natural gas**	**Pure hydrogen**	**Syngas**
y_{CO2}	0.0051	0.0051	0.0051	0.0035
y_{H2O}	0.0062	0.0063	0.0051	0.0083
y_{N2}	0.7764	0.7753	0.7121	0.7141
y_{O2}	0.1982	0.1979	0.1818	0.1823
y_{CO}	0	0	0	0
y_{H2}	0	0	0	0

Table A.3 Equilibrium Mole Fractions

Mole Fractions of	**Pure gasoline**	**Natural gas**	**Pure hydrogen**	**Syngas**
CO_2	0.0775	0.0771	0.0838	0.0548
H_2O	0.1064	0.1072	0.0941	0.1512
N_2	0.7203	0.7199	0.7251	0.7026
O_2	0.0359	0.0358	0.0366	0.0333
CO	0.0191	0.019	0.0204	0.014
H_2	0.0036	0.0037	0.0032	0.0054
H	0.0013	0.0014	0.0013	0.0016
O	0.003	0.003	0.0031	0.0029
OH	0.0133	0.0133	0.0125	0.0155
NO	0.0196	0.0196	0.0199	0.0187

Table A.4 Stoichiometric Constant Pressure Adiabatic Flame Temperature

Fuel	**T_f (K)**
Pure gasoline	2191.87
Natural gas	2192.52
Pure hydrogen	2259.25
Syngas	1950.04

Table A.5 Thermal Curve Coefficient Corresponding to Fuels

300K<T<1000K					
Fuel	$\boldsymbol{a1}$	$\boldsymbol{a2}$	$\boldsymbol{a3}$	$\boldsymbol{a6}$	$\boldsymbol{a7}$
Pure Gasoline	4.0652	0.060977	-1.88E-05	-3.59E+04	15.45
Natural Gas	3.96442451	0.055146952	-1.75E-05	-32390.89047	13.67502944
Syngas	2.31738493	0.007091626	-3.67E-06	-19676.25005	6.88546659
Pure Hydrogen	3.05744	0.00267	-5.81E-06	-988.9047	-2.2997

Table A.6 Composition of simulated fuels in percentage

S.N.	**Composition of simulated fuels**	**H_2 (%)**	**CO_2(%)**	**CH_4 (%)**	**C_7H_{17} (%)**
1	Pure Gasoline	0	0	0	100
2	Natural Gas	10	0	0	90
3	Syngas	20	30	50	0
4	Pure Hydrogen	100	0	0	0

Table A.7 NOx (ppm) emissions for different gas at phi=0.8, ST 20 BTDC, CR10, at different engine speed (rpm)

Engine Speed(RPM)	Gasoline(ppm)	Syngas(ppm)	Natural gas(ppm)	Hydrogen (ppm)
500.0	4316.2	7420.6	3720.4	7836.2
550.0	4552.3	7639.9	3950.2	8067.7
600.0	4733.4	7819.1	4126.4	8257.0
650.0	4871.5	7968.6	4260.1	8414.8
700.0	4975.5	8095.3	4360.3	8548.6
750.0	5052.7	8204.1	4433.5	8663.5
800.0	5108.1	8298.1	4485.1	8762.8
850.0	5145.9	8380.6	4519.2	8849.9
900.0	5169.4	8453.1	4539.0	8926.5
950.0	5180.8	8517.0	4547.0	8994.0
1000.0	5182.5	8573.6	4545.5	9053.7
1050.0	5175.9	8623.5	4536.0	9106.4
1100.0	5162.6	8667.7	4519.9	9153.1
1150.0	5143.6	8706.7	4498.6	9194.3
1200.0	5119.7	8741.1	4472.7	9230.6
1250.0	5091.9	8771.2	4443.2	9262.4
1300.0	5060.7	8797.6	4410.7	9290.3
1400.0	4990.6	8839.7	4338.8	9334.7
1500.0	4912.7	8869.8	4260.4	9366.5
1600.0	4829.8	8889.2	4178.1	9387.0
1700.0	4743.6	8899.4	4093.7	9397.8
1800.0	4655.8	8901.4	4008.3	9399.9
1900.0	4567.2	8896.1	3923.0	9394.3
2000.0	4478.9	8884.3	3838.5	9381.8
2100.0	4391.2	8866.6	3755.5	9363.1
2200.0	4304.6	8843.6	3673.9	9338.8
2300.0	4219.6	8816.0	3594.4	9309.7
2400.0	4136.2	8784.1	3516.9	9276.0
2500.0	4054.6	8748.5	3441.6	9238.4
2600.0	3975.1	8709.7	3368.4	9197.4
2700.0	3897.7	8667.4	3297.4	9152.8
2800.0	3822.3	8622.6	3228.7	9105.5
2900.0	3749.1	8575.4	3162.2	9055.6
3000.0	3677.9	8525.9	3097.9	9003.4

Table A.8 Measured NOx(ppm) emission for different gas at CR 8:1, ST 15 BTDC,1500RPM as a function of equivalence ratio

Equivalence ratio(ϕ)	**Gasoline**	**Syngas A**	**Syngas B**	**Natural Gas**	**Hydrogen**
0.500	2.3	65.9	92.2	2.1	97.4
0.525	5.4	130.4	180.0	4.9	190.1
0.550	11.9	244.0	332.7	10.7	351.3
0.575	25.0	433.7	583.5	22.2	616.2
0.600	49.9	733.6	973.3	43.9	1027.8
0.625	95.0	1181.7	1544.5	82.7	1631.0
0.650	173.1	1812.2	2327.9	149.1	2458.3
0.675	302.3	2639.3	3322.3	258.1	3508.3
0.700	506.5	3639.6	4472.4	429.3	4722.9
0.725	814.5	4736.8	5662.9	686.4	5980.0
0.750	1255.1	5809.5	6742.6	1054.5	7120.2
0.775	1847.9	6724.3	7579.0	1553.2	8003.4
0.800	2586.9	7382.0	8103.7	2185.0	8557.5
0.825	3420.5	7745.1	8317.2	2918.7	8783.0
0.850	4243.2	7829.5	8264.4	3677.5	8727.2
0.875	4913.0	7681.6	8002.1	4341.2	8450.2
0.900	5300.5	7351.9	7582.4	4780.2	8007.0
0.925	5338.4	6886.7	7046.6	4901.4	7441.2
0.950	5033.0	6322.1	6426.8	4678.8	6786.7
0.975	4440.8	5688.5	5749.5	4147.3	6071.5
1.000	3644.2	5014.1	5039.6	3384.9	5321.8
1.025	2805.5	4347.7	4343.7	2568.5	4586.9
1.050	2104.3	3737.4	3714.5	1894.4	3922.5
1.075	1582.6	3208.6	3176.0	1402.9	3353.9
1.100	1205.0	2762.4	2726.7	1053.1	2879.4
1.125	929.1	2390.3	2355.6	800.7	2487.5
1.150	723.0	2080.5	2049.2	613.8	2164.0
1.175	565.1	1822.0	1795.3	471.6	1895.8
1.200	441.2	1604.9	1583.6	361.2	1672.3

Table A.9 Measured NOx (ppm) emission for different gas at CR 10:1, ST 15 BTDC, 2000RPM

Equivalence ratio(ϕ)	Gasoline	Syngas A	Syngas B	Natural Gas	Hydrogen
0.500	3.7	145.3	199.6	3.6	210.8
0.525	8.2	286.9	388.9	8.0	410.7
0.550	17.4	534.6	714.6	16.7	754.6
0.575	35.0	941.8	1240.3	33.2	1309.8
0.600	67.3	1596.6	2032.8	63.1	2146.6
0.625	123.8	2470.5	3135.9	114.8	3311.5
0.650	218.6	3655.7	4572.2	200.4	4828.2
0.675	370.8	5057.3	6077.4	336.6	6417.7
0.700	604.8	6507.2	7555.8	544.2	7978.9
0.725	948.2	7780.2	8720.0	847.3	9208.3
0.750	1426.6	8689.9	9431.5	1268.8	9959.7
0.775	2053.2	9168.1	9698.2	1822.9	10241.3
0.800	2812.9	9261.2	9617.4	2502.3	10156.0
0.825	3646.9	9067.1	9300.3	3264.0	9821.1
0.850	4447.9	8680.4	8831.6	4020.2	9326.2
0.875	5083.6	8168.6	8265.7	4651.8	8728.6
0.900	5439.6	7575.0	7634.8	5041.2	8062.3
0.925	5459.8	6925.7	6958.4	5114.3	7348.1
0.950	5151.8	6237.5	6248.6	4857.4	6598.5
0.975	4566.1	5523.4	5515.9	4307.6	5824.8
1.000	3778.7	4798.3	4773.5	3538.4	5040.8
1.025	2944.6	4099.5	4059.3	2717.1	4286.6
1.050	2232.0	3478.1	3428.5	2026.6	3620.5
1.075	1689.9	2953.4	2900.5	1512.7	3062.9
1.100	1290.8	2520.6	2468.7	1141.7	2606.9
1.125	996.1	2166.8	2118.2	871.7	2236.8
1.150	774.8	1877.4	1833.4	671.0	1936.1
1.175	605.0	1639.5	1600.5	518.3	1690.1
1.200	472.0	1422.6	1408.5	399.7	1487.4

Table A.10 NOx (ppm) emissions for different gas at phi=0.8, 1500rpm, CR8, at different spark timing

Spark timing BTDC	Gasoline	Syngas	Natural gas	Hydrogen gas
15.0	2471.3	6821.9	2088.5	7203.9
16.0	2694.9	7107.8	2286.9	7505.8
17.0	2936.4	7388.0	2502.4	7801.7
18.0	3196.0	7660.1	2735.5	8089.1
19.0	3474.3	7922.3	2986.5	8365.9
20.0	3770.5	8172.0	3255.8	8629.6
21.0	4084.3	8407.8	3543.5	8878.6
22.0	4414.8	8628.4	3848.8	9111.6
23.0	4760.3	8832.0	4171.1	9326.6
24.0	5119.4	9018.3	4509.3	9523.3
25.0	5489.4	9186.5	4861.7	9700.9
26.0	5867.6	9336.6	5226.1	9859.4
27.0	6250.8	9468.8	5599.8	9999.1
28.0	6635.1	9583.5	5980.2	10120.2
29.0	7017.0	9681.8	6363.6	10224.0
30.0	7392.2	9764.9	6746.4	10311.7

Table A.11 Gasoline, syngas, natural gas and hydrogen test result for peak pressure vs crank angle at CR 8:1,1500RPM, ST 20 BTDC for different equivalence ratio

Crank angle	Equivalence ratio(ϕ)=0.8				Equivalence ratio(ϕ)=0.9				Equivalence ratio(ϕ)=1			
	Gasoline	Syngas	Natural gas	Hydrogen	Gasoline	Syngas	Natural gas	Hydrogen	Gasoline	Syngas	Natural gas	Hydrogen
-180	100	100	100	100	100	100	100	100	100	100	100	100
-170	101	101	101	101	101	101	101	101	101	101	101	101
-160	103.3	103.5	103.5	103.5	103.3	103.5	103.5	103.5	103.3	103.5	103.5	103.5
-150	107.2	107.5	107.5	107.5	107.2	107.5	107.4	107.5	107.2	107.5	107.4	107.5
-140	112.9	113.4	113.3	113.4	112.8	113.4	113.3	113.4	112.8	113.4	113.2	113.4
-130	120.8	121.5	121.3	121.5	120.7	121.5	121.3	121.5	120.6	121.5	121.3	121.5
-120	131.4	132.5	132.3	132.5	131.3	132.5	132.2	132.5	131.2	132.5	132.2	132.5
-110	145.8	147.4	147.1	147.4	145.6	147.4	147	147.4	145.5	147.4	146.9	147.4
-100	165.3	167.6	167.1	167.6	165.1	167.6	167	167.6	164.8	167.6	167	167.6
-90	192	195.4	194.7	195.4	191.6	195.4	194.5	195.4	191.2	195.4	194.4	195.4
-80	229.1	234.2	233	234.2	228.5	234.2	232.8	234.2	227.9	234.1	232.6	234.1
-70	281.5	289.3	287.3	289.3	280.6	289.2	287	289.2	279.7	289.1	286.7	289.1
-60	356.8	369	365.8	369	355.4	368.9	365.3	368.9	354	368.7	364.8	368.7
-50	466.6	486	480.6	486	464.3	485.8	479.7	485.8	462.1	485.5	478.9	485.5
-40	626.3	657.8	648.5	657.8	622.7	657.4	647.1	657.4	619.1	657	645.7	657
-30	851.2	901.6	886	901.6	845.4	901	883.6	901	839.8	900.3	881.3	900.3
-28	904.3	959.4	942.2	959.4	897.9	958.7	939.6	958.7	891.8	958	937	958
-26	959.6	1019.1	1000.9	1019.8	952.7	1019	998	1019	946	1018	995.2	1018
-24	1016.9	1082.5	1061.6	1143.12	1009.4	1081	1058.5	1141.536	1002.1	1080	1055	1140.48
-22	1075.6	1146	1123.9	1210.176	1067.4	1145	1120.5	1209.12	1059.6	1144	1117	1208.064
-20	1135	1211	1187	1278.816	1126.2	1210	1183.3	1277.76	1117.7	1209	1179	1276.704
-18	1209	1290	1263.8	1362.24	1200.8	1289	1260.9	1361.184	1192.8	1289	1257	1361.184
-16	1325.6	1407	1380.4	1485.792	1322	1409	1381.9	1487.904	1317.3	1410	1382	1488.96
-14	1482.1	1560	1534.1	1647.36	1486.8	1566	1543.1	1653.696	1488.2	1570	1548	1657.92
-12	1677.8	1746	1723.7	1843.776	1694.4	1759	1743.4	1857.504	1704.6	1767	1756	1865.952
-10	1909.7	1963	1946.1	2072.928	1941.6	1984	1979.4	2095.104	1963.2	1997	2002	2108.832
-8	2172.8	2206	2196.2	2329.536	2223.1	2236	2245.7	2361.216	2258.5	2255	2280	2381.28
-6	2460.1	2466	2467.1	2604.096	2531.3	2507	2535	2647.392	2582.7	2532	2583	2673.792
-4	2762.6	2737	2750.4	2890.272	2857	2789	2838.2	2945.184	2926	2822	2901	2980.032
-2	3070.4	3008	3036.4	3176.448	3189.2	3072	3145.2	3244.032	3277.1	3113	3223	3287.328
0	3372.3	3271	3315	3454.176	3516.2	3347	3445.2	3534.432	3623.5	3395	3539	3585.12

2	3657.2	3515	3576	3711.84	3826.1	3603	3727.1	3804.768	3952.8	3659	3837	3863.904
4	3914.8	3733	3809.8	3942.048	4107.4	3831	3980.8	4045.536	4252.8	3895	4106	4113.12
6	4135.8	3916	4008.2	4135.296	4350.3	4025	4197.4	4250.4	4512.8	4095	4336	4324.32
8	4312.8	4059	4164.6	4286.304	4546.5	4176	4369.8	4409.856	4724.2	4253	4520	4491.168
10	4440.5	4158	4274.6	4390.848	4690.2	4283	4493	4522.848	4880.6	4364	4653	4608.384
12	4515.9	4211	4335.8	4446.816	4778.2	4341	4564.4	4584.096	4978.4	4426	4733	4673.856
14	4538.5	4218	4347.9	4454.208	4809.4	4352	4583.5	4595.712	5016.5	4439	4757	4687.584
16	4509.7	4180	4312.4	4414.08	4785.3	4316	4551.7	4557.696	4996.2	4405	4728	4651.68
18	4432.4	4102	4232.5	4331.712	4709.1	4238	4472.3	4475.328	4920.8	4326	4649	4568.256
20	4311.1	3985	4112.2	4208.16	4585.3	4121	4349.7	4351.776	4795.2	4208	4525	4443.648
22	4151.3	3837	3956.7	4051.872	4419.7	3970	4189.2	4192.32	4625.3	4055	4361	4282.08
24	3958.7	3660	3771.5	3864.96	4218.6	3790	3996.6	4002.24	4417.7	3872	4163	4088.832
26	3740.3	3462	3562.9	3655.872	3989.3	3587	3778.6	3787.872	4180.3	3666	3939	3871.296
28	3528.3	3270	3360.6	3453.12	3766.5	3390	3566.9	3579.84	3949.8	3466	3721	3660.096
30	3324.9	3085	3166.4	3257.76	3552.6	3201	3363.7	3380.256	3728.4	3275	3512	3458.4
40	2458.1	2295	2339.3	2423.52	2638.3	2393	2495.4	2527.008	2782.3	2455	2618	2592.48
50	1834.9	1722	1745.1	1818.432	1977.1	1806	1868.1	1907.136	2097.1	1860	1971	1964.16
60	1401.7	1321	1332.2	1394.976	1515	1392	1430.1	1469.952	1616.1	1441	1517	1521.696
70	1100.9	1040	1045.5	1098.24	1192.6	1101	1124.7	1162.656	1278.7	1146	1198	1210.176
80	889.4	842.5	844	889.68	965.2	894	909.4	944.064	1039.1	935.7	972.8	988.0992
90	737.9	699.8	699.6	738.9888	802	744.1	755	785.7696	866.2	782.5	809.8	826.32
100	627.5	595.3	594.4	628.6368	682.9	633.9	642.1	669.3984	739.2	669.3	690.2	706.7808
110	545.6	517.5	516.4	546.48	594.3	551.7	558.3	582.5952	644.5	584.3	601	617.0208
120	484	458.8	457.6	484.4928	527.7	489.5	495.2	516.912	573	519.6	533.6	548.6976
130	437.2	414	413	437.184	477	442	447.1	466.752	518.5	469.9	482.3	496.2144
140	401.5	379.6	378.8	400.8576	438.3	405.4	410.4	428.1024	476.7	431.5	442.8	455.664
150	374.2	353.2	352.8	372.9792	408.7	377.3	382.3	398.4288	444.8	401.9	412.7	424.4064
160	353.8	333.2	333.2	351.8592	386.5	356	361.1	375.936	420.8	379.3	389.9	400.5408
170	338.9	318.5	318.9	336.336	370.3	340.3	345.6	359.3568	403.3	362.6	373.2	382.9056
180	328.9	308.3	309.2	325.5648	359.4	329.3	335	347.7408	391.5	351	361.8	370.656

Table A.12 Gasoline, syngas, natural gas and hydrogen test result for peak pressure vs crank angle at ϕ=1,1500RPM, ST 20 BTDC for different compression ratio

Crank angle	**Compression ratio 8**				**Compression ratio 9**				**Compression 10**			
	Gasoline	**Syngas**	**Natural gas**	**Hydrogen**	**Gasoline**	**Syngas**	**Natural gas**	**Hydrogen**	**Gasoline**	**Syngas**	**Natural gas**	**Hydrogen**
-180	100	100	100	100	100	100	100	100	100	100	100	100
-170	101	101	101	101	101	101	101	101	101	101.1	101	101.1
-160	103.3	103.5	103.5	103.5	103.4	103.5	103.5	103.5	103.4	103.6	103.5	103.6
-150	107.2	107.5	107.4	107.5	107.3	107.6	107.5	107.6	107.4	107.7	107.6	107.7
-140	112.8	113.4	113.2	113.4	113	113.6	113.5	113.6	113.2	113.7	113.6	113.7
-130	120.6	121.5	121.3	121.5	121	121.8	121.7	121.8	121.2	122.1	122	122.1
-120	131.2	132.5	132.2	132.5	131.8	133.1	132.8	133.1	132.3	133.6	133.3	133.6
-110	145.5	147.4	146.9	147.4	146.4	148.4	147.9	148.4	147.2	149.2	148.7	149.2
-100	164.8	167.6	167	167.6	166.3	169.2	168.6	169.2	167.6	170.5	169.9	170.5
-90	191.2	195.4	194.4	195.4	193.7	198	197	198	195.8	200.1	199.1	200.1
-80	227.9	234.1	232.6	234.1	232	238.4	236.9	238.4	235.4	242	240.4	242
-70	279.7	289.1	286.7	289.1	286.6	296.5	294	296.5	292.4	302.7	300	302.7
-60	354	368.7	364.8	368.7	366.1	381.7	377.5	381.7	376.3	392.7	388.2	392.7
-50	462.1	485.5	478.9	485.5	483.9	509.3	502	509.3	502.7	529.7	521.9	529.7
-40	619.1	657	645.7	657	659.7	701.6	688.9	701.6	695.6	741.2	727.3	741.2
-30	839.8	900.3	881.3	900.3	915.7	984.8	962.8	984.8	985.7	1062	1038	1062
-28	891.8	958	937	958	977.6	1053	1029	1053	1057.4	1143	1115.1	1143
-26	946	1018	995.2	1018	1042.8	1126	1099	1126	1133.5	1228	1197.1	1228
-24	1002.1	1080	1055	1140.48	1110.9	1202	1172	1269.312	1213.8	1318	1283.6	1391.808
-22	1059.6	1144	1117	1208.064	1181.3	1281	1248	1352.736	1297.7	1412	1374	1491.072
-20	1117.7	1209	1179	1276.704	1253.3	1362	1325	1438.272	1384.2	1510	1467.5	1594.56
-18	1192.8	1289	1257	1361.184	1344.5	1459	1421	1540.704	1492.4	1626	1581.3	1717.056
-16	1317.3	1410	1382	1488.96	1490.8	1603	1568	1692.768	1661.4	1794	1751.6	1894.464
-14	1488.2	1570	1548	1657.92	1689.2	1791	1762	1891.296	1888.5	2011	1975.2	2123.616
-12	1704.6	1767	1756	1865.952	1939.2	2020	2004	2133.12	2173.2	2273	2251.1	2400.288
-10	1963.2	1997	2002	2108.832	2237.1	2286	2288	2414.016	2511.9	2578	2574.9	2722.368
-8	2258.5	2255	2280	2381.28	2576.5	2584	2608	2728.704	2897.1	2917	2939.3	3080.352
-6	2582.7	2532	2583	2673.792	2948.3	2903	2955	3065.568	3318.2	3279	3333.6	3462.624
-4	2926	2822	2901	2980.032	3340.6	3234	3319	3415.104	3761	3653	3744.2	3857.568
-2	3277.1	3113	3223	3287.328	3739.7	3564	3686	3763.584	4209.2	4024	4155.8	4249.344

0	3623.5	3395	3539	3585.12	4130.4	3882	4041	4099.392	4644.6	4377	4551.8	4622.112
2	3952.8	3659	3837	3863.904	4497.7	4175	4372	4408.8	5049.3	4698	4915.9	4961.088
4	4252.8	3895	4106	4113.12	4827.2	4432	4666	4680.192	5406.5	4974	5233.2	5252.544
6	4512.8	4095	4336	4324.32	5106.5	4643	4912	4903.008	5702.2	5194	5491.5	5484.864
8	4724.2	4253	4520	4491.168	5326	4803	5101	5071.968	5926	5352	5681.9	5651.712
10	4880.6	4364	4653	4608.384	5479.2	4906	5229	5180.736	6071.5	5444	5799.6	5748.864
12	4978.4	4426	4733	4673.856	5563.1	4952	5293	5229.312	6136.8	5469	5843.3	5775.264
14	5016.5	4439	4757	4687.584	5577.9	4941	5293	5217.696	6123.5	5430	5815.3	5734.08
16	4996.2	4405	4728	4651.68	5526.5	4877	5233	5150.112	6036.7	5333	5720.5	5631.648
18	4920.8	4326	4649	4568.256	5414	4765	5118	5031.84	5883.7	5183	5566	5473.248
20	4795.2	4208	4525	4443.648	5247.2	4609	4955	4867.104	5673.3	4988	5360.1	5267.328
22	4625.3	4055	4361	4282.08	5034	4417	4749	4664.352	5415.1	4756	5111.6	5022.336
24	4417.7	3872	4163	4088.832	4782.3	4196	4509	4430.976	5118.8	4496	4829.4	4747.776
26	4180.3	3666	3939	3871.296	4501.6	3953	4244	4174.368	4794.9	4215	4523.1	4451.04
28	3949.8	3466	3721	3660.096	4231.6	3718	3989	3926.208	4486.2	3947	4231.1	4168.032
30	3728.4	3275	3512	3458.4	3974.7	3496	3746	3691.776	4194.8	3694	3955.6	3900.864
40	2782.3	2455	2618	2592.48	2902.3	2565	2732	2708.64	3004.2	2660	2829.8	2808.96
50	2097.1	1860	1971	1964.16	2151.6	1913	2023	2020.128	2195.4	1956	2065.4	2065.536
60	1616.1	1441	1517	1521.696	1637.9	1465	1538	1547.04	1653.9	1483	1553.9	1566.048
70	1278.7	1146	1198	1210.176	1284.2	1155	1204	1219.68	1286.9	1160	1207.5	1224.96
80	1039.1	935.7	972.8	988.0992	1036.6	936.5	970.9	988.944	1032.9	936.1	967.9	988.5216
90	866.2	782.5	809.8	826.32	859.7	779.3	804.2	822.9408	853	775.7	798.4	819.1392
100	739.2	669.3	690.2	706.7808	730.8	664	682.8	701.184	722.9	658.8	675.8	695.6928
110	644.5	584.3	601	617.0208	635.4	577.9	592.9	610.2624	627	572	585.4	604.032
120	573	519.6	533.6	548.6976	563.7	512.7	525.3	541.4112	555.3	506.5	517.7	534.864
130	518.5	469.9	482.3	496.2144	509.2	462.9	473.9	488.8224	500.9	456.6	466.5	482.1696
140	476.7	431.5	442.8	455.664	467.6	424.5	434.6	448.272	459.5	418.3	427.4	441.7248
150	444.8	401.9	412.7	424.4064	435.9	395	404.7	417.12	428.1	389	397.7	410.784
160	420.8	379.3	389.9	400.5408	412.1	372.6	382.1	393.4656	404.5	366.7	375.3	387.2352
170	403.3	362.6	373.2	382.9056	394.8	356	365.6	375.936	387.4	350.3	359	369.9168
180	391.5	351	361.8	370.656	383.2	344.5	354.4	363.792	376	338.9	348	357.8784

Table A.13 Gasoline, syngas, natural gas and hydrogen test result for peak pressure vs crank angle at ϕ=1,1500RPM, ST 20 BTDC for different compression ratio

Crank angle	**Spark timing 15 BTDC**				**Spark timing 20 BTDC**				**Spark timing 25 BTDC**			
	Gasoline	**Syngas**	**Natural gas**	**Hydrogen**	**Gasoline**	**Syngas**	**Natural gas**	**Hydrogen**	**Gasoline**	**Syngas**	**Natural gas**	**Hydrogen**
-180.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
-170.0	101.0	101.0	101.0	101.0	101.0	101.0	101.0	101.0	101.0	101.0	101.0	101.0
-160.0	103.3	103.5	103.5	103.5	103.3	103.5	103.5	103.5	103.3	103.5	103.5	103.5
-150.0	107.2	107.5	107.4	107.5	107.2	107.5	107.4	107.5	107.2	107.5	107.4	107.5
-140.0	112.8	113.4	113.2	113.4	112.8	113.4	113.2	113.4	112.8	113.4	113.2	113.4
-130.0	120.6	121.5	121.3	121.5	120.6	121.5	121.3	121.5	120.6	121.5	121.3	121.5
-120.0	131.2	132.5	132.2	132.5	131.2	132.5	132.2	132.5	131.2	132.5	132.2	132.5
-110.0	145.5	147.4	146.9	147.4	145.5	147.4	146.9	147.4	145.5	147.4	146.9	147.4
-100.0	164.8	167.6	167.0	167.6	164.8	167.6	167.0	167.6	164.8	167.6	167.0	167.6
-90.0	191.2	195.4	194.4	195.4	191.2	195.4	194.4	195.4	191.2	195.4	194.4	195.4
-80.0	227.9	234.1	232.6	234.1	227.9	234.1	232.6	234.1	227.9	234.1	232.6	234.1
-70.0	279.7	289.1	286.7	289.1	279.7	289.1	286.7	289.1	279.7	289.1	286.7	289.1
-60.0	354.0	368.7	364.8	368.7	354.0	368.7	364.8	368.7	354.0	368.7	364.8	368.7
-50.0	462.1	485.5	478.9	485.5	462.1	485.5	478.9	485.5	462.1	485.5	478.9	485.5
-40.0	619.1	657.0	645.7	657.0	619.1	657.0	645.7	657.0	619.1	657.0	645.7	657.0
-30.0	839.8	900.3	881.3	900.3	839.8	900.3	881.3	900.3	839.8	900.3	881.3	900.3
-28.0	891.8	958.0	937.0	958.0	891.8	958.0	937.0	958.0	891.8	958.0	937.0	958.0
-26.0	946.0	1018.0	995.2	1018.0	946.0	1018.0	995.2	1018.0	946.0	1018.0	995.2	1018.0
-24.0	1002.1	1080.0	1055.0	1080.0	1002.1	1080.0	1055.0	1080.0	1002.9	1081.0	1056.0	1081.0
-22.0	1059.6	1144.0	1117.0	1208.1	1059.6	1144.0	1117.0	1208.1	1100.4	1179.0	1155.0	1245.0
-20.0	1117.7	1209.0	1179.0	1276.7	1117.7	1209.0	1179.0	1276.7	1242.8	1316.0	1296.0	1389.7
-18.0	1175.7	1274.0	1242.0	1345.3	1192.8	1289.0	1257.0	1361.2	1431.5	1492.0	1479.0	1575.6
-16.0	1232.5	1338.0	1303.0	1412.9	1317.3	1410.0	1382.0	1489.0	1666.5	1706.0	1706.0	1801.5
-14.0	1287.8	1400.0	1362.0	1478.4	1488.2	1570.0	1548.0	1657.9	1945.4	1955.0	1971.0	2064.5
-12.0	1386.4	1497.0	1461.0	1580.8	1704.6	1767.0	1756.0	1866.0	2264.1	2235.0	2273.0	2360.2
-10.0	1530.4	1632.0	1602.0	1723.4	1963.2	1997.0	2002.0	2108.8	2615.9	2539.0	2603.0	2681.2
-8.0	1718.3	1802.0	1782.0	1902.9	2258.5	2255.0	2280.0	2381.3	2992.0	2860.0	2953.0	3020.2
-6.0	1946.0	2002.0	1997.0	2114.1	2582.7	2532.0	2583.0	2673.8	3381.7	3187.0	3313.0	3365.5
-4.0	2207.0	2227.0	2241.0	2351.7	2926.0	2822.0	2901.0	2980.0	3772.6	3511.0	3673.0	3707.6
-2.0	2492.9	2468.0	2506.0	2606.2	3277.1	3113.0	3223.0	3287.3	4151.1	3821.0	4018.0	4035.0

0.0	2793.5	2717.0	2782.0	2869.2	3623.5	3395.0	3539.0	3585.1	4503.8	4105.0	4338.0	4334.9
2.0	3097.8	2965.0	3059.0	3131.0	3952.8	3659.0	3837.0	3863.9	4817.5	4353.0	4620.0	4596.8
4.0	3394.3	3201.0	3326.0	3380.3	4252.8	3895.0	4106.0	4113.1	5081.1	4557.0	4854.0	4812.2
6.0	3672.1	3418.0	3574.0	3609.4	4512.8	4095.0	4336.0	4324.3	5285.5	4711.0	5033.0	4974.8
8.0	3921.0	3609.0	3794.0	3811.1	4724.2	4253.0	4520.0	4491.2	5424.4	4809.0	5151.0	5078.3
10.0	4132.7	3766.0	3978.0	3976.9	4880.6	4364.0	4653.0	4608.4	5494.9	4851.0	5206.0	5122.7
12.0	4300.8	3885.0	4121.0	4102.6	4978.4	4426.0	4733.0	4673.9	5496.6	4836.0	5198.0	5106.8
14.0	4421.0	3965.0	4220.0	4187.0	5016.5	4439.0	4757.0	4687.6	5432.4	4768.0	5131.0	5035.0
16.0	4491.2	4003.0	4273.0	4227.2	4996.2	4405.0	4728.0	4651.7	5307.0	4651.0	5007.0	4911.5
18.0	4511.4	4001.0	4281.0	4225.1	4920.8	4326.0	4649.0	4568.3	5127.2	4490.0	4834.0	4741.4
20.0	4483.3	3960.0	4245.0	4181.8	4795.2	4208.0	4525.0	4443.6	4897.0	4289.0	4616.0	4529.2
22.0	4410.0	3883.0	4168.0	4100.4	4625.3	4055.0	4361.0	4282.1	4650.7	4075.0	4383.0	4303.2
24.0	4295.7	3775.0	4054.0	3986.4	4417.7	3872.0	4163.0	4088.8	4407.4	3864.0	4153.0	4080.4
26.0	4145.1	3638.0	3908.0	3841.7	4180.3	3666.0	3939.0	3871.3	4169.7	3658.0	3929.0	3862.8
28.0	3963.6	3477.0	3735.0	3671.7	3949.8	3466.0	3721.0	3660.1	3939.7	3458.0	3711.0	3651.6
30.0	3753.4	3294.0	3536.0	3478.5	3728.4	3275.0	3512.0	3458.4	3718.8	3267.0	3502.0	3450.0
40.0	2801.7	2469.0	2636.0	2607.3	2782.3	2455.0	2618.0	2592.5	2774.7	2449.0	2611.0	2586.1
50.0	2112.5	1871.0	1985.0	1975.8	2097.1	1860.0	1971.0	1964.2	2091.0	1855.0	1965.0	1958.9
60.0	1628.6	1451.0	1528.0	1532.3	1616.1	1441.0	1517.0	1521.7	1611.1	1437.0	1512.0	1517.5
70.0	1289.0	1154.0	1208.0	1218.6	1278.7	1146.0	1198.0	1210.2	1274.5	1143.0	1194.0	1207.0
80.0	1047.8	942.4	980.9	995.2	1039.1	935.7	972.8	988.1	1035.6	932.7	969.4	984.9
90.0	873.6	788.4	816.8	832.6	866.2	782.5	809.8	826.3	863.1	779.9	806.9	823.6
100.0	745.7	674.6	696.3	712.4	739.2	669.3	690.2	706.8	736.5	667.0	687.7	704.4
110.0	650.3	589.0	606.4	622.0	644.5	584.3	601.0	617.0	642.2	582.2	598.8	614.8
120.0	578.2	523.9	538.5	553.2	573.0	519.6	533.6	548.7	570.9	517.7	531.6	546.7
130.0	523.3	473.8	486.6	500.3	518.5	469.9	482.3	496.2	516.6	468.1	480.4	494.3
140.0	481.1	435.2	446.9	459.6	476.7	431.5	442.8	455.7	475.0	429.9	441.2	454.0
150.0	448.9	405.4	416.4	428.1	444.8	401.9	412.7	424.4	443.2	400.4	411.1	422.8
160.0	424.7	382.6	393.4	404.0	420.8	379.3	389.9	400.5	419.2	377.9	388.4	399.1
170.0	407.0	365.8	376.6	386.3	403.3	362.6	373.2	382.9	401.8	361.2	371.8	381.4
180.0	395.1	354.0	365.1	373.8	391.5	351.0	361.8	370.7	390.0	349.7	360.5	369.3

APPENDIX B: MATLAB code

B.1 airdata.m

```
function B=airindexdata
switch scheme
case 'GMcB_low'
B=[  0.237E+01    0.86E-02  -0.65E-05    0.20E-08  0.61E-15    -0.49E+05    0.97+01
%Carbon dioxide
0.41E+01 -0.12E-02  -2.6E-05 -0.30E-08 0.81E-12 -0.32E+05 -0.33E+00 %Water
0.371E+01 -0.13E-02 0.24E-05 -0.62E-09 -0.23E-12 -0.11E+04 0.24E+01 %Nitrogen
0.37E+01 -0.19E-02  0.71E-05 -0.68E-08 0.22E-11  -0.11E+04  0.44E+01%Oxygen
0.38E+01 -0.17E-02   0.38E-05 -0.21E-08 0.24E-12   -0.13E+05   0.30E+01%Carbon
monoxide
0.29E+01     0.28E-02   -0.59E-05     0.56E-08   -0.19E-11   -1.0   E+03   -0.19E+01
%Hydrogen
0.27E+01  0+00  0+    0+00  0.00000000E+00      0.26E+05   -0.47E+00  %Hydrogen
isotope
0.30E+01  -0.17E-02 0.25E-05 -0.17E-08  0.41E-12  0.30E+05  0.31E+01  %Oxygen
atom
0.39E+01     -0.12E-02   0.97E-06     0.19E-09     -0.23E-12   0.37E+04     0.51E+00
%Hydrooxide
0.41E+01       -0.35E-02       0.80E-05       -0.62E-08       0.16E-11       1.0       E+04
0.29974988E+01];%Nitrogen monooxide
end
```

B.2 fuel.m

```
function[a,b,c,d,enthalpy,entropy,cp,mw,Fs,q ] = fuel( id, T )
FuelProposition = [ [ 1.971324, 7.871586e-3, -1.048592e-06, -9.930422e+3, 8.873728
]; ... % Methane One
[ 4.0652, 6.0977e-2, -1.8801e-05, -3.588e+4, 1.545e+1 ]; ... % Gasoline Two
[ 7.971, 1.1954e-01, -3.6858e-05, -1.9385e+4,-1.7879 ]; ... % Diesel Three
[ 1.779819, 1.262503e-02, -3.624890e-6,-2.525420e+4, 1.50884e+1 ]; ... % Methanol
Four
[ 1.412633, 2.0871e-02, -8.14213e-6, -1.02635e+4, 1.917126e+1 ]; % Nitromethane
Five
[3.42151,   0.0002874,-5.4337e-07,-7942.8456376,   0.619329432];%syngas data
[3.96442451,   0.055146952,   -1.750189162e-05,   -32390.890474     ,13.67502944];
%Natural gas data
[3.05744,     2.67e-03,  -5.8099e-6,  -0.98890474e+03,  -0.229970e+01];   %Hydrogen
eight
FuelInfo = [[ 1 4 0 0 ]; ... % Methane one
[ 7.1 17.1 0.1 0.1 ]; ... % Gasoline two
[ 14.5 24.8 0.1 .1 ]; ... % Diesel three
[ 1 4 1 0 ]; ... % Methanol four
[ 1 3 2 1 ];% Nitromethane... five
[ 0.52 0.88 0.52 0.08 ]; %... syngas six
[ 6.3 15.5 0 0 ];%...Hydrogen ten Natural gas
[ 1 2 0 0 ];%... Hydrogen eight
F = [ 0.0584 0.06548 0.06907 0.1555 0.5924 0.2381 0.0709 0.0294 0.1337 0.1461];
ac = [ 52420 47870 45730 22680 12430 15300 50381 119520 30000 30000]; % Table
```

```
Fs = F(id);
% Remaining energy
q = ac(id);
alpha = FuelInfo(id, 1);
beta = FuelInfo(id, 2);
gamma = FuelInfo(id, 3);
delta = FuelInfo(id, 4);
ao = FuelProposition(id, 1);
bo = FuelProposition(id, 2);
co = FuelProposition(id, 3);
do = FuelProposiiton(id, 4);
eo = FuelProposition(id, 5);
Enthalpy = ao + bo/2*T +co/3*T^2 +do/T;
Entropy= ao*log(T) + bo*T +co/2*T^2 + eo;
cp = ao + bo*T + co*T^2;
mw = 12.01*a + 1.008*b+ 16.00*c+ 14.01*d;
fprintf('h=\t%6.4f\n',h);
fprintf('s=\t%6.4f\n',s);
fprintf('cp=\t%6.4f\n',cp);
fprintf('mw=\t%6.4f\n',mw);
fprintf('Fs=\t%6.4f\n',Fs);
fprintf('q=\t%6.4f\n',q);
```

B.3 fargH.M

```
function [Y,h,u,s,v,R,Cp,MW,dvdT,dvdP]=fargH2(T,P,phi,f,fuel_id)
 [alpha,beta,gamma,delta,h_fuel,so_fuel,cp_fuel,m_fuel ]=fuelH2( fuel_id, T );
Cp/R = b1 + b2*T + b3*T^2 + b4*T^3 + b5*T^4
 h/RT = b1 + b2/2*T + b3/3*T^2 + b4/4*T^3 + b5/5*T^4 + b6/T
 so/R = b1*ln(T) + b2*T + b3/2*T^2 + b4/3*T^3 + b5/4*T^4 + b7
B = [[0.25e+1, 0.88e-2, -0.67e-5, 0.21e-8, 0.64e-15, -0.49e+5, 0.977e+1 ];  % carbon
[0.4e+1, -0.1e-2, 0.41e-5, -0.30e-8,0.81e-12, -0.31e+5, -0.33 ]; % water
[0.37e+1, -0.13e-2, 0.22e-5, -0.64e-9,-0.21e-12, -0.11e+4, 0.24e+1 ]; % nitrogen
[0.37e+1, -0.19e-2, 0.71e-5, -0.68e-8, 0.22e-11, -0.11e+4, 0.44e+1 ]; % Oxygen
[ 0.38e+1, -0.17e-2, 0.37e-5, -0.21e-8, 0.24e-12, -0.15e+5, 0.30e+1 ];% Carbon mono
oxide
[ 0.31e+1, 0.27e-2, -0.59e-5, 0.56e-8, -0.19e-11, -0.99e+3, -0.23e+1 ]; % Hydrogen
[3.5,    0.00029, -5.44e-07, 1.35e-09, -6.9e-13, -8000.2, 0.619329432]];%Syngas
Mi = [ 44.01, 18.02, 28.013, 32.00, 28.01, 2.016 ];
a_s = alpha + beta/4 - gamma/2;
y_1 = 1 / (1 + 4.76*a_s/phi);
y_fuel = y_1;
y_O2 = a_s/phi * y_1;
y_N2 = a_s/phi*3.76 * y_1;
m_fa = y_fuel*m_fuel + y_O2*32.00 + y_N2*28.013;
Y = zeros(6,1);
m_r = 0; y_r = 0;
n = zeros(6,1);
dcdt = 0;
if ( phi <= 1 )
n(1) = alpha;
```

```
n(2) = beta/2;
n(3) = delta/2 + 3.76*a_s/phi;
n(4) = a_s*(1/phi - 1);
else
d1 = 2*a_s*(1-1/phi);
z = T/1000;
K = exp( 2.743 - 1.761/z - 1.611/z^2 + 0.2803/z^3 );
a1 = 1-K;
b1 = beta/2 + alpha*K - d1*(1-K);
c1 = -alpha*d1*K;
n(5) = (-b1 + sqrt(b1^2 - 4*a1*c1))/(2*a1);
dkdt = -K*(-1.761+z*(-3.222+z*.8409))/1000;
dn5dk = -((alpha - n(5))*(n(5) + 2*a_s*(1/phi - 1)))/(beta/2 + n(5)+ 2*a_s*(1/phi -
1));
dcdt = dn5dk * dkdt;
n(1) = alpha - n(5);
n(2) = beta/2 - d1 + n(5);
n(3) = delta/2 + 3.76*a_s/phi;
n(6) = d1 - n(5);
end
N = sum(n);
m_r = 0;
for i=1:6
Y(i) = n(i)/N;
m_r = m_r + Y(i)*Mi(i);
end
y_r = 1/(1 + m_r/m_fa * (1/f-1));
fprintf('%6.1f',y_r);
for i=1:6
Y(i) = Y(i)*y_r;
fprintf('%6.1f\t',Y(i));
end
y_fuel = y_fuel*(1 - y_r);
Y(3) = Y(3) + y_N2*(1 - y_r);
Y(4) = Y(4) + y_O2*(1 - y_r);
h = h_fuel*y_fuel;
s = (so_fuel-log(max(y_fuel,1e-15)))*y_fuel;
Cp = cp_fuel*y_fuel;
MW = m_fuel*y_fuel;
cpo = zeros(6,1);
ho = zeros(6,1);
so = zeros(6,1);
for i=1:6
cpo(i) = A(i,1) + A(i,2)*T + A(i,3)*T^2 + A(i,4)*T^3 + A(i,5)*T^4;
ho(i) = A(i,1) + A(i,2)/2*T + A(i,3)/3*T^2 + A(i,4)/4*T^3+A(i,5)/5*T^4 + A(i,6)/T;
so(i) = A(i,1)*log(T) + A(i,2)*T + A(i,3)/2*T^2 + A(i,4)/3*T^3+A(i,5)/4*T^4
+A(i,7);
end
table = [-1,1,0,0,1,-1];
for i=1:6
```

```
if(Y(i)>1.e-25)
h = h + ho(i)*Y(i);
s = s + Y(i)*(so(i)-log(Y(i)));
Cp = Cp+cpo(i)*Y(i)+ho(i)*T*table(i)*dcdt*y_r/N;
MW = MW + Y(i)*Mi(i);
end
end
R = 8.31434/MW; h = R*T*h;
u = h-R*T;
v = R*T/P;
s = R*(-log(P/101.325)+s);
Cp = R*Cp; dvdT = v/T; dvdP = -v/P;
fprintf('\nMixture Properties\n');
fprintf('\nh (kJ/kg)=%6.1f\n',h);
fprintf('u (kJ/kg)=%6.1f\n',u);
fprintf('s (kJ/kgK)=%6.1f\n',s)
fprintf('v (m3/kg)=%6.1f\n',v);
fprintf('Cp (kJ/kgK)=%6.1f\n',Cp);
fprintf('Molecular mass =%6.1f\n',MW);
fprintf('dvdt =%6.1f\n',dvdT);
fprintf('dvdP =%6.1f\n',dvdP);
```

B.4 ecpH2.m

```
function [ierr,Y,h,u,s,v,R,Cp,MW,dvdT,dvdP]=ecpH2(T,P,phi,ifuel )
y(1) : CO2
y(2) : H2O
y(3) : N2
y(4) : O2
y(5) : CO
y(6) : H2
y(7) : H
y(8) : O
y(9) : OH
y(10) : NO
Y = zeros(10,1);
h = 0;
u = 0;
s = 0;
v = 0;
R = 0;
Cp = 0;
MW = 0;
dvdT = 0;
dvdP = 0;
prec = 1e-3;
MaxIter = 20;
PATM = P/101.325;
sqp = sqrt(PATM);
if ( T < 600 || T > 3500 )
```

```
ierr = 8;
return;
end
if ( P < 20 || P > 30000 )
ierr = 9;
return;
end
if ( phi < 0.01 )
ierr = 10;
return;
end
 [ alpha, beta, gamma, delta ] = fuelH2( ifuel, T );
Kp = [ [ 0.44-0.2e+5, 0.27e+1, -0.75e-4, 0.25e-8 ];
[ 0.32, -0.13e+5, 0.33e+1, -0.4e-4, 0.35e-8 ];
[ -0.15, -0.22e+4, 0.86, 0.35e-4, -0.32e-8 ];
[ 0.16e-1, -0.48e+4, 0.67, 0.28e-5, -0.16e-8 ];
[ -0.76, 0.13e+5, -0.27e+1, 0.26e-3, -0.17e-7 ];
[ -0.42e-2, 0.15e+5, -0.48e+1, 0.13e-3, -0.91e-8 ] ];
K = zeros(6,1);
for i=1:6
log10ki = Kp(i,1)*log(T/1000) + Kp(i,2)/T + Kp(i,3) + Kp(i,4)*T + Kp(i,5)*T*T;
K(i) = 10^log10ki;
end
c1 = K(1)/sqp;
c2 = K(2)/sqp;
c3 = K(3);
c4 = K(4);
c5 = K(5)*sqp;
c6 = K(6)*sqp;
[ierr,y3,y4,y5,y6 ] = guess( T, phi, alpha, beta, gamma, delta, c5, c6 );
if ( ierr ~= 0 )
return;
end
a_s = alpha + beta/4 - gamma/2;
D1 = beta/alpha;
D2 = gamma/alpha + 2*a_s/(alpha*phi);
D3 = delta/alpha + 2*3.7619047619*a_s/(alpha*phi);
A = zeros(4,4);
final = 0;
for jj=1:MaxIter
sqy6 = sqrt(y6);
sqy4 = sqrt(y4);
sqy3 = sqrt(y3);
y7= c1*sqy6;
y8= c2*sqy4;
y9= c3*sqy4*sqy6;
y10= c4*sqy4*sqy3;
y2= c5*sqy4*y6;
y1= c6*sqy4*y5;
d76 = 0.5*c1/sqy6;
```

```
d84 = 0.5*c2/sqy4;
d94 = 0.5*c3*sqy6/sqy4;
d96 = 0.5*c3*sqy4/sqy6;
d103 = 0.5*c4*sqy4/sqy3;
d104 = 0.5*c4*sqy3/sqy4;
d24 = 0.5*c5*y6/sqy4;
d26 = c5*sqy4;
d14 = 0.5*c6*y5/sqy4;
d15 = c6*sqy4;
A = [ [ 1+d103, d14+d24+1+d84+d104+d94, d15+1, d26+1+d76+d96 ];
[ 0, 2.*d24+d94-D1*d14, -D1*d15-D1, 2*d26+2+d76+d96; ];
[ d103, 2*d14+d24+2+d84+d94+d104-D2*d14,2*d15+1-D2*d15-D2, d26+d96 ];
[ 2+d103, d104-D3*d14, -D3*d15-D3,0 ] ];
if ( final )
break;
end
B = [ -(y1+y2+y3+y4+y5+y6+y7+y8+y9+y10-1);
-(2.*y2 + 2.*y6 + y7 + y9 -D1*y1 -D1*y5);
-(2.*y1 + y2 +2.*y4 + y5 + y8 + y9 + y10 -D2*y1 -D2*y5);
-(2.*y3 + y10 -D3*y1 -D3*y5) ];
[ B, ierr ] = gauss( A, B );
if ( ierr ~= 0 )
return;
end
y3 = y3 + B(1);
y4 = y4 + B(2);
y5 = y5 + B(3);
y6 = y6 + B(4);
nck = 0;
if ( abs(B(1)/y3) > prec )
nck = nck+1;
end
if ( abs(B(2)/y4) > prec )
nck = nck+1;
end
if ( abs(B(3)/y5) > prec )
nck = nck+1;
end
if ( abs(B(4)/y6) > prec )
nck = nck+1;
end
if( nck == 0 )
final = 1;
continue;
end
end
if (jj>=MaxIter)
ierr = 3;
return;
end
```

```
Y = [ y1 y2 y3 y4 y5 y6 y7 y8 y9 y10 ];
if( abs( sum(Y)-1 ) > 0.0000001 )
ierr = 4;
return;
end
dkdt = zeros(6,1);
for i=1:6
dkdt(i)=2.302585*K(i)*( Kp(i,1)/T - Kp(i,2)/(T*T)+ Kp(i,4)+2*Kp(i,5)*T );
end
dcdt = zeros(6,1);
dcdt(1) = dkdt(1)/sqp;
dcdt(2) = dkdt(2)/sqp;
dcdt(3) = dkdt(3);
dcdt(4) = dkdt(4);
dcdt(5) = dkdt(5)*sqp;
dcdt(6) = dkdt(6)*sqp;
dcdp = zeros(6,1);
dcdp(1) = -0.5*c1/P;
dcdp(2) = -0.5*c2/P;
dcdp(5) = 0.5*c5/P;
dcdp(6) = 0.5*c6/P;
x1 = Y(1)/c6;
x2 = Y(2)/c5;
x7 = Y(7)/c1;
x8 = Y(8)/c2;
x9 = Y(9)/c3;
x10 = Y(10)/c4;
dfdt(1) = dcdt(6)*x1 + dcdt(5)*x2 + dcdt(1)*x7 +dcdt(2)*x8 +dcdt(3)*x9 +
dcdt(4)*x10;
dfdt(2) = 2.*dcdt(5)*x2 + dcdt(1)*x7 + dcdt(3)*x9 -D1*dcdt(6)*x1;
dfdt(3) = 2.*dcdt(6)*x1+dcdt(5)*x2+dcdt(2)*x8+dcdt(3)*x9+dcdt(4)*x10 -
D2*dcdt(6)*x1;
dfdt(4) = dcdt(4)*x10 -D3*dcdt(6)*x1;
dfdp(1) = dcdp(6)*x1 + dcdp(5)*x2 + dcdp(1)*x7 +dcdp(2)*x8;
dfdp(2) = 2.*dcdp(5)*x2 + dcdp(1)*x7 -D1*dcdp(6)*x1;
dfdp(3) = 2.*dcdp(6)*x1 + dcdp(5)*x2 + dcdp(2)*x8 - D2*dcdp(6)*x1;
dfdp(4) = -D3*dcdp(6)*x1;
sb = -1.0 .* dfdt';
[b, ierr] = gauss(A,b);
if ( ierr ~= 0 )
return;
end
dydt(3) = b(1);
dydt(4) = b(2);
dydt(5) = b(3);
dydt(6) = b(4);
dydt(1) = sqrt(Y(4))*Y(5)*dcdt(6) + d14*dydt(4) + d15*dydt(5);
dydt(2) = sqrt(Y(4))*Y(6)*dcdt(5) + d24*dydt(4) + d26*dydt(6);
dydt(7) = sqrt(Y(6))*dcdt(1) + d76*dydt(6);
dydt(8) = sqrt(Y(4))*dcdt(2) + d84*dydt(4);
```

```
dydt(9) = sqrt(Y(4)*Y(6))*dcdt(3) + d94*dydt(4) + d96*dydt(6);
dydt(10) = sqrt(Y(4)*Y(3))*dcdt(4) + d104*dydt(4) + d103*dydt(3);
b = -1.0 .* dfdp'; [b,ierr] = gauss(A,b);
if ( ierr~=0 )
return;
end
dydp(3) = b(1);
dydp(4) = b(2);
dydp(5) = b(3);
dydp(6) = b(4);
dydp(1) = sqrt(Y(4))*Y(5)*dcdp(6) + d14*dydp(4) + d15*dydp(5);
dydp(2) = sqrt(Y(4))*Y(6)*dcdp(5) + d24*dydp(4) + d26*dydp(6);
dydp(7) = sqrt(Y(6))*dcdp(1) + d76*dydp(6);
dydp(8) = sqrt(Y(4))*dcdp(2) + d84*dydp(4);
dydp(9) = d94*dydp(4) + d96*dydp(6);
dydp(10)= d104*dydp(4) + d103*dydp(3);
Mi = [ 44.01, 18.02, 28.013, 32.00, 28.01, 2.016, 1.009, 16., 17.009, 30.004];
if ( T > 1000 )
AAC = [[.446080e+1,.309817e-2,-.123925e-5,.227413e-9, -.155259e-13, -
.489614e+5,-.986359 ];
[.271676e+1,.294513e-2,-.802243e-6,.102266e-9, -.484721e-14, -
.299058e+5,.663056e+1 ];
[.289631e+1,.151548e-2,-.572352e-6,.998073e-10,-.652235e-14, -
.905861e+3,.616151e+1 ];
[.362195e+1,.736182e-3,-.196522e-6,.362015e-10,-.289456e-14, -
.120198e+4,.361509e+1 ];
[.298406e+1,.148913e-2,-.578996e-6,.103645e-9, -.693535e-14, -
.142452e+5,.634791e+1 ];
[.310019e+1,.511194e-3, .526442e-7,-.349099e-10,.369453e-14,-.877380e+3,-
.196294e+1 ];
[.25e+1,0,0,0,0,.254716e+5,-.460117 ];
[.254205e+1,-.275506e-4,-.310280e-8,.455106e-11,-.436805e-
15,.292308e+5,.492030e+1 ];
[.291064e+1,.959316e-3,-.194417e-6,.137566e-10,.142245e-
15,.393538e+4,.544234e+1 ];
[.3189e+1,.133822e-2,-.528993e-6,.959193e-10,-.648479e-
14,.982832e+4,.674581e+1 ]; ];
elseif ( T <= 1000 )
AAC = [ [ 0.24007797e+1, 0.87350957e-2, -0.66070878e-5, 0.20021861e-8,
0.63274039e-15, -0.48377527e+5, 0.96951457e+1 ]; % CO2
[ 0.40701275e+1, -0.11084499e-2, 0.41521180e-5, -0.29637404e-8, 0.80702103e-12,
-0.30279722e+5, -0.32270046 ]; % H2O
[ 0.36748261e+1, -0.12081500e-2, 0.23240102e-5, -0.63217559e-9, -0.22577253e-
12, -0.10611588e+4, 0.23580424e+1 ]; % N2
[ 0.36255985e+1, -0.18782184e-2, 0.70554544e-5, -0.67635137e-8, 0.21555993e-11,
-0.10475226e+4, 0.43052778e+1 ]; % O2
[ 0.37100928e+1, -0.16190964e-2, 0.36923594e-5, -0.20319674e-8, 0.23953344e-12,
-0.14356310e+5, 0.2955535e+1 ]; % CO
[ 0.30574451e+1, 0.26765200e-2, -0.58099162e-5, 0.55210391e-8, -0.18122739e-11,
-0.98890474e+3, -0.22997056e+1 ]; % H2
```

```
[ 0.25000000e+1, 0, 0, 0, 0, 0.25471627e+5, -0.46011762e+0 ]; % H
[ 0.29464287e+1, -0.16381665e-2, 0.24210316e-5, -0.16028432e-8, 0.38906964e-12,
0.29147644e+5, 0.29639949e+1 ]; % O
[ 0.38375943e+1, -0.10778858e-2, 0.96830378e-6, 0.18713972e-9, -0.22571094e-12,
0.36412823e+4, 0.49370009e+0 ]; % OH
[ 0.40459521e+1, -0.34181783e-2, 0.79819190e-5, -0.61139316e-8, 0.15919076e-11,
0.97453934e+4, 0.29974988e+1 ]; % H2
end
MW = 0;
Cp = 0;
h = 0;
s = 0;
dMWdT = 0;
dMWdP = 0;
for i=1:10
cpo = AAC(i,1) + AAC(i,2)*T + AAC(i,3)*T^2 + AAC(i,4)*T^3 + AAC(i,5)*T^4;
ho = AAC(i,1) + AAC(i,2)/2*T + AAC(i,3)/3*T^2 + AAC(i,4)/4*T^3 +
AAC(i,5)/5*T^4 + AAC(i,6)/T;
so = AAC(i,1)*log(T) + AAC(i,2)*T + AAC(i,3)/2*T^2 + AAC(i,4)/3*T^3 +
AAC(i,5)/4*T^4 +AAC(i,7);
h = h + ho*Y(i); % h is h/rt here
MW = MW + Mi(i)*Y(i);
dMWdT = dMWdT + Mi(i)*dydt(i);
dMWdP = dMWdP + Mi(i)*dydp(i);
Cp = Cp+Y(i)*cpo + ho*T*dydt(i);
if (Y(i)> 1.0e-37)
s = s + Y(i)*(so - log(Y(i)));
end
end
R = 8.31434/MW;
v = R*T/P;
Cp = R*(Cp - h*T*dMWdT/MW);
h = h*R*T;
s = R*(-log(PATM) + s);
u=h-R*T;
dvdT = v/T*(1 - T*dMWdT/MW);
dvdP = v/P*(-1 + P*dMWdP/MW);
ierr = 0;
fprintf('\nMixture Properties\n');
fprintf('\nh (kJ/kg)=%6.1f\n',h);
fprintf('u (kJ/kg)=%6.1f\n',u);
fprintf('s (kJ/kgK)=%6.1f\n',s)
fprintf('v (m3/kg)=%6.1f\n',v);
fprintf('Cp (kJ/kgK)=%6.1f\n',Cp);
fprintf('Molecular mass =%6.1f\n',MW);
fprintf('dvdt =%6.4f\n',dvdT);
fprintf('dvdP =%6.4f\n',dvdP);
fprintf('\nMole Fractions\n')
fprintf('\nCO2=\t%6.4f \n', Y(1) );
fprintf('H2O=\t%6.4f \n', Y(2) );
```

```
fprintf('N2=\t %6.4f \n', Y(3) );
fprintf('O2=\t %6.4f \n', Y(4) );
fprintf('CO=\t %6.4f \n', Y(5) );
fprintf('H2=\t %6.4f \n', Y(6) );
fprintf('H=\t %6.4f \n', Y(7) );
fprintf('H=\t %6.4f \n', Y(8) );
fprintf('OH=\t %6.4f \n', Y(9) );
fprintf('NO=\t %6.4f \n', Y(10) );
return;
function [ierr,y3,y4,y5,y6] = guess(T,phi,alpha,beta,gamma,delta,c5,c6)
ierr = 0;
y3 = 0;
y4 = 0;
y5 = 0;
y6 = 0;
n = zeros(6,1);
a_s = alpha + beta/4 - gamma/2;
if ( phi <= 1 )
n(1) = alpha;
n(2) = beta/2;
n(3) = delta/2 + 3.76*a_s/phi;
n(4) = a_s*(1/phi - 1);
else
d1 = 2*a_s*(1-1/phi);
z = T/1000;
KK = exp( 2.743 - 1.761/z - 1.611/z^2 + 0.2803/z^3 );
aa = 1-KK;
bb = beta/2 + alpha*KK - d1*(1-KK);
cc = -alpha*d1*KK;
n(5) = (-bb + sqrt(bb^2 - 4*aa*cc))/(2*aa);
n(1) = alpha - n(5);
n(2) = beta/2 - d1 + n(5);
n(3) = delta/2 + 3.76*a_s/phi;
n(6) = d1 - n(5);
end
nIterMax=40;
for ii=1:nIterMax
f = 2*N*ox - gamma - (2*a_s)/phi + (alpha*(2*c6*ox^(1/2) + 1))/ (c6*ox^(1/2) + 1)
+ (beta*c5*ox^(1/2))/(2*c5*ox^(1/2) + 2);
if ( f < 0 )
break;
else
ox = ox*0.1;
if ( ox < 1e-37 )
ierr = 5;
return;
end
end
end
for ii=1:nIterMax
```

```
f = 2*N*ox - gamma - (2*a_s)/phi + (alpha*(2*c6*ox^(1/2) + 1))/ (c6*ox^(1/2) + 1)
+ (beta*c5*ox^(1/2))/(2*c5*ox^(1/2) + 2);
df = 2*N - (beta*c5^2)/(2*c5*ox^(1/2) + 2)^2 + (alpha*c6)/ (ox^(1/2)*(c6*ox^(1/2)
+ 1)) +(beta*c5)/ (2*ox^(1/2)*(2*c5*ox^(1/2) + 2))-(alpha*c6*(2*c6*ox^(1/2) + 1))/
(2*ox^(1/2)*(c6*ox^(1/2) + 1)^2);
dox = f/df;
ox = ox - dox;
if ( ox < 0.0 )
ierr = 6;
return;
end
if ( abs(dox/ox) < 0.001 )
break;
end
end
if( ii == nIterMax )
ierr = 7;
return;
end
y3 = 0.5*(delta + a_s/phi*2*3.76)/N;
y4 = ox;
y5 = alpha/N/(1+c6*sqrt(ox));
y6 = beta/2/N/(1+c5*sqrt(ox));
end % guess
function [B, IERQ] = gauss( A, B )
IERQ = 0;
for N=1:3
NP1=N+1;
BIG = abs( A(N,N) );
if ( BIG < 1.0e-05)
IBIG=N;
for I=NP1:4
if( abs(A(I,N)) <= BIG )
continue;
end
BIG = abs(A(I,N));
IBIG = I;
end
if(BIG <= 0.)
IERQ=2;
return;
end
if( IBIG ~= N)
for J=N:4
TERM = A(N,J);
A(N,J) = A(IBIG,J);
A(IBIG,J) = TERM;
end
TERM = B(N);
B(N) = B(IBIG);
```

```
B(IBIG) = TERM;
end
end
for I=NP1:4
TERM = A(I,N)/A(N,N);
for J=NP1:4
A(I,J) = A(I,J)-A(N,J)*TERM;
end
B(I) = B(I)-B(N)*TERM;
end
end
if( abs(A(4,4)) > 0.0 )
B(4) = B(4)/A(4,4);
B(3) = (B(3)-A(3,4)*B(4))/A(3,3);
B(2) = (B(2)-A(2,3)*B(3)-A(2,4)*B(4))/A(2,2);
B(1) = (B(1)-A(1,2)*B(2)-A(1,3)*B(3)-A(1,4)*B(4))/A(1,1);
else
IERQ=1;
return;
end
end
End
```

B.5 AdiabaticFlameTempH2.m

```
T1 = 298.15;
P1 = 101.3;
PHI = 1;
f = 0.05;
ifuel=10;
[~, H1, ~, ~, ~, ~, CP, ~, ~, ~] = fargH2( T1, P1, PHI, f, ifuel );
fprintf('Initial Enthalpy H1 = %7.1f Initial CP = %7.3f \n',H1,CP);
P2 = P1;
T2 = 2000;
MAXITS = 50;
TOL = 0.00001;
for i=1:MAXITS
[~,~, H2, ~, ~, ~, ~, CP, ~, ~, ~] = ecpH2( T2, P2, PHI, ifuel );
DELT2 = (H1-H2)/CP;
T2 = T2 + DELT2;
fprintf('Iterated Adiabatic Flame Temp (K) = %8.2f \n',T2);
if ( abs(DELT2)/T2 < TOL )
break;
end
end
fprintf('Final Adiabatic Flame Temp (K) = %8.2f \n',T2);
```

A.6 HomogeneousH2.m

```
function [ ETA, IMEP, NOX_ppm ] = HomogeneousH2(varargin)
R = 8; B = 0.1016;
S = 0.0762;
EPS = 0.24788;
```

```
RPM = 3000;
HEAT = 500;
BLOWBY = 0.8;
THETAS = -20; THETAB = 45;
PHI=0.8; F = 0.05;
TW = 400;
fuel_type = 2;
FS = 0.1461;
A0 =  30000
T1 = 350; %K
P1 = 100; % kPa
if ( nargin == 3 )
PHI = varargin{1};
F = varargin{2};
RPM = varargin{3};
end
OMEGA = RPM*pi/30;
to_ppm = 10^6;
MW_NO = 30;
THETA = -180;
DTHETA = 1;
THETAE = THETA+DTHETA;
[ VOL, X, EM ] = auxiliary( THETA );
NNOX = THETAB/DTHETA;
NY = 6+NNOX;
Y = zeros(NY,1);
Y(1) = P1;
Y(2) = nan;
Y(3) = T1;
[~, ~, ~, ~, vU, ~, ~, ~, ~, ~] = fargH2( Y(3), Y(1), PHI, F, fuel_type );
MNOT = VOL/vU;
M = EM*MNOT;
NN = 360*1; %Graph Plot
SAVE.THETA = zeros( NN, 1 );
SAVE.VOL = zeros( NN, 1 );
SAVE.T = zeros(NN, 1 );
SAVE.P = zeros( NN, 1 );
SAVE.MDOTFI = zeros( NN, 1 );
SAVE.NOx = zeros(NN,5);
fprintf( 'BURN FRAC \n' );
fprintf( ' --   \n' );
fprintf('%3.3f \n',  X );
fprintf('%7.1f \n',  THETA );
fprintf('%6.1f \n',  Y(1) );%Pressure
fprintf('%6.1f \n',  Y(2) );%Burn Temp
fprintf('%6.1f \n',  Y(3) );%UnBurn Temp
fprintf('%6.1f \n',  0.0 );
II = 1;
for III=1:360 % 360 72 36
for JJJ=1:1 % 1 5 10
```

```
[ Y ] = integrate( THETA, THETAE, Y );
[ VOL, X, EM ] = auxiliary( THETA );
M = EM*MNOT;
THETA=THETAE;
THETAE=THETA+DTHETA;
% save data for plotting later
SAVE.THETA(II) = THETA;
SAVE.VOL(II) = VOL;
SAVE.P(II) = Y(1);
SAVE.TB(II) = Y(2);
SAVE.TU(II) = Y(3);
SAVE.X(II) = X;
SAVE.NOX(II,:) = [ Y(6+1), Y(round(6+0.25*NNOX)),Y(round(6+0.5*NNOX)),
Y(round(6+0.75*NNOX)), Y(6+NNOX) ]*to_ppm;
II=II+1;
if ( THETAS >= THETA && THETAS < THETAE )
Y(2) = tinitial( Y(1), Y(3), PHI, F );
end
if ( THETA > THETAS + THETAB )
Y(3) = nan;
end
end
%fprintf('%3.3f\n',X);
end
 NOX_ppm = 0;
for nn=1:NNOX
THETA = THETAS + (nn-1)/(NNOX-1)*THETAB;
dxbdtheta = 0.5*sin(pi*(THETA-THETAS)/THETAB)*pi/THETAB;
dxb = dxbdtheta*DTHETA;
NOX_ppm = NOX_ppm + Y(6+nn)*dxb*to_ppm;
end
ETA = Y(4)/MNOT*(1+PHI*FS*(1-F))/PHI/FS/(1-F)/A0;
IMEP = Y(4)/(pi/4*B^2*S);
fprintf( '%7.3f\n',NOX_ppm );
fprintf( '%7.3f\n',IMEP );
fprintf( '%1.4f\n',ETA );
if ( nargin == 0 )
sTitle = sprintf('Homogenous 2 zone, gasoline, PHI=%.2f F=%.2f
RPM=%.1f\nETA=%.3f IMEP=%.2f kPa NOx=%.1f ppm ', PHI, F, RPM, ETA,
IMEP, NOX_ppm );
 figure;
plot( SAVE.THETA, SAVE.X, 'linewidth',2 );
set(gca,'fontsize',16,'linewidth',2,'Xlim',[-100 100]);
xlabel( 'theta','fontsize',16);
ylabel('burn fraction','fontsize',16);
title( sTitle );
figure;
plot( SAVE.THETA, SAVE.P,'linewidth',2 );
set(gca,'fontsize',16,'linewidth',2,'Xlim',[-100 100]);
xlabel( '\theta','fontsize',16);
```

```
ylabel('pressure (kPa)','fontsize',16);
figure;
plot( SAVE.THETA, SAVE.TU, '-',SAVE.THETA, SAVE.TB,'--','linewidth',2 );
set(gca,'fontsize',16,'linewidth',2,'Xlim',[-100 100]);
xlabel( '\theta','fontsize',16);
ylabel( 'temperature (K)', 'fontsize',16);
legend('Unburned','Burned', 'Location', 'SouthEast');
figure;
plot( SAVE.THETA, SAVE.NOX,'linewidth',1);
grid on;
set(gca,'fontsize',16,'linewidth',2,'Xlim',[-100 100]);
xlabel('theta','fontsize',16);
ylabel('NOx (ppm)','fontsize',16);
axis( [ THETAS, 110, 0, max(max(SAVE.NOX)*1.1) ] );
legend( 'X=0', 'X=0.25', 'X=0.5', 'X=0.75', 'X=1', 'Location', 'SouthEast' );
figure;
NVE1=[0.85 6483.4;0.9  6747.4;1    3917.6;1.1  1313.1;1.2  549.6;1.3  248.3];
NVEx=NVE1(:,1);
NVEy=NVE1(:,2);
plot(NVEx,NVEy);
xlabel('Equivalence Ratio','fontsize',16);
ylabel('NOx (ppm)','fontsize',16);
legend('f=0');
 end
function [ TB ] = tinitial( P, TU, PHI, F )
TB = 2000;
[~, HU,~, ~, ~, ~, ~, ~, ~, ~] = fargH2( TU, P, PHI, F, fuel_type );
 for ITER=1:50
[ierr, ~, HB,~, ~, ~, ~, CP, ~, ~, ~] = ecpH2( TB, P, PHI, fuel_type );
 if ( ierr ~= 0 )
fprintf('Error in ecpH2(%g, %g, %g): %d\n', TB, P, PHI, ierr )
end
DELT = +(HU-HB)/CP;
TB = TB + DELT;
if ( abs(DELT/TB) < 0.001 )
break;
end
end
end
function [ VOL, X, EM ] = auxiliary( THETA )
VTDC = pi/4*B^2*S/(R-1); % m3
VOL = VTDC*(1 + (R-1)/2*(1-cosd(THETA) + 1/EPS*(1-sqrt(1-(EPS*sind(THETA))^2))));
X = 0.5*(1-cos(pi*(THETA-THETAS)/THETAB));
if ( THETA <= THETAS )
X = 0.;
end
if ( THETA >= THETAS+THETAB )
X = 1.;
end
```

```
EM = exp(-BLOWBY*(THETA*pi/180 + pi)/OMEGA);
end
function [Y] = integrate( THETA, THETAE, Y )
[TT, YY ] = ode23( @rates, [ THETA, THETAE ], Y );
for J=1:NY
Y(J) = YY(length(TT),J);
end
function [ YPRIME ] = rates( THETA, Y )
YPRIME = zeros(NY,1);
[ VOL, X, EM ] = auxiliary( THETA );
M = EM*MNOT;
DUMB = sqrt(1-(EPS*sind(THETA))^2);
DV = pi/8*B^2*S*sind(THETA)*(1+EPS*cosd(THETA)/DUMB);
AA = (DV + VOL*BLOWBY/OMEGA)/M;
C1 = HEAT*(pi*B^2/2 + 4*VOL/B)/OMEGA/M/1000;
C0 = sqrt(X);
P = Y(1);
TB = Y(2);
TU = Y(3);
if ( X > 0.999 )
[ierr,YB,HL, ~, ~,VB, ~,CP, ~,DVDT,DVDP]=ecpH2(TB,P,PHI,fuel_type);
 if ( ierr ~= 0 )
fprintf('Error in ecpH2(%g, %g, %g): %d\n', TB, P, PHI, ierr );
end
BB = C1/CP*DVDT*TB*(1-TW/TB);
CC = 0;
DD = 1/CP*TB*DVDT^2 + DVDP;
EE = 0;
YPRIME(1) = (AA + BB + CC)/(DD + EE);
YPRIME(2) = -C1/CP*(TB-TW) + 1/CP*DVDT*TB*YPRIME(1);
YPRIME(3) = 0;
elseif ( X > 0.001 )
% COMBUSTION
[~,HU, ~, ~,VU, ~,CPU, ~,DVDTU,DVDPU]=fargH2(TU,P,PHI,F,fuel_type);
 [ierr,YB,HB, ~, ~,VB, ~,CPB, ~,DVDTB,DVDPB]=ecpH2(TB,P,PHI,fuel_type);
if ( ierr ~= 0 )
fprintf('Error in ecpH2(%g, %g, %g): %d\n', TB, P, PHI, ierr );
end
BB = C1*(1/CPB*TB*DVDTB*C0*(1-TW/TB) + 1/CPU*TU*DVDTU*(1-C0)*(1-
TW/TU));
DX = 0.5*sin( pi*(THETA-THETAS)/THETAB )*180/THETAB;
CC = -(VB-VU)*DX - DVDTB*(HU-HB)/CPB*(DX-(X-
X^2)*BLOWBY/OMEGA);
DD = X*(VB^2/CPB/TB*(TB/VB*DVDTB)^2 + DVDPB);
EE = (1-X)*(1/CPU*TU*DVDTU^2 + DVDPU);
HL = (1-X^2)*HU + X^2*HB;
YPRIME(1) = (AA + BB + CC)/(DD + EE);
YPRIME(2) = -C1/CPB/C0*(TB-TW) + 1/CPB*TB*DVDTB*YPRIME(1)+(HU-
HB)/CPB*(DX/X - (1-X)*BLOWBY/OMEGA);
YPRIME(3) = -C1/CPU/(1+C0)*(TU-TW) + 1/CPU*TU*DVDTU*YPRIME(1);
```

```
else
 [~, HL, ~, ~, ~, ~,CP, ~,DVDT,DVDP]=fargH2(TU,P,PHI,F,fuel_type);
BB = C1*1/CP*TU*DVDT*(1-TW/Y(3));
CC = 0;
DD = 0;
EE = 1/CP*TU*DVDT^2 + DVDP;
YPRIME(1) = ( AA + BB + CC )/(DD + EE);
YPRIME(2) = 0;
YPRIME(3) = -C1/CP*(Y(3)-TW) + 1/CP*Y(3)*DVDT*YPRIME(1);
end
YPRIME(4) = Y(1)*DV;
YPRIME(5) = 0;
if ( ~isnan(TB) )
YPRIME(5) = YPRIME(5) + C1*M*C0*(TB-TW);
end
if ( ~isnan(TU) )
YPRIME(5) = YPRIME(5) + C1*M*(1-C0)*(TU-TW);
end
YPRIME(6) = BLOWBY*M/OMEGA*HL;
if ( X > 0.001 )
for k=1:NNOX
if ( THETA >= THETAS + (k-1)/(NNOX-1)*THETAB )
YPRIME(6+k) = zeldovich( TB, P/100, YB, Y(6+k)/(MW_NO*VB*1000) )*MW_NO*VB*1000/OMEGA;
end
end
end
for JJ=1:NY
YPRIME(JJ) = YPRIME(JJ)*pi/180;
end
end
end
function [ dNOdt ] = zeldovich( T, P, y, NO )
k1 = 7.6*10^13*exp(-38000/T);
k2r = 1.5*10^9*T*exp(-19500/T);
k3r = 2*10^14*exp(-23650/T);
N_V = (100000*P)/(8.314*T)*(1/100)^3;
N2e = y(3)*N_V;
He = y(7)*N_V;
Oe = y(8)*N_V;
NOe = y(10)*N_V;
R1 = k1*Oe*N2e;
R2 = k2r*NOe*Oe;
R3 = k3r*NOe*He;
alpha = NO/NOe;
dNOdt = 2*R1*(1-alpha*alpha)/(1+alpha*R1/(R2+R3));
end
end
```