"Mathematical Modeling of Bioethanol Fueled DI Diesel Engine"

(A thesis submitted in partial completion of the requirements for the degree of B.Tech in Mechanical Engineering)

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CERTIFICATE

This is to certify that the thesis submitted by Mr. Soham Acharya in partial completion of the requirements for the felicitation of Bachelor of Technology Degree in Mechanical Engineering at National Institute of Technology, Rourkela is a valid work carried out by him under my guidance. To the best of my knowledge the matter embodied in the thesis has not been submitted to any University/Institute for the award of any Degree or Diploma.

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ABSTRACT

In the present scenario, the energy security and environmental issues are matter of concern for every nation. The discovery of a new ecofriendly renewable fuel source is extremely important to overcome this problem. Biofuels mainly biodiesel and bioethanol are gaining importance as an alternative fuel for transportation sector due to their biodegradable and renewable nature. Bioethanol can be explored from different feed stock such as sugar, starch and waste material. It is an oxygenated fuel and able to reduce both NOx and particulate matters in large amount. So it is a good alternative fuel for CI engine. In this project, a zero dimensional, quasi steady diesel engine simulation model is developed to prove the bioethanol as a fuel for diesel engine. By using modern analysis and simulation tool like MATLAB we can drastically decrease the need for experiment and hence save a lot of time and money. Thus by taking some assumptions and applying basic thermodynamic properties a model to predict the pressure and volume variation in the cylinder of the CI engine with the given fuel has been developed in this project.

CONTENTS

SYMBOLS AND ABBREVIATIONS

dQ/dH	rate of heat release from cylinder walls=A
P	pressure
V	instantaneous cylinder volume
m	mass
r	gas constant
T	temperature
dT/dθ	change of temperature with crank angle=B
dP/dθ	change of pressure with crank angle=C
dV/dθ	change of volume with crank angle=D
h	heat transfer coefficient
A	heat transfer area
Tw	wall temperature
Vcl	cylinder clearance volume
λ	crank radius to piston length ratio
k	thermal conductivity of the cylinder gas
d	cylinder bore
R	Reynolds number
BC	cylinder bulk gas temperature
Q	heat losses
Qc	cumulative heat release rate
LCV	lower calorific value of fuel
n	engine speed
ρf	density of fuel
cos(theta)	angular position of crank shaft=F

Chapter 1

Introduction

1. General

The engine converts heat energy obtained from the chemical combination of fuel with oxygen, into mechanical energy. Since the heat energy is derived from the fuel, a fundamental knowledge of the types of fuel and their characteristics is essential in order to understand the combustion phenomenon. The characteristics of the fuel used have considerable influence on the design, efficiency, output and particularly, the reliability and durability of the engine. IC engines can be operated on different types of fuels such as liquid, gaseous and even solid fuels depending upon the types of fuels to be used in the engine has to be designed accordingly.

1.1. Types of fuel

Different types of fuels are used in IC engine which are explained below:

1.1.1. Solid fuels

The solid fuels find little practical application at present because of the problems in handling the fuel as well as in disposing off, the solid residue or ash after combustion. However, in the initial stages of the engine development, solid fuels such as finely powdered coal were attempted. Compared to gaseous and liquid fuels, the solid fuels are quite difficult to handle and storage and feeding are quite cumbersome. Because of the complications in the design of the fuel feed systems these fuels have become unsuitable in solid forms. Attempts are being made to generate gaseous or liquid fuels from charcoal for the use in IC Engine.

1.1.2. Gaseous fuels

Gaseous fuels are ideal and pose no problems what so ever in using them in IC engine. Being gaseous, they mix more homogenously with air and eliminate the distribution and starting problems that are encountered with liquid fuels. Even though the gaseous fuels are the most ideal for IC engines, storage and handling problems restrict their use in automobiles. Consequently, they are more commonly used for stationery power plants locate near the source of availability of fuel. Some of the gaseous fuels can be liquefied under pressure for reducing the storage volume. But this arrangement is very expensive as well as risky. Because of the energy crisis in the recent years, considerable research efforts are being made to improve the design and performance of the gas engines, which became obsolete when liquid fuels, came into use. The different types of gaseous fuels are given below;

1.1.2.1. Natural gas

Natural gas can be obtained from the earth surface found naturally. The gas is produced due to the thermogenic action i.e. when plants and animals are buried under the earth surface over the period of thousand years, and exposed to intense heat and pressure then gas will generated. It is colourless, odourless gas and mostly composed of methane. This natural gases are mainly available in the market is in the form of compressed natural gas (CNG) and liquefied natural gas (LNG). Natural gas can also be converted into liquid fuel like gasoline, diesel or jet fuel by gas to liquid (GTL) technologies. Natural gas is a clean burning fuel, emits less emission to the atmosphere, can be efficiently and safely stored. Natural gas can also be produce by biogenic mechanisms from methanogenic organisms in marshes bogs, landfills and shallow sediments. It is also known as renewable natural gas or biogas.

1.1.2.2. CNG

CNG is a compressed natural gas (mostly methane), stored and distributed at a pressure of 200-248 bar in a cylindrical and spherical container. It can be used in place of gasoline, diesel fuel and propane/LPG. It is safer, low cost and produces fewer undesirable gases compared to above mentioned fuel. CNG is used increasingly in large cities of India like Delhi, Ahmedabad, Mumbai, and Kolkata. In world it is also used in Latin America, Europe and North America. The highest numbers of CNG vehicles run in world are India, Pakistan, Iran, Argentina and Brazil. Advantages of CNG are better mixing characteristics, no lead content, increased life of lubricating oil, low maintenance cost compared to other hydrocarbon fuelled vehicles, prevent spill and evaporation losses, and provide less pollution and more efficiency.

1.1.2.3. LNG

Liquefied natural gas (LNG) is liquid form of natural gas. It is formed when natural gas is condensed into a liquid at close to atmospheric pressure set at around 25 kPa by cooling it to approximately -162°C. LNG has higher volumetric or energy density compared to CNG, approximately 2.4 times greater than the CNG which makes it economical to transport natural gas. The energy density of LNG is comparable to propane and ethanol, but is only 60% compared to that of diesel and 70% that of gasoline. The specially designed cryogenics sea vessels or cryogenic road tankers are used for the transportation of LNG. LNG application in heavy duty engine achieves significantly lower NOx and particulate emission compared to diesel.

1.1.2.4. LPG

Liquefied petroleum gas (LPG) is propane or butane a by-product of natural gas processing and petroleum refining. The processing of natural gas involves removal of butane, propane, and large amounts of ethane from the raw gas and cracking of petroleum into gasoline or heating oil produces by product of propane. Propane vehicles are used almost all over the world. There are two types of propane vehicles used such as dedicated and bi-fuel. Dedicated propane vehicles are designed to run only on propane, while bi-fuel propane vehicles have two separate fuelling systems that enable the vehicle to use either propane or liquid fuel. The power, acceleration, and cruising speed of propane vehicles are similar to those of conventionally-fueled vehicles. Due to low maintenance cost it is widely used in light duty vehicles such as pickup trucks and taxis, and in heavy-duty vehicles. There will be no cold start problems due to better fuel air mixture which is associated with liquid fuel. Depending upon the vehicle type and drive cycle, propane vehicles can produce less harmful emission compared to diesel and gasoline.

1.1.2.5. Hydrogen

Hydrogen (H_2) is a potentially emissions-free/zero emission alternative fuel that can be produced from steam reforming process of methane, electrolysis, and steam electrolysis. Hydrogen is gas at room temperature, so it can be stored in compressed gas cylinder or in liquid form with high pressure. Liquid hydrogen storage is preferred to compressed gas storage since more hydrogen can be stored in the liquid state than in the gaseous state. Small vacuum tanks with a 100-liter capacity are available with a super insulation consisting of some 30 aluminum foil layers separated by plastic foil. Research work demonstrated that compressed hydrogen or liquid hydrogen can be a possible alternative fuels for ICE's, gas turbine engines, or fuel cells. Hydrogen has higher energy density which supplies more energy per unit volume than gasoline, diesel, or kerosene, lower the emission, abundantly available and can be easily produces by water.

Hydrogen can also be generated from renewable sources such as thermochemical gasification coupled with water gas shift, fast pyrolysis followed by reforming of carbohydrate fractions of bio-oil, direct solar gasification, biomass derived syngas conversion, microbial conversion of biomass etc. Hydrogen can be produced by following oxidative pyrolysis process,

$$\text{Biomass} + O_2 \longrightarrow CO + H_2 + CO_2 + \text{energy}$$

1.1.2.6. Biogas

Biogas is produced from the biodegradable waste material or energy crops by the process of anaerobic digestion with the help of anaerobes. The solid by-products are used in fertilizer. The present sources of biogas are mainly landfills, sewage, and animal/agri-waste. This is efficient way of energy conversion, renewable energy, reduce the unemployment, better energy security, increase economy. It is used in IC engine in dual fuel mode.

1.1.2.7. Syngas

It is produced by partial combustion of biomass. It consists of mixture of carbon monoxide, hydrogen and other hydrogen. Before partial combustion, the biomass is dried, and sometimes pyrolysed. Syngas are burned directly in internal combustion engines, turbines or high-temperature fuel cells. The wood gas generator, a wood fuelled gasification reactor, can be connected to an IC engine. Syngas can be used to produce methanol, DME and hydrogen, or converted via the Fischer-Tropsch process to produce a diesel substitute, or a mixture of alcohols that can be blended into gasoline. Gasification normally relies on temperatures greater than 700°C.

1.1.3. Liquid fuels

In most of the modern IC engines, liquid fuels which are derived from fossil fuels, biomass and waste of institute, industries are mostly used. However, petroleum products such as gasoline and diesel are the main fuels for IC engines as on today. Other liquid fuels such as biodiesel, bioethanol, hydrogen fuel are gaining importance in transportation sector due to their availability and less pollution. The types of liquid fuels are discussed below,

1.1.3.1. Biodiesel

It is produced from vegetable oils of edible or non edible type or animal fat or algae by transesterification method using some catalyst. Edible feed stocks such as sunflower oil, soy etc. or non edible feed stocks such as jatropha, karanja, mahua etc. are commonly used. Biodiesel has better lubricating properties and much higher cetane ratings than today's low sulfur diesel fuels. Biodiesel addition reduces fuel system wear. Biodiesel can be used in pure form (B100) or may be blended with petroleum diesel at any concentration in most injection pump diesel engines for transportation purpose. But engine may face problem of low temperature operation, durability and drop in power. Blends of 20% biodiesel and lower can be used in diesel equipment with no, or only minor modifications.

1.1.3.2. Ethanol/Bioethanol

Ethanol can be produce from the chemical method in petrochemical industry. Bioethanol is produced from biomass feed stock by fermentation process in the presence of yeast or enzyme. Ethanol/bioethanol can be produced from corn, maize, wheat, grain, cellulosic material, waste of industries, institution etc. Ethanol can be used in petrol engines as a replacement for gasoline; it can be mixed with gasoline to any percentage. Most existing car petrol engines can run on blends of up to 15% bioethanol with petroleum/gasoline. Ethanol has a smaller energy density than that of gasoline; which requires more fuel (volume and mass) to produce the same amount of work. It can also be used in diesel engine by adopting different techniques such as blending, emulsion, addition of ignition improver, fumigation, and dual fuel operation. Advantage of using ethanol/bioethanol is its renewable nature, lower GHG emission, high octane rating.

1.1.3.3. Pyrolysis oil

Pyrolysis oil is another type of fuel derived from the lignocellulosic fraction of biomass by rapidly heating the biomass in the absence of oxygen (pyrolysis) with or without help of catalyst. It consumes more energy to break down the complex compound. It can also use the wastage material such as plastics, tire etc. to produce oil.

1.1.3.4. Green diesel

It is produced by the hydrocracking of vegetable oils and animal fats in the presence of catalyst at an elevated temperature, pressure where the larger molecules are break down into smaller molecule chain. It has similar properties as in petro-diesel. It does not require new engines, pipelines or infrastructure to distribute and use, but has not been produced at a cost that is competitive with petroleum. The development of green diesel is still in infant stage.

1.1.3.5. Bio ethers

These are oxygenated fuels produced by the reaction of reactive iso-olefins, such as iso-butylene, with bioethanol. The examples are dimethyl ethers (DME), diethyl ether (DEE), methyl tertiary-butyl ether (MTBE), ethyl tertiary-butyl ether (ETBE), tertiary-amyl methyl ether (TAME), tertiary-amyl ethyl ether (TAEE). The MTBE and ETBE are used as additive instead of lead in Europe. Some are used in diesel engine. They enhance the engine performance, reduce engine wear and toxic emission mostly reduce the ground level ozone emission.

Chapter 2

Literature Survey

Many models have been developed by many researchers to solve the complex heterogeneous combustion process of diesel engines [1-9]. The rapid development of computer technology has encouraged the use of complex simulation techniques to quantify the effect of the fundamental processes in the engine systems. The advances achieved by current automotive engines would have been impossible without the simulation models providing these insights [10-11]. Lyn et al. [12] analyzed the effects of injection timing, injection velocity and fuelling rate on the delay period. An increase in speed at constant load increases the peak pressure and temperature, due to the decrease in heat transfer, resulting in a slight decrease in delay period as analysed by Wong et al. [13].

For engineering applications a semi-empirical relation based on chemical chain reactions called as Weibe's function is used to find heat release rate [14-15]. However a single Weibe's function is not able to predict the heat release rate during early premixed burning. Thus a double Weibe's function is required for accurate prediction direct injection diesel engine [14, 6].

Bioethanol has a relatively low flash point, a high heating value, high density and high viscosity comparable to those of petroleum derived diesel. Many studies show that unburned hydrocarbons (HC), carbon monoxide (CO) and sulfur levels are significantly less in the exhaust gas while using bioethanol as fuel. However, a noticeable increase in the oxides of nitrogen (NOx) levels is reported with bioethanol [17-20]. Bioethanol blends reduce levels of global warming gases such as CO_2. Its additional advantages are biodegradability, higher combustion efficiency and low toxicity as compared to other fuels. Bioethanol is a fuel with high octane number which makes it suitable for spark ignition engines. It can also be used in CI engine by adopting technologies such as emulsion/blends, fumigation, dual fuel mode, surface ignition method and addition of ignition improver.

Chapter 3

Model Description

3.1. Assumptions made

1) Zero dimensional flow condition is assumed

2) The gas in the cylinder is always in a state of equilibrium

3) There is no leakage of gas i.e. mass of the system remains constant

4) The speed of the crank remains uniform throughout the motion

5) The gas is air which follows all ideal gas laws

6) The specific heat is a function of temperature

7) The pressure and temperature are only functions of the crank angle

Pressure and temperature is found by solving the differential equation

For temperature solve

B= (1/MCv)*A-(hA(T(theta)-T(w))/mc)-RT/(V*Cv)*D

For pressure

C= (A-(Y/(Y-1)PD)/((Y-1)/Y)

Rate of heat release from the cylinder walls

A= hA(T(theta)-T(w))

Gas properties during combustion is calculated assuming the gas to be undergoing isentropic processes through out.

P(theta+1)= P(theta)(V(theta)/V(theta+1))^n

T(theta+1)=T(theta)(V(theta+1)/V(theta))^(n-1)

Chapter 4

Weibe's Combustion Model

Wiebe function is used to predict the mass fraction burn and burn rate in internal combustion engines operating with different combustion systems and fuels [14]. Wiebe linked chain chemical reactions with the fuel reaction rate in internal combustion engines and his approach was based on the premise that a simple one-step rate equation will not be adequate to describe complex reacting systems such as those occurring in an internal combustion engine. Moreover, developing and solving rate equations which account for the simultaneous and sequential interdependent chain and chain branching reactions would be time consuming and tedious task. He argued that for engineering application the details of chemical kinetics of all the reactions could be bypassed and a general macroscopic reaction rate expression could be developed based on the concept of chain reactions. The Wiebe's functions for the non-dimensional burn fraction x and its derivative w (burn rate) as functions of degrees crank angle.

Net Soot Formation Model

The exhaust of CI engines contains solid carbon soot particles that are generated in the fuel rich regions inside the cylinder during combustion. Soot particles are clusters of solid carbon spheres with HC and traces of other components absorbed on the surface. They are generated in the combustion chamber in the fuel rich zones where there is not enough oxygen to convert all carbon to CO_2. Subsequently as turbulence motion continues to mix the components most of these carbon particles find sufficient oxygen to react and form CO_2. Thus soot particles are formed and consumed simultaneously in the combustion chamber. The model is given as,

dm(soot)/dt=Cbs*(phi)*Mf*p^0.5*e^(-Esf/RaT)

The constant Cbs needs to be defined and modified.

Friction power calculation

Friction losses are extremely detrimental in the determination of the power lost and thus the net efficiency of the system. Friction losses happen due to,

1) Pressure lost to overcome friction caused by the gas behind the rings

2) Losses due to wall tension of rings

3) Pressure lost due to friction between the piston and ring

Thermal energy balance

$Q=Cv*Mf$ (kJ/h)

Q is the latent heat supplied by fuel

Cv calorific value of fuel in (kJ/kg)

Mf= mass of fuel consumption (kg/h)

Useful work (q1) = brake power *3600 (kJ/h)

Percentage of useful work = useful work/Q*100 Heat loss through exhaust

$q2=(Ma+Mf)*Cpg*(Tg-Ta)$ (kJ/h) Ma = mass of air consumption (kJ/h)

Cpg= specific heat of gas t different exhaust temperature (kJ/kg °C)

Ta=atmospheric temperature (°C)
Tg=exhaust gas temperature (°C)

Chapter 5

MATLAB Codes

1) For calculating the indicative power

function ip = calcIP(imep,l,a,n,k)

ip=(imep*l*a*n*k)/(60*1000);

end;

2) Calculate the mean effective pressure lost due to gas behind the cylinder function

fmep1=0.42*(Pa-Pimf)*(S/d^2)+1.82*(r^(1.33-0.34)*(sp/1000)*10; end;

3) Calculate the mean effective pressure absorbed by friction due to wall tension of rings

function fmep2=calcfmep2(snpr,d2)

fmep2=(10*0.377*snpr)/d2;

end;

4) Mean effective pressure absorbed by friction due to piston and ring function

fmep3=calc fmep3(pst,ds,sp) fmep3=12.85*((pst/ds)+(100*sp/1000));

end;

5) For pressure assuming isentropic property function pt1=calcPt1(pt,vt,vt1,n)

pt1=pt*(vt/vt1)^n;

end;

(at the start pressure is 1 bar and initial volume is 250 cc)

6) For temperature

function tt1=calcTt1(tt,vt,vt1,n) tt1=tt*(vt1/vt)^(n-1);

end;

7) For calculating brake power function

bp=calc(Bp(TP,ip) bp=ip-fp;

end;

8) Calculate brake thermal efficiency function

nth=calcBth(bp,mf,cv) bth=bp/(mf*cv);

end;

9) For calculating volume

function vtheta=calcVtheta(Vd,r,theta,l,s) a=cos(theta);

b=sin(theta);

c=L/S; d=r/(r-1);

vtheta=Vd*(d*(1-a)/2+c-0.5sqrt(4*(c^2)-b^2)); end;

(Here we take Vd=250,l=110,r=50,s=100)

For plotting graphs

1) For v(theta) Vtheta=0:6; theta=0:6; for

i=0:6

vtheta(i+0.1)=calcVtheta(250,55,i,110,100); end

plot(theta,vtheta);

2) For p(theta) theta=0:6; ptheta=0:6; for i=

0:6

ptheta(i+0.1)=calc pt1(2,calcVtheta(250,55,i,110,100);

calcVtheta(250,55,1+0.1,110,100),1.414);

end plot(theta,ptheta);

Chapter 6

Results and Discussion

5.1. Pressure-crank angle diagram

Figure 1 is the pressure curve with respect to the crank angle for the fuel under full load condition. In a compression ignition engine, cylinder pressure depends on the burned fuel fraction during the initial stage of combustion and the ability of the fuel to mix well with air and burn. High peak pressure and maximum rate of pressure rise are corresponding to large amount of fuel burned in the initial stage. It is found out from the experiment that the peak pressure for diesel, bioethanol are 77.23, 90.61 bar respectively. For the simulated conditions the peak pressure values are 71 .48, 73 .88 bar respectively. In both the cases the combustion of bioethanol starts before the diesel. The peak cylinder pressure of bioethanol is higher than diesel. It is due to high viscosity and low volatility.

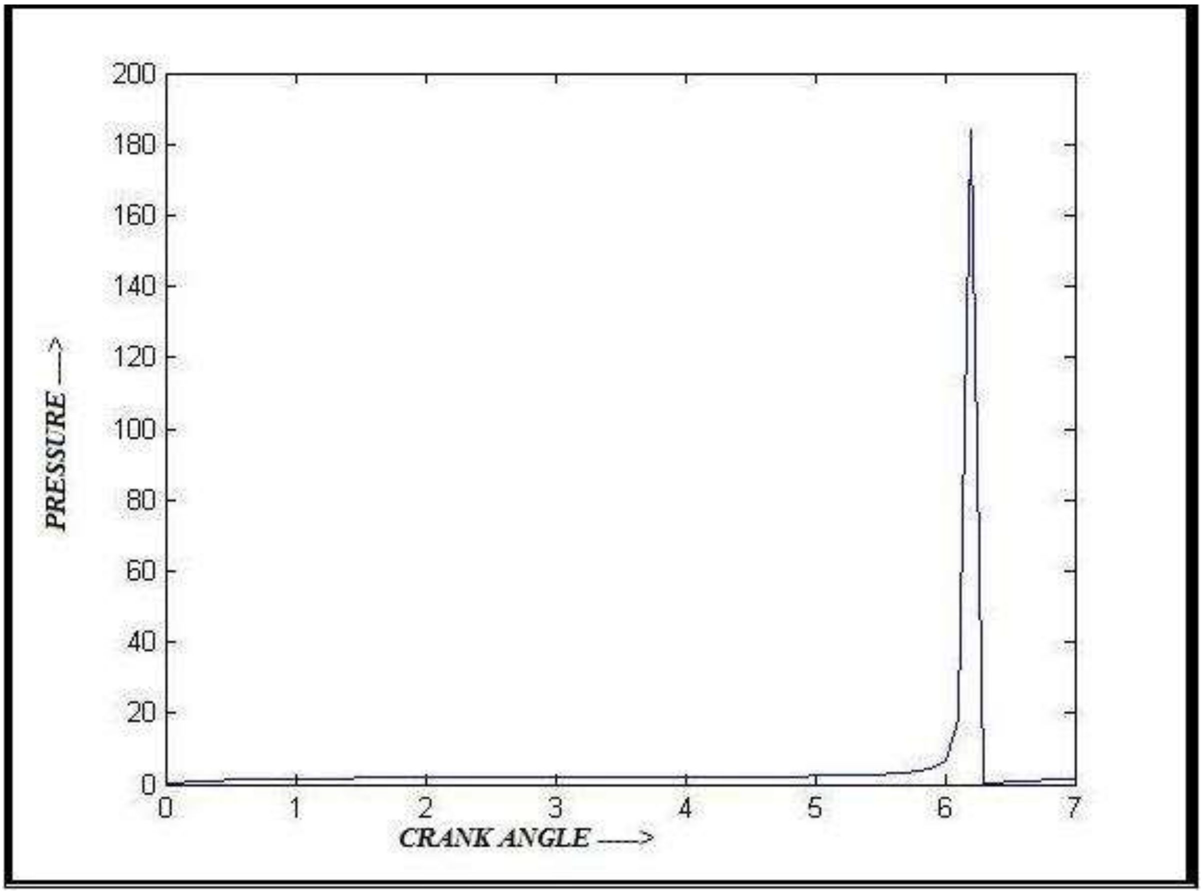

Figure 1. Variation of pressure with crank angle

5.2. Apparent or Net heat release rate

The net heat release rate is found out from the heat transferred to the cylinder walls, crevice volume, blow-by and the fuel injection effects from heat energy liberated by burning the fuel. Maximum net heat release rate for diesel and bioethanol are 52.31 and 50.01 J/°CA respectively at full load. At simulated conditions, it is found to be 54.12 and 50.03 J/°CA respectively at full load. It is also seen that combustion is shorter for bioethanol due to the rate of burning being high in these two and also the presence of oxygen in the molecular structure.

5.3. NO formation

In diesel engine exhaust, NOx is primarily composed of NO, with lesser amounts of NO_2. Other oxides of nitrogen, such as N_2O, N_2O_5, NO_3 are negligible. Under most diesel engine combustion conditions, thermal NOx is believed to be the predominant contributor to total NOx. At high temperatures, occurring within the combustion chamber of a diesel engine, N_2 and O2 can react through a series of chemical steps known as the Zeldovich mechanism. NOx formation occurs at temperatures around 1500 °C, and the rate of formation increases rapidly with increasing temperature.

5.4. Volume variations

The volume during the combustion of fuel can be computed with the help of MATLAB code which is shown in Figure 2.
The variation of volume with crank angle is as follows;

For

1)theta =0 ;V=0

2)theta=1 ;V=79.437

3)theta=2 ;V=204.8850

4)theta=3 ;V=253.8219

5)theta=4 ;V=227.316

6)theta=5 ;V= 118.6984

When we compare these with the values for diesel which has been computed through experimentation we find out that bioethanol engine shows a greater volumetric efficiency.

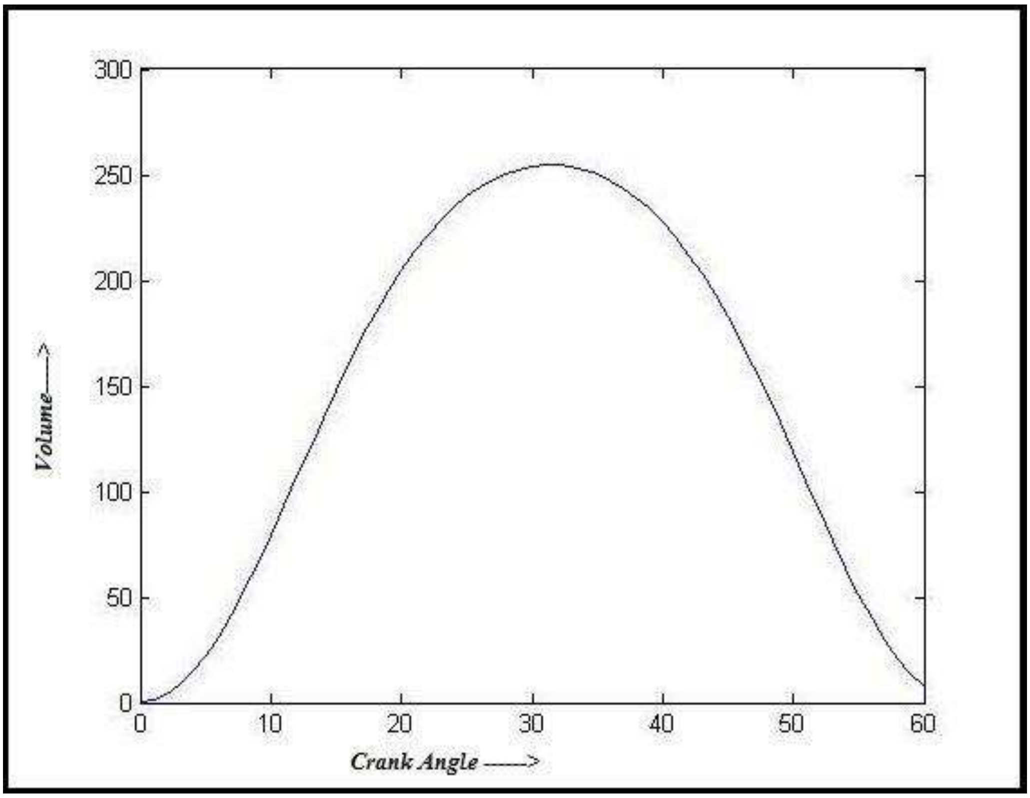

Figure 2. Variation of volume with crank angle

Chapter 7

Conclusions

The zero dimensional simulation for bioethanol fueled diesel engine was done successfully and results have compared with diesel and conclude that,

1) The peak cylinder pressure for bioethanol is higher than that of diesel.

2) The maximum heat release rate of bioethanol is lower than that for diesel.

3) The NO emission for diesel is higher than that for bioethanol due to the presence of oxygen in the molecular structure of bioethanol which leads to a more complete combustion.

4) The soot is emission also decreased due to similar reason as above.

5) Bioethanol shows a higher volumetric efficiency than diesel.

6) The presented model can predict the combustion and emission characteristics like pressure in the cylinder, heat exchanged, NO emissions, soot densities, volumetric efficiency and the results obtained are quite similar to those obtained through experimentation.

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