MODELING AND SIMULATION OF BIO-FUELED CONVENTIONAL ENGINE

by

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DECLARATION

I hereby declare that this submission is my own work and that, to the best of my knowledge and belief, it contains no material previously published or written by another person nor material which has been accepted for the award of any other degree or other institute of higher learning, except where due acknowledgement has been made in the text.

(Bhanu Pratap Singh)

CERTIFICATE

This is to certify that the thesis entitled entitled "Modeling and simulation of biofueled conventional engine" submitted by Bhnau Pratap Singh to University of Petroleum & Energy Studies for the award of the degree of Doctor of Philosophy is a bonafide record of the research work carried out by him under my supervision and guidance. The content of the thesis, in full or parts have not been submitted to any other Institute or University for the award of any other degree.

(Dr. P.K.Sahoo)

Place: Date:

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EXECUTIVE SUMMARY

There were more than 50 million cars produced worldwide in 2007. The car production increase by 5% every year. This development of automotive market brings many negative aspects that need to be seriously considered by automotive industry. Firstly, the internal combustion engine has become one of the major polluting contributors to our environment. Secondly, the oil prices increase every year as the oil is being depleted at high rates. These circumstances force the engine manufacturers to develop and apply new ideas for combustions engines. New technologies coming from this development allow producing less polluting and much more efficient combustion engines. These modern engines face several other challenges: to reduce emissions of pollutant species and fuel consumption, to increase power and safety, to improve drivability and passengers comfort.

The current interest regarding how to stop the global warming has put focus on the automobile industry and forced them to produce vehicles/engines that are more environmental friendly. This has led to the development of increasingly complex control system of the engines. The introduction of common-rail systems in regular automotives increased the demand of physical models that in an accurate way can describe the complex cycle within the combustion chamber. With these models implemented it is possible to test new strategies on engine steering in a cost- and time efficient way.

All the above mentioned issues can be solved only by using advanced electronic control systems. Nowadays, these control systems are mainly based on experimental data. For every type of engine the measurements concerning the fuel economy and pollutants emissions are made. These measurements include successive changes of each of the many parameters involved in order to cover all the operating conditions of the engine. This is very expensive and time consuming. There is an obvious alternative to the experimental approach, a computer simulation of the engine processes using a mathematical model. This approach allows easily trying and examining the effects of various designs and setups. The reliable model reduces the need for complex experimental analysis of the engine and consequently reduces the financial costs in the development.

There are two primary objectives of this thesis. The first aim is to modify and validate a mathematical model. This model should allow simulating the pressure and temperature in the cylinder during the engine cycle as well as the engine performance parameters. This model is not meant to be used in real-time applications and cannot be directly incorporated into the electronic control unit. At the same time the model should be easily adjustable to any engine. The second aim is to control the engine performance. Various control strategies will be implemented and compared.

The objectives of this thesis can be summed up as modify mathematical model for predicting the variation of fuel injection angle by using diesel and jatropha oil as fuel, model for observing the effect of injection pressure, model for analyzing the effect of fuel inlet temperature on engine performance and simulation of the modified model for engine performance by F-Chart Software.

The combustion process can be described with varying complexity and accuracy. Normally the degree of complexity is decided by the number of zones in which the cylinder has been divided. An engine model therefore is either single-zone or multi-zone. In a single-zone model the gas mixture within the cylinder is considered to be homogenous for each sample. It is also assumed to be made up strictly of ideal gases. In a multi-zone model, for example the two-zone model, the gases are still considered ideal. However, the homogenous approach has been replaced by a heterogeneous one. Here the cylinder is also divided into two zones, one containing burned zone and the other unburned. Each zone itself is homogenous and no heat transfer occurs between the two zones. The simplicity of the single-zone model is its biggest advantage. This makes it fast and therefore applicable in real time systems. The multi-zone model is more complex and more accurate compared to the single-zone model. A multi-zone model is often needed for combustion chamber design, but for most aspects of control design a two-zone model is good enough.

The equations of the model adopted in the thesis are suitable for any hydrocarbon fuel as diesel, vegetable oil and biodiesel etc. These equations are solved numerically using with time step size of $0.5⁰$ crank angle. The engine geometrical parameters, molecular weight of gaseous products and various constants used in the model are defined. The input parameters used in model are injection pressure, crank angle and the molecular formula of the diesel and jatropha oil. The several physical, chemical and thermal properties are also measured and calculated as input parameters .The properties of gaseous constituents such as enthalpy, internal energy and specific heats are calculated as a function of temperature. The pressure and temperature of the gases in the combustion chamber are calculated for every half degree crank angle. From the typical design of the engine, the combustion chamber volume at every degree crank angle is calculated with the help of modified model equation. In the combustion modeling the molecular formula of diesel fuel is taken as $C_{10}H_{22}$. From the fatty acid composition, jatropha classifies it as linoleic or oleic acid types, which are unsaturated fatty acids. So based on these properties, the molecular formula of jatropha oil is approximated as $C_{18}H_{32}O_2$. In general, this combustion model, developed for C.I engine analysis is suitable for any hydrocarbon fuel. This includes diesel, biodiesel or their blends as well as vegetables oil. The engine model is analyzed for the variation in fuel injection pressure, point of fuel injection and fuel inlet temperature for the diesel as well as jatropha oil.

To validate the model, a comparison is given in the present work between the results obtained from the simulation model and the ones obtained from an

experimental investigation conducted in the U.P.E.S.Dehradun. The comparison between the calculated and experimental value determined for 1000 rpm engine speed and 7.35 kW load examined. The coincidence between calculated and experimental values is good, verifying the accuracy of the simulation model. The values obtained from the proposed model and the detailed one are practically the same for all test conditions examined. Furthermore, in order to validate the model against existing sophisticated models and to find the level of significance in case of diesel fuel BTE, a chi-square test is performed.

A two zone thermodynamic model is modified for analyzing the performance characteristics of the compression ignition engine. The model is modified in such a way that it can be used for characterizing any hydrocarbon-fueled engines, as diesel or biodiesel. The modeling results showed that, with increase in fuel injection pressure brake thermal efficiency is increased and brake specific fuel consumption and smoke opacity are decreased. The performance characteristics of the engine follow the same trend for all fuels as diesel, preheated jatropha and unheated jatropha oil. The predicted results are compared with the experimental results of the engine fueled by diesel, jatropha (PH) and jatropha (UH). This model predicted the engine performance characteristics in closer approximation to that of experimental results. Hence, it is concluded that this modified model can be used for the prediction of the performance characteristics of the compression ignition engine fueled by any type of hydrocarbon fuel.

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LIST OF SYMBOLS

- A_n cross sectional area of nozzle, m²
- d cylinder bore, m
- k thermal conductivity, $W/m K$
- L connecting rod length, m
- l stroke length, m
- m mass of the mixture $air + fuel$ contained in the combustion chamber, kgs
- N engine speed, rpm
- Pcylinder pressure, pascal
- Q heat energy, joule
- R universal gas constant, kJ/mol K
- Re Reynolds's number
- T temperature, K
- V instantaneous cylinder volume, $m³$
- V_p mean piston speed, m/s
- V_{θ} volume at any crank angle, $m³$
- V_c clearance volume, $m³$

Greek

- θ crank angle ,degrees
- $\Delta\theta$ computational step, ^oCA
- Δ*P* pressure difference, pascal
- ρ density, kg/m³
- ϕ fuel air equivalence ratio, dimensionless
- v kinematic viscosity, m^2 /sec
- σ surface tension of fuel, N/m
- *γ* specific heat ratio, dimensionless
- µ dynamic viscosity, kg/m s

Subscripts

- a air
- b burned zone
- c carbon
- com combustion
- f fuel
- h hydrogen
- inj fuel injection
- min minimum
- n species number, or nozzle hole
- o oxygen
- p piston
- u unburned zone
- w wall

LIST OF ABBREVIATIONS

- BTE brake thermal efficiency
- BSFC brake specific fuel consumption (kg/kWh)
- BTDC before top dead center
- CN cetane number
- EVO exhaust valve opening
- EES engineering equation solver
- IVC inlet valve closing
- NO nitric oxide (ppm)
- PM particulate matter
- PAHs polycyclic aromatic hydrocarbons
- rpm revolutions per minute
- SMD sauter mean diameter (m)
- TDC top dead center
- PPO pure plant oil
- HM heavy metals

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 at speed 1000 rpm, 80% of full load and static 17.5 MPa injection pressure

Jatropha oil (preheated) fueled engine

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CHAPTER 1 INTRODUCTION

The majority of the world's energy needs are supplied through petrochemical sources, such as coal and natural gases. With the exception of hydroelectricity and nuclear energy, all of these sources are finite and at current usage rates will be consumed shortly. The high energy demand in the industrialized world as well as in the domestic sector and pollution problems caused due to the widespread use of fossil fuels make it increasingly necessary to develop renewable energy sources of limitless duration and smaller environmental impact than our traditional sources. This has stimulated recent interest in alternative sources for petroleum-based fuels [1]. Petroleum based fuels became the primary source of energy for transportation needs in the 20th century. This has continued in the beginning of the 21st century with almost all vehicles running on gasoline, diesel or natural gas [2]. As time passed, the oil industry invested in infrastructure to enable long-distance diffusion of easily exploitable and thus cheaper petroleum resources, thereby halting the development of biofuels as alternatives to mineral oil-based petrol and diesel. After the oil crises of the 1970s, bio-fuels briefly gained new momentum, but interest declined when oil prices returned to lower levels [3].

The bio-fuels to be considered as relevant technologies by both developing and industrialized countries are due to a number of factors, including energy security reasons, environmental concerns, foreign exchange savings, and socioeconomic issues related to the rural sector. Increasing use of bio-fuels for energy generation purposes is of particular interest nowadays because they allow mitigation of greenhouse gases, provide means of energy independence, and may even offer new employment possibilities [4]. Bio-fuels are thought to be the best

hope in these and Power's are also eco-friendly. These fuels are non-toxic, biodegradable, and free of sulphur and carcinogenic compounds like benzene [5]. Bio-fuels are being investigated as potential substitutes for current high pollutant fuels obtained from conventional sources [6]. Bio-fuels are liquid or gaseous fuels made from plant matter and residues, such as agricultural crops, municipal wastes and agricultural and forestry by-products. Liquid biofuels being considered the world over fall into the following categories: (a) vegetable oils and biodiesels; (b) alcohols; and (c) biocrude and synthetic oils. Liquid bio-fuels can be used as an alternative fuel for transport, as can other alternatives such as liquid natural gas (LNG), compressed natural gas (CNG), liquefied petroleum gas (LPG) and hydrogen. Figure 1.1 shows the resources of main liquid bio-fuels for automotives.

Figure 1.1 Resources of main liquid bio-fuels for automotives

Main advantages of bio-fuels are to represent a carbon dioxide $(CO₂)$ cycle. In combustion, most of them have better emissions, are biodegradable and contribute to sustainability. Also bio-fuels have considerable environmentally friendly potential.

1.1 GLOBAL BIO FUEL SCENARIOS

Brazil and the United States have the largest programs promoting bio-fuels in the world. The European Union (EU) is in the third rank of bio-fuel production worldwide, behind Brazil and the United States. In Europe, Germany is the largest and France the second largest producer of bio-fuels. In 2002, the German Parliament decided to exempt all bio-fuels from the gasoline tax. The exemption is in force only until the end of 2009, and a report by the government on progress in market introduction of bio-fuels and on the price development of biomass, crude oil and fuels is required every other year to allow for adaptations if necessary According to the International Energy Agency (IEA), scenarios developed for the USA and the EU indicate that near term targets of up to 6% displacement of petroleum fuels with bio-fuels appear feasible using conventional bio-fuels, given available crop land. A 5% displacement of gasoline in the EU requires about 5% of available crop land to produce ethanol, while in the USA, 8% is required. A 5% displacement of diesel requires 13% of USA crop land and 15% in the EU. Land requirements for bio-diesel are greater, primarily because average yields (liters of final fuel per hectare of crop land) are considerably lower than for ethanol. Land requirements to achieve 5% displacement of both gasoline and Diesel would require the combined land total of 21% in the USA and 20% in the EU $[8]$.

Worldwide interest reflects convergence of developed and developing country perspectives on the role bio-fuels can play in energy for sustainable development [7]. The increase in bio-fuels utilization has also been accompanied over the past 3–4 years with policy decisions that encourage future growth of these fuels. The United States and several EU member states already pursue successful bio-fuel policy [9].

The recent commitment by the United States government to increase bioenergy three-fold in 10 years has added impetus to the search for viable biofuels [10]. Future conditions for an international bio-fuel market in Europe will largely be decided by the EU policies on renewable energy and their interplay with

national energy policies. So far, the Commission has indicated that biomass will play an important role in the future [11]. The most important piece of legislation for biofuels in Europe is the Biofuels Directive. Adopted in May 2003, it aims to promote the use in transport of fuels made from biomass, as well as other renewable fuels. The directive sets a reference value of 5.75% for the market share of bio-fuels in 2010, measured in terms of energy content [12]. In the Commission's view, mandating the use of bio-fuels will (a) improve energy supply security and (b) reduce greenhouse gas (GHG) emissions and (c) boost rural incomes and employment. Current regulations would preclude a notable negative impact on the rural environment [13]. In South America, Brazil also continued policies that mandate at least 22% bioethanol on motor fuels and encourage the use of vehicles that use hydrous ethanol to replace gasoline [14].

Figure1.2 shows the shares of alternative fuels compared to the total automotive fuel consumption in the world as a futuristic view. Hydrogen is currently more expensive than conventional energy sources. There are different technologies presently being practiced to produce hydrogen economically from biomass. Biohydrogen technology will play a major role in the future because it can utilize the renewable sources of energy.

Figure 1.2 Shares of alternative fuels compared to the total automotive fuel consumption in the world.

1.2 COMPETING FUELS

Bio fuels would not be the one and only substitute for fossil fuels is that biomass is that not only used for transport fuels, but also for other purposes. Besides all that, there are other fuels under development .The most promising competing fuels are as following.

- i. Bio diesels or methyl esters are produced by esterification of plant oil.Jatropha methyl ester is the biodiesel made of Jatropha oil. But other biodiesels are like Rape methyl ester(from Rapeseeds) and Sunflower methyl ester (from sun flower seeds).The properties of biodiesel are like those of fossil diesel and therefore can be used in most diesel engines without any or with little adjustments to the engine. It is also possible to use a blend of biodiesel and normal diesel, which is already very common in some countries.Esterification, is a process in which methanol reacts with the plant oil, producing the oil methyl ester and the side product glycerin.
- ii. Bio-ethanol is traditionally produced by fermentation of crops containing sugar or starch, like sugar beet, corn or grain. The biomass is converted by enzymes and bacteria at low temperature and pressure. A recent technology is to produce bio ethanol from lignocellulosic bio mass, which is woody and grassy material like poplar and eucalyptus.Bio ethanol can be used in conventional or adapted Otto engines. Just as with biodiesels it can be used in blends with gasoline as well.
- iii. Bio-methanol is produced from the products of biomass gasification. The gas mixture is converted by means of methanol synthesis.Bio-methanol can be used as bioethanol or in certain fuel cells it can directly substitute hydrogen. The fuel cell produces electricity with which the engine is driven.
- iv. Bio-DME (dimethylether) can be produced from the combination of gasification and DME-synthesis. This process is similar to that of methanol production. Another method is catalytic dehydratation of biomethanol, which is a chemical process with catalysis.Bio-DME has approximately the same properties as natural gas and it can be used in conventional diesel engines.
- v. Bio-ETBE (ethyl tertiary butyl ether) is bio–ethanol that has reacted with isobutylene. It is added to gasoline in order to raise the oxygen content. The result is reduction of emissions and higher octane number, which reduces the risk of knocking.
- vi. Bio-MTBE (methyl tertiary butyl ether) is similar to bio-ETBE, but is produced from bio methanol instead of bio-ethanol. It has the same application as bio-ETBE.
- vii. Biogas is the product of the fermentation of biomass. Fermentation is the degradation of wet biomass by microorganisms at low temperature and without the presence of oxygen. In order to be used as a transport fuel, the biogas should be upgraded to 98% methane content. If that is the case, it can be used in a gas engine.
- viii. Fischer –Tropsch diesel can be produced by gasifying biomass and converting the gas mixture into a liquid by the so –called Fischer-Tropsch synthesis process. The products are long hydrocarbons called waxes, from which by hydro cracking diesel fractions can be produced. This can be used in conventional diesel engines, either in a blend or pure.
- ix. SNG (Substitute Natural Gas) can be produced by several gasifying techniques, followed by a methanisation step, which increases the methane content in the gas. SNG is similar to natural gas and therefore can be used in normal gas engines.
- x. Bio-hydrogen is produced by gasifying or fermentation. The gasifying process is the same as for bio methanol, Fischer-Tropsch diesel and SNG.Fermentation is described in the biogas explanation. After one of

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these processes, the hydrogen content is increased by the steam-reforming step.Biohydrogen can be used either in fuel cells combined with an electric motor or in a combustion engine.

xi. HTU-diesel is diesel produced by the Hydro Thermal Upgrading process, which is developed only in the Netherlands. It is a conversion technique to convert wet biomass in to a liquid similar to crude oil and is therefore called biocrude.By the process of hydride oxygenation (HDO) bio crude can be converted in a fuel like diesel.

Several types of vegetable oils, with a diversified composition in fatty acids, can be used for the preparation of biodiesel. Soybean, rapeseed, sunflower and palm oils are the most studied. However, there are no technical restrictions to the use of other types of vegetable oils. Considering the type of alcohol, the use of methanol is advantageous as it allows simultaneous separation of the glycerol. The same reaction using ethanol is more complicated as it requires a water free alcohol, as well as oil with low water content in order to obtain glycerol separation

The use of vegetable oils as alternative renewable fuel competing with petroleum was proposed in the beginning of the 1980s. The advantages of vegetable oils as Diesel fuel are liquid nature-portability, ready availability; renewability, higher heat content, lower sulfur content, lower aromatic content and iodegradability.The disadvantages of vegetable oils as Diesel fuel are higher viscosity, lower volatility and the reactivity of unsaturated hydrocarbon chains.

In Figure 1.3 as shown below all options and processes are schematically shown. Between brackets is indicated in what kind of engine the product can be used.

Figure1.3 Schematic overview of the most common biomass conversion processes and their products

1.3 VEGETABLE OILS AS DIESEL FUELS

Vegetable oils, also known as triglycerides, comprise of 98% triglycerides and small amounts of mono- and diglycerides. Triglycerides are esters of three fatty acids and one glycerol. These contain substantial amounts of oxygen in its structure. The fatty acids vary in their carbon chain length and in the number of double bonds. Different types of vegetable oils have different types of fatty acids. Table 1.1 shows the empirical formula and chemical name of various fatty acids present in vegetable oils.

Table 1.1 Chemical name and formula of common fatty acids

The disadvantages of vegetable oils as diesel fuel are higher viscosity, lower volatility and the reactivity of unsaturated hydrocarbon chains. Vegetable oils have their own advantages as first of all, they are available everywhere in the world. Secondly, they are renewable as the vegetables which produce oil seeds can be planted year after year. Thirdly, they are ''greener" to the environment, as they seldom contain sulfur element in them.

In 1970, scientists discovered that the viscosity of vegetable oils could be reduced by a simple chemical process and that it could perform as diesel fuel in modern engine. Fundamentally, high viscosity appears to be a property at the root of many problems associated with direct use of vegetable oils as engine fuel. The

vegetable oils, as alternative engine fuels, are all extremely viscous with viscosities ranging from 10 to 20 times greater than that of petroleum-derived diesel fuel. The injection and atomization characteristics of the vegetable oils are significantly different than those of petroleum-derived diesel fuels, mainly as the result of their high viscosities. Modern diesel engines have fuel-injection systems that are sensitive to viscosity changes. A way to avoid these problems is to reduce the viscosity of vegetable oil in order to improve its performance. Four techniques can be used to reduce the viscosity of vegetable oils; namely heating/pyrolysis, dilution/blending, micro-emulsion, and transesterification.

Several experimental studies showed that vegetable oils can be used as alternative fuel for diesel engines. Some of these vegetable oils are as follows: sunflower, rapeseed, cottonseed, jojoba and Jatropha curcas.

1.4 BIO-DIESEL AS A VEHICULAR FUEL

Bio-diesel is a cleaner-burning diesel replacement fuel made from natural, renewable sources such as new and used vegetable oils and animal fats. Just like petroleum diesel, bio-diesel operates in compression-ignition engines or Diesel engines. Bio-diesel has physical properties very similar to conventional diesel. The bio-diesel was characterized by determining its density, viscosity, high heating value, cetane index, cloud and pour points, characteristics of distillation, and flash and combustion points according to ISO norms. Selected properties of diesel and bio-diesel fuels are given in Table 1.2 .Viscosity is the most important property of bio-diesel since it affects the operation of the fuel injection equipment, particularly at low temperatures when the increase in viscosity affects the fluidity of the fuel. Bio-diesel has a viscosity close to that of diesel fuels. The higher viscosity range of bio-diesel helps to reduce barrel/plunger leakage and increase injector efficiency in engines. Viscosity measurements have been made over the temperature range $20-100^{\circ}$ C for blends of different bio-diesel diesel fuel. The viscosity of the distillate was 10.2 mm²/s at 38⁰C, which is higher than the ASTM specification for diesel fuel $(1.9-4.1 \text{ mm}^2/\text{s})$ but considerably below that

of soybean oil $(32.6$ mm²/s). Bio-diesel offers safety benefits over petroleum diesel because it is much less combustible, with a flash point greater than 150 0C , compared to 77 $\mathrm{^0C}$ for petroleum diesel. The cetane number of bio-diesel is generally higher than conventional diesel. The cetane number of bio-diesel is around 50. Bio-diesel has lower volumetric heating values (about 12%) than diesel fuels but has a high cetane number and flash point.

Density is another important property of bio-diesel. It is the weight of a unit volume of fluid. Specific gravity is the ratio of the density of a liquid to the density of water. Specific gravity of bio-diesels ranges between 0.87 and 0.89. Fuel injection equipment operates on a volume metering system, hence a higher density for bio-diesel results in the delivery of a slightly greater mass of fuel .Two important parameters for low temperature applications of a fuel are Cloud Point (CP) and Pour Point (PP). The CP is the temperature at which wax first becomes visible when the fuel is cooled. The PP is the temperature at which the amount of wax out of solution is sufficient to gel the fuel, thus it is the lowest temperature at which the fuel can flow. Bio-diesel has higher CP and PP compared to conventional diesel. The esters have CP and PP that are $15-25^{\circ}$ C higher than those of diesel fuels. Methyl esters of vegetable oils have several outstanding advantages among other new-renewable and clean engine fuel alternatives. A number of technical advantages of biodiesel fuel : (a) it prolongs engine life and reduces the need for maintenance (bio-diesel has better lubricating qualities than fossil diesel); (b) it is safer to handle, being less toxic, more biodegradable, and having a higher flash point; (c) it reduces some exhaust emissions (although it may, in some circumstances, raise others). Bio-diesel fuels have many advantages over petroleum diesel fuel: produce less smoke and particles, have higher cetane number, produce lower carbon monoxide and hydrocarbon emissions, are renewable, biodegradable and non-toxic. When ethyl esters are used as fuel the advantage of totally recyclable carbon dioxide cycle is obtained since ethyl alcohol could be of vegetal origin.

Table 1.2 Specifications of diesel and bio-diesel fuels

1.5 TRANSESTERIFICATION OF VEGETABLE OIL

The vegetable oil was transesterified using methanol in the presence of sodium hydroxide (NaOH) as a catalyst shown in Figure 1.4. The parameter involved in the processing such as catalyst amount, molar ratio of alcohol to oil, reaction temperature and reaction time are optimized [15].

CH ₂ OCCR		CH_3OH	CH ₃ OOCR	CH ₂ OH
CHOOCR	$+$		$CH_3OH \rightarrow CH_3OOCR + CH_2OH$	
CH ₂ OOCR		CH_3OH	CH ₃ OOCR	CH ₂ OH
Vegetable oil $+$			Methanol \rightarrow Methyl Ester + Glycerol	

Figure1.4 Transesterification chemistry of vegetable oil

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The reaction shows why the viscosity of pure vegetable oil is higher than that of biodiesel. The large molecules of vegetable oil are split into smaller molecules, those of the methyl ester. About the molecules in Jatropha oil and Jatropha methyl ester only little is known.

1.6 JATROPHA CURCUS

It is non-edible oil being singled out for large-scale plantation on wastelands. Jatropha curcas plant can thrive under adverse conditions. It is a drought-resistant, perennial plant, living up to fifty years and has capability to grow on marginal soils. It requires very little irrigation and grows in all types of soils (from coastline to hill slopes). The production of Jatropha seeds is about 0.8 kg per square meter per year. The oil content of Jatropha seed ranges from 30% to 40% by weight and the kernel itself ranges from 45% to 60% [16]. Fresh Jatropha oil is slow-drying, odorless and colorless oil, but it turns yellow after aging.

The only limitation of this crop is that the seeds are toxic and the press cake can not be used as animal fodder. The press cake can only be used as organic manure. The fact that Jatropha oil can not be used for nutritional purposes without detoxification makes its use as energy/fuel source very attractive. In Madagascar, Cape Verde and Benin, Jatropha oil was used as mineral diesel substitute during the Second World War. Forson et al., [17] used Jatropha oil and diesel blends in compression ignition engines and found its performance and emissions characteristics similar to that of mineral diesel at low concentration of Jatropha oil in blends. Pramanik tried to reduce viscosity of Jatropha oil by heating it and also blending it with mineral diesel.

Figure 1.5 Unit process of Jatropha oil production

1.7 ENVIRONMENTAL ISSUES

The main advantage of biofuels is of course that it is $CO₂$ neutral. But $CO₂$ is not the only issue, other gasses are important as well. The effects of different emissions and how they harm the environment are explained below.

1.7.1 EMISSIONS FROMBIODIESELCOMBUSTIONIN CI ENGINE

Research shows that biodiesel generally produces less carbon monoxide (CO), hydrocarbons (HC), particulate matter (PM) and sulphur dioxide $(SO₂)$ than diesel. Even blends can already lower these emissions. For nitric oxide (NOx) this is not always the case. Depending on fuel system design and manufacturers approach towards NO_x , NO_x emissions are either slightly higher or slightly lower than for fossil fuels. In order to examine the emissions in greater detail the emissions will be divided into two groups, emissions from complete and incomplete combustion.

1.7.1.1 EMISSIONS FROM COMPLETE COMBUSTION

Emissions from complete combustion are those emitted to the atmosphere with combustion, these are carbon dioxide (CO_2) , nitric oxides (NO_x) , nitrous oxide (N_2O) , sulphur oxides(SO_x), hydrogen chloride (HCl) and heavy metals (HM). Figure 1.6 shows the variations of NO_x , PM, CO and HC. On average the

emissions of CO, PM and HC are substantially lower than for fossil diesel. However, the data also show an increase in emissions of NOx. NOx emissions vary with the iodine number of the fuel that was tested. The iodine number is a measure of the degree of saturation, which is the number of carbon-carbon double bonds in the biodiesel fatty acid chain [18].The higher is the saturation rate (or iodine number), the lower the NOx emissions. Other emissions from complete combustion like heavy metals and SOx are very low compared to those of fossil diesel, because biofuels do not contain as much Sulphur as fossil fuels and no heavy metals at all.

Figure1.6. Variations of NO_x , CO and HC with biodiesel

1.7.1.2 EMISSIONS FROM INCOMPLETE COMBUSTION

Incomplete combustion occurs if the amount of oxygen is too low, or by inadequate air/fuel mixing. Also low combustion temperatures, short resident times and low radical concentration can result in incomplete combustion. Emissions from incomplete combustion are carbon monoxide (CO), methane (CH4), no methane volatile organic components (NMVOC), particulate matter (PM), polychlorinated dioxins and furans (PCDD/F), ammonia and ozone (O_3) .

1.7.2 EFFECTS OF EMISSIONS ON THE ENVIRONMENT

All emissions mentioned above are harmful, but the effect that these emissions have on the environment and on human health is not always known. Not all emissions from vehicles are greenhouse gases, but unfortunately they have other serious consequences. The main green house gas is evidently $CO₂$, but also $CH₄$ and N₂O cause an increased greenhouse effect. Another effect acidification is caused by emissions of NH3, NOx, PM and NMVOC.These gases are converted in acids and case acid deposits, which can damage soil, vegetation, fresh water, building and coastal ecosystems. Emissions of diesels are seen as an important cause of soil contamination. Air pollutants from deposits and end up in the ground water. Besides effects on the environment in general, there are effects of pollutants that are very specifically harmful for animals and humans. Almost every part of the human body is affected by one pollutant or another. In general, pollutants emitted by traffic, especially CO, SOx and PM cause severe health problems. CO is odorless, colorless and tasteless gas, but it can cause fatal poisoning. Exposure to low levels of carbon monoxide can produce symptoms like a throbbing headache, dizziness fatigue and shortness of breath. Very high levels of carbon monoxide can lead to seizures, coma, respiratory failure and some times death also. Table 1.3 summarizes the environmental effects and emissions from traffic that cause the problems.

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Table 1.3 Environmental effects and the emissions

CHAPTER 2 LITERATURE REVIEW

2.1 INTRODUCTION

The use of vegetable oils as a fuel for compression ignition engines is restricted by some unfavorable properties like high viscosity, low cetane rating, low calorific value and higher emission characteristics. Viscosity increased with molecular weight but decreased with increasing unsaturated level and temperature. At room temperature the kinematic viscosity of Jatropha oil was detected 48.7 cSt. The viscosity of Jatropha oil seed must be reduced for biodiesel application since the kinematic viscosity of biodiesel were very low compared to vegetable oils. High viscosity of the jatropha oil seed are not suitable if its use directly as engine fuel, often results in operational problems such as carbon deposits, oil ring sticking, and thickening and gelling of lubricating oil as a result of contamination by the vegetable oils. Different methods such as preheating, blending, ultrasonically assisted methanol transesterification and supercritical methanol transesterification are being used to reduce the viscosity and make them suitable for engine applications [19]. The density of vegetable oil is lower than of water and the differences between vegetables oil are quite small, particularly amongst the common vegetable oils. Generally, the density of oil decreases with molecular weight, yet increase with unsaturation level. At room temperature the density of Jatropha seed oil was 0.917 g/ml.

2.2 SEVERAL PROPERTIES OF JATROPHA OIL

The production of Jatropha seeds is about 0.8 kg per square meter per year. The oil content of Jatropha seed ranges from 30% to 40% by weight and the
kernel itself ranges from 45% to 60%. Fresh Jatropha oil is slow-drying, odorless and colorless oil, but it turns yellow after aging. The only limitation of this crop is that the seeds are toxic and the press cake can not be used as animal fodder. The press cake can only be used as organic manure. The fact that Jatropha oil can not be used for nutritional purposes without detoxification makes its use as energy/fuel source very attractive.

The several physical, chemical and thermal properties of diesel and Jatropha oil are shown in Table 2.1 Density, cloud point and pour point of Jatropha oil was found higher than diesel. Higher cloud and pour points reflect unsuitability of Jatropha oil as diesel fuel in cold climatic conditions. The flash and fire points of Jatropha oil was quite high compared to diesel. Hence, Jatropha oil is extremely safe to handle. Higher carbon residue from Jatropha oil may possibly lead to higher carbon deposits in combustion chamber of the engine. Low sulfur content of Jatropha oil results in lower SOx emissions. Presence of oxygen in fuel improves combustion properties and emissions but reduces the calorific value of the fuel. Jatropha oil has approximately 90% calorific value compared to diesel. Nitrogen content of the fuel also affects the NOx emissions (by formation of fuel NOx).

Higher viscosity is a major problem in using vegetable oil as fuel for diesel engines. The viscosity was reduced by (i) heating and (ii) blending the oil with diesel. Viscosity of Jatropha oil was found at different temperatures in the range of 40–100 0 C. The viscosity variations are shown in Fig. 2.1. Viscosity of Jatropha oil decreases remarkably with increasing temperature and it becomes close to diesel at temperature above 90° C (within ASTM limits). Viscosity of diesel was 2.44 cSt at 40° C. For Jatropha oil, viscosity was found below 6 cSt at a temperature above 100⁰C. Therefore, Jatropha oil should be heated to 100° C before injecting it into the engine in order to bring its physical properties close to mineral diesel (at 40° C).

Table 2.1.Properties of diesel and Jatropha oil

Figure 2.1.Variation of viscosity with temperature

2.3 DIFFERENT TYPES OF MODEL

Researchers have experimentally evaluated the performance characteristics of conventional diesel engines fueled by biofuel its blends. However, experiments require enormous effort, money and time. A realistic numerical simulation model could reduce such effort. Numerical simulation based on mathematical modeling of diesel engine processes have long been used as an aid by design engineers to develop new design concepts. However, with biofuel, very few works have been done and it is still a newer area of research.

The process of diesel combustion is very complex and heterogeneous in nature. Diesel engine combustion models are mainly described as thermodynamic and fluid dynamic models. Models based on Thermodynamics can be further classified as single zone heat release model, phenomenological jet based model and quasidimensional multi-zone model. Single zone models assume that the cylinder content is uniform in composition and temperature and are suitable for prediction of engine performance. Phenomenological combustion models are based on each individual processes occurring in engine cycle such as fuel injection, mixture formation, heat release, heat transfer and emission formation.Quasi-dimensional multi-zone models incorporate the development of the fuel spray with time and simplified quasi steady equations are used to describe

processes like fuel injection, atomization, air entrainment, droplet formation, evaporation, wall impingement, ignition, heat release, heat transfer and so on. Fluid dynamic based models, often called multi-dimensional or computational fluid dynamics (CFD) models are based on solving the governing equations for conservation of mass, momentum and energy and species concentration through a definite discretization procedure.

C. D. Rakopoulos et al., [20] developed a multi-zone model of a diesel engine cycle, in order to examine the influence of insulating the combustion chamber on the performance and exhaust pollutants emissions of a naturallyaspirated, direct injection (DI), four-stroke, and water cooled diesel engine. The heat insulation was taken into account by the corresponding rise of wall temperature, since this was the final result of insulation useful for the study. It was found that there is no remarkable improvement of engine efficiency, since the decrease of volumetric efficiency had a greater influence on it than the decrease of heat loss to the coolant, which was converted mainly to exhaust gas enthalpy (significant rise of the exhaust gas temperature). As far as the concentration of exhaust pollutant emissions was concerned, it was found that the rising heat insulation leads to a significant increase of the exhaust nitric oxide (NO) and to a moderate increase of the exhaust soot concentration, Plots of temperature, equivalence ratio, NO and soot distributions at various instants of time inside the combustion chamber, emanating from the application of the multi-zone model, aid the correct interpretation of the insulation effects gaining insight into the mechanisms.

Yukio Matsui et al., [21] developed a fuel injection simulation code with an approximate lumped-parameter network scheme. Pressure and flow rate at every part, and motion of movable elements, are represented by respective differential equations on the assumption that fuel velocity in the injection pipe is sufficiently small compared with sound velocity, and every structural member has so high rigidity that the part is not deformed at all. For convenience of numerical calculation, functions of pressure and flow rate are defined pre- liminarily.

On the other hand, if a pressure difference exists before and after the orifice having effective area *,* then the flow rate passing through this orifice is given as, taking into consideration both cases of pressure of plunger. The injection pipe is approximated by a lumped parameter system having finite parameters. The pipe having a total length of L and a cross sectional area of *F* is divided into n parts. If the pressure in the ith volume element is p_i , and the flow rate passing through the boundary between the $(i - 1)$ th volume element and the ith volume element is q_i , the equation of motion of the fluid in each volume element is written as, using resistance. This code has many improvements for obtaining better computational accuracy.

These include a new iteration approach, a no uniform dividing method of injection pipe, a large number of injection system elements and consideration of kinematic viscosity of the fuel and its flow resistance through the injector during the throttling period. This simulation code was used to evaluate various control systems of injection rate for IDI diesel engines. Based on the results, a comparison was carried out among control characteristics of fuel injection rate of these systems, and clear correlation was shown between operating conditions of the injection pump and injection rates.

D. T. Hountalas and A. D. Kouremenos, [22] proposed a simple algorithm for the simulation of fuel injection systems that was very fast, requiring little computational time and the least possible geometrical data. The main purpose of the proposed model is to examine the behaviour of the fuel injection system and to predict the effect of engine operation parameters (i.e. speed and load) upon it. The following control volumes are considered, pertaining to a DI (direct injection) engine:

- (i) High pressure pump chamber
- (ii) Delivery valve chamber
- (iii) Delivery tube from pump to injector
- (iv) Injector

At each instant of time the pressure inside the previous control volumes is obtained. This allows the computation of the injection profile. The fuel is considered to be compressible with a bulk modulus of compressibility given by the expression. All elastic deformations of solid parts of the system, due to pressure changes, are neglected. The foregoing assumptions yield a pressuredependent wave propagation velocity which is a function of fluid compressibility only. The error in wave propagation velocity, as a result of neglecting pipeline deformation, is less than 5% for the maximum pressure variation.

Simulation of pump chamber-delivery valve chamber-injector as mentioned above, the fuel is considered to be compressible, with a compressibility defined by the relation, where P_i is the corresponding control volume pressure and V_i its instantaneous volume. The volumetric flow rate through orifices, various openings or ports is given by the formula where j is the corresponding volume. The simulation of each control volume is accomplished by considering equation and the incoming and outgoing volume flow rates, thus obtaining the following relation .For the fuel pump, the rate of volume change is obtained from the motion of the piston which is driven by the fuel injection system cam. As already stated, the modeling of the delivery valve is accomplished in a fairly simple way, compared to a previous detailed model developed by the authors, by considering it as a check valve allowing the flow to take place only from the pump chamber to the fuel pipeline.

The proposed model aims to overcome the difficulties during field applications where it was impossible to know details of the geometry of the system and especially about the delivery valve and the injector. The algorithm was written in FORTRAN-77 language and provides the fuel injection rate and the conditions at the nozzle exit with reasonable accuracy. The method was applied to a high speed direct injection diesel engine and the results were compared with experimental data. Furthermore, in order to validate the proposed model against other detailed models, a comparison was given between the present model and a detailed simulation model developed by the present research group.

From this comparison, a good accuracy of the model was revealed when compared against experimental data and the predictions of the previous detailed model, despite its simplicity.

A Chow and M L Wyszynski, [23] developed an engine systems model by first and second law analysis. Early efforts were focused on the closed part of the engine cycle, i.e. the compression combustion expansion sequence. These models have evolved from the ideal cycle calculations in the 1950s to simple component matching models in the 1960s, full thermodynamic models during the late 1970s and multi zone and multidimensional combustion models in the 1980s and early 1990s. The high-resolution multidimensional models, such as KIVA II 3-D, are often used for specific problem areas in design, where details of fluid transport processes or those involving subtle geometry changes dominate.

These models are capable of simulating detailed airflow, spray and combustion events in local geometries. The lower-resolution multi zone combustion models, such as ISIS, are able to predict power output, emissions and losses in the engine, fuel consumption and efficiency. For these reasons, multi zone combustion models are used in the conceptual and development stages of design in order to explore a larger range of alternatives within acceptable time and cost limits. The later introduction of concepts such as turbo charging, manifold tuning, exhaust gas recirculation (EGR) and the use of exhaust gas treatment devices to enhance the engine performance (output and emissions) prompted the need to develop models to describe the flows in the engine system.

The models developed, in order of increasing complexity, are the quasisteady' filling and emptying' and the wave dynamics models. The quasi-steady simulations are dependent on empirical knowledge and do not allow for mass accumulation between components. The filling and emptying models are based on solving the mass and energy conservation equations of a thermodynamic control volume. This method represents the unsteady flow phenomena more realistically as it models the time varying properties off low and allows for mass accumulation between the engine system components. The wave dynamics method analyses

even more detail as it tracks the pressure wave and temperature discontinuity along manifolds. Such models are more accurate in representing long pipes where pressure wave effects are prevalent. A detailed manifold design requires the use of a wave action model. The combined use of both the in-cylinder (thermodynamic and multi zone) and flow models is an important tool in the analysis of engine systems. Engine developers have successfully utilized engine system models to evaluate the performance of their system. Then second law analysis is briefly outlined. The model then presents some future concepts in power plant systems and discusses how certain aspects need to be addressed in order to model these new concepts. The final two sections review existing gas composition tracking methods and the TWC models.

Complex engine systems are becoming more commonly implemented to meet the increasing demands of fuel efficiency and emission legislation. Future engine systems may also include both exhaust gas treatment and fuel processing devices. This leads to complex interactions within the thermodynamics and chemistry of power plant systems. There is therefore a need to improve the systems modeling methods. This concerns first of all the composition tracking and the models of three-way catalytic exhaust converters and fuel processors. The applicability of gas dynamics modeling to chemically complex systems was also discussed. All these processes need to be modeled as interacting parts of one system. Developers proposed a great variety of traditional engine systems have been modeled successfully by using first law analysis. The concepts of future engine systems, however, demonstrate the need for a more flexible and comprehensive model that allows the simultaneous incorporation of several new modeling strategies in an engine system design (such as the ability to cope with the chemistry of a system in transients and in the description of gas dynamics). Such a model should enable an optimum configuration and corresponding regimes of operation to be produced.

A comprehensive mathematical model of the engine system was well developed and is now a standard tool for the engine designer. However, the

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development of composition tracking, TWC and fuel reformer models is lagging behind. A gas dynamics model that is accurate in tracking pressure, temperature and composition is fundamental to the development of transient models of a complete engine system consisting of the engine and TWC elements. Such a model will be useful in the investigation of the effects of the warm-up characteristics of the system on emission levels. Second law analysis, although supplementary, allows further insight into the distribution of the quality of energy in the system and the analysis of lost potential to do mechanical work.

Y H Zweiri et al, [24] developed an analytical non-linear dynamic model for single-cylinder diesel engines. The model describes the dynamic behavior between fuelling and engine speed and includes models of the non-linear engine and dynamometer dynamics, the instantaneous friction terms and the engine thermodynamics. The model operates in the crank angle domain. The dynamometer model enables the study of the engine behaviour under loading. The instantaneous friction model takes into consideration the viscosity variations with temperature. Inertia variations with piston pin offset were presented. In-cycle calculations were performed at each crank angle, and the correct crank angles of ignition, speed variations, fuel supply and air as well as fuel burning rate are predicted. The model treats the cylinder strokes and the manifolds as thermodynamic control volumes by using the filling and emptying method. The model was validated using experimentally measured cylinder pressure and engine instantaneous speeds, under transient operating conditions, and gives good agreement. The model can be used as an engine simulator to aid diesel engines control system design and fault diagnostics.

A.S. Kuleshov, [25] developed a multi-zone model of diesel sprays evolution and combustion named as RK-model. The combustion process in a direct injection diesel is very sensitive to engine parameters such as the sprayer design and location, the injection profile, the piston bowl shape, swirl, the composition, the pressure and the temperature of charge. To optimize of combustion and improve emissions of DI diesel with the thermodynamic engine

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model, the development of a high-accuracy combustion model taking into account the above parameters is actual. The choice of the thermodynamic engine model is conditioned by requirements of the high computational rate, because numbers of engine simulation sessions in optimization over the whole operating range come up to 30000 and more.

The diesel combustion model presented, named the RK model, as well as the Hiroyasu model, includes separate emissions sub models, the NOx formation sub model based on the Zeldovich's scheme, and the soot formation sub model. The first was developed by Zvonov and the last was developed by Razleytsev . Soot and NOx formation processes are simulated by combustion modeling with separate procedures. The main equations of the RK-model were developed by Razleytsev in 1990-1994. This method afterwards was modified and complemented by Kuleshov. The method takes into account conditions of evolution of each fuel spray and wall surface flows generated by sprays, and also interaction between sprays and swirl as well as between wall surface flows formed by adjacent sprays. These features of the RK-model allow predicting diesel combustion and emission for the following varying parameters, piston bowl shape and sprayer location, swirl intensity, number, diameter and direction of sprayer nozzles, shape of the injection profile including split injection

The model with sub models of NO and soot formation has been implemented into ICE thermodynamic analysis software (DIESEL-RK). The RKmodel takes into account, the shape of injection profile, including split injection, drop sizes, direction of each spray in the combustion chamber; the swirl intensity, the piston bowl shape. Evolution of wall surface flows generated by each spray depends on the spray and wall impingement angle and the swirl intensity. Interaction between near wall flows (further named wall surface flows) generated by the adjacent sprays is taken into account. The method considers hitting of fuel on the cylinder head and liner surfaces. The evaporation rate in each zone is determined by Nusselt number for the diffusion process, the pressure and the temperature, including temperatures of different walls where a fuel spray gets.

A parametric study of the swirl intensity effect had been performed and a good agreement with experimental data was obtained. The calculations results allow describing the phenomenon of increased fuel consumption with increase of swirl ratio over the optimum value. The model has been used for simulation of different engines performances. The calculated results obtained for high-speed, truck and medium speed diesels have shown a good agreement of SFC, power, smoke and NO emissions with the experimental data over the whole operating range, including modes of idling and 7 to 10% capacity. The model does not require recalibration for different operating modes of a diesel engine.

M. Nikian et al, [26] calculated the cylinder working fluid mean temperature, rate of heat fluxes to combustion chamber and temperature distribution on combustion chamber surface. The engine studied in this work was an Isuzu Diesel engine developed by Isuzu Ceramics Research Institute (ICRI). It is a ceramic, single cylinder DI Diesel engine. The piston crown, head, linear, cylinder and valves are made of Silicon Nitride (Kyocera SN235). This material has the following properties at room temperature, density $= 3240 \text{ kgm}^{-3}$, thermal conductivity $k=31$ W/m-k, and specific heat cp=680 J/kg-k. Additional insulation is provided by air gaps and insulating rings between the ceramics and the metal components of the engine.

The engine has limited cooling of the cylinder wall and of the bottom of the metal skirt of the piston. Both of these regions are cooled by lubricating oil. The primary feature used in the development of this cycle simulation is the first law of thermodynamics which is utilized to derive an expression for the crank angle (time) derivative of the overall gas temperature interims of engine design variables, operating conditions, and sub-model parameters. By simulating thermodynamic cycle of engine, temperature distribution of combustion chamber has calculated by the Crank- Nicolson method. An implicit finite difference method was used in this code. Special treatments for piston movement and a grid transformation for describing the realistic piston bowl shape were designed and utilized. The results were compared with a finite element method and were

verified to be accurate for simplified test problems. In addition, the method was applied to realistic problems of heat transfer in an Isuzu Diesel engine, and gave good agreement with available experimental.

H. F. Quintero, [27] presented a model for the calculation of in-cylinder parameters in an internal combustion engine with a noncircular gear based modified crank-slider mechanism. This work proposes a novel modified crankslider mechanism of an internal combustion engine, by introducing a noncircular gear pair. The noncircular tooth bodies enable to adjust the piston speed throughout the entire cycle, so that the performance of the engine can be improved. In this engine, the improvement of performance is constrained by the non-variability of the piston velocity law in accordance with the needs of the combustion process. With the introduction of an on circular gear pair in the engine mechanism, the duration of the portion during which the non burned charge is subjected to high pressures and temperatures can be diminished. Thus, the knock tendency of the engine would be reduced.

This modification also reduces the rejected heat. Since, to the knowledge of the authors, a mathematical model for piston velocity that optimizes the combustion process has not been developed, this work proposes a design for the displacement law of the noncircular gear set based on B-spline curves. These curves provide a powerful tool for designing displacement laws, because they give the designer a higher-level interface and the curve design is thus more intuitive. The primary input in mechanical design analyses is the data of the dynamic pressure of the cylinder.

A design process, a predictive model for the combustion process has to be selected. For simplicity, a zero dimensional or single zone model has been chosen in this work. With a zero-dimensional model, the cylinder charge is assumed to be homogeneous in both temperature and composition. Models for in-cylinder thermodynamics and dynamics of the crank-slider mechanism are integrated in this work to configure a concise methodology for an easy simulation of an internal combustion engine. Based on this methodology, a computer program to

analyze pressure, temperature, heat release, forces, and torques is developed. The program is written in the MathematicaTMsoftware language. Results for an example case are presented, with an angular resolution of 0.25 degree of crank angle (2880 data points per engine cycle) and under steady operation conditions. Finally, a noncircular gear pair is designed in order to optimize the operation of the engine.

With the introduction of noncircular gears, the instantaneous velocity of the piston can be accommodated to improve combustion performance. The displacement law of the noncircular gears is obtained using a B-spline curve, so that the appropriate instantaneous velocity of the piston is obtained. The gas pressure and temperature required for the determination of mechanical and thermal loads on engine components were found. The influence of the noncircular gears on the loads that act on all the components of the crank-slider mechanism, as well as the theoretical output torque for a given geometrical structure and inertial properties, were presented. To obtain the pressure and temperature inside the cylinder, under different operating parameters, such as air fuel ratio and spark angle advance, a zero dimensional model was applied. The proposed mechanism enables the optimisation of the combustion cycle; therefore, greater power may be achieved.

C.D. Rakopoulos et al [28], presented a multi-zone model for calculation of the closed cycle of a direct injection (DI) Diesel engine and applied for the interesting case of its operation with vegetable oil (cottonseed) or its derived biodiesel (methyl ester) as fuels, which were considered as promising alternatives (bio-fuels) to petroleum distillates. Although there were many experimental studies, there was an apparent scarcity of theoretical models scrutinizing the formation mechanisms of combustion generated emissions when using these fuels. The model was multi-zone with the issuing jets (from the nozzle) divided into several discrete volumes, called 'zones', formed along the direction of the fuel injection and across it. The model follows each zone, with its own time history, as the spray penetrates into the swirling air environment (forming the

non-burning zone) of the combustion chamber, before and after wall impingement. Droplet evaporation and jet mixing models were used to determine the amount of fuel and entrained air in each zone available for combustion. The mass, energy and state equations were applied in each zone to yield local temperatures and cylinder pressure histories. The concentrations of the various constituents were calculated by adopting a chemical equilibrium scheme for the C–H–O–N system of 11 species considered, together with the chemical rate equations for the calculation of nitric oxide (NO). A model for evaluation of soot formation and oxidation rates was included. The results from the relevant computer program for the in cylinder pressure, exhaust nitric oxide concentration (NO) and soot density are compared favorably with the corresponding measurements from an experimental investigation conducted on a fully automated test bed, standard 'Hydra', DI Diesel engine installed at the authors' laboratory. Iso-contour plots of equivalence ratio, temperature, NO and soot inside the combustion chamber at various instants of time when using these fuels against Diesel fuel (baseline fuel) shed light on the mechanisms underlying the combustion and pollutants formation and reveal how the widely differing properties of these fuels, against the normal Diesel fuel, affect greatly the spray formation, combustion mechanism and the related emissions.

T. Ganapathy et al, [29] proposed a methodology for thermodynamic model analysis of Jatropha biodiesel engine in combination with Taguchi's optimization approach to determine the optimum engine design and operating parameters. A thermodynamic model based on the First law of thermodynamics for the closed cycle period has been developed to study the performance of Jatropha biodiesel engine. This closed cycle simulation program models the compression, combustion, and expansion processes in the engine. The compression process is analyzed with ideal gas equation and polytropic process. The combustion process is modeled using two-zone model in which the rate of heat release is calculated using an empirical equation of double Weibe's function to adequately model the combustion in the premixed and the diffusive zones. The

ignition delay is also taken into account in the model and it is calculated by using the Wolfer's relation .The heat transfer is accounted for throughout the closed form cyclic process. These calculations are based on the well known Hohenberg's equation. The exhaust and intake processes are also analyzed in the cycle simulation by treating the gas exchange processes using the control volume approach. The various empirical equations proposed by Bishop have been incorporated in the model to account for different frictional power losses.

The model based on Weibe's heat release function has been employed to simulate the Jatropha biodiesel engine performance. Among the important engine design and operating parameters 10 critical parameters were selected assuming interactions between the pair of parameters. Using linear graph theory and Taguchi method an L16 orthogonal array has been utilized to determine the engine test trials layout. In order to maximize the performance of Jatropha biodiesel engine the signal to noise ratio (SNR) related to higher-the-better (HTB) quality characteristics has been used. The methodology correctly predicted the compression ratio, Weibe's heat release constants and combustion zone duration as the critical parameters that affect the performance of the engine compared to other parameters.

B. Rajendra Prasath et al, [30] were made an effort taken to simulate the combustion and performance characteristics of biodiesel fuel in direct injection (D.I) low heat rejection (LHR) diesel engine. Thermal barrier coatings are used to improve the engine performance and efficiency of internal combustion engines. The engine with thermal barrier coating is called low heat rejection (LHR) engine, which is based on suppressing the heat rejection to the coolant and recovering the energy. The engines parts such as piston, cylinder head, cylinder liners and valves are coated with partially stabilized zirconia (PSZ). The superior advantages of LHR engines are improved fuel economy, higher energy in exhaust gases and capability of handling higher viscous fuel. The transesterification process brings down the properties of fuel closer to the diesel fuel. The higher temperature of the LHR engine increases the possibility of using biodiesel without preheating.

Comprehensive analyses on combustion characteristics such as cylinder pressure, peak cylinder pressure, heat release and performance characteristics such as specific fuel consumption and brake thermal efficiency were carried out. Compression ignition (C.I) engine cycle simulation was developed and modified in to LHR engine for both diesel and biodiesel fuel. On the basis of first law of thermodynamics the properties at each degree crank angle was calculated. Preparation and reaction rate model was used to calculate the instantaneous heat release rate. A gas-wall heat transfer calculations were based on the ANNAND's combined heat transfer model with instantaneous wall temperature to analyze the effect of coating on heat transfer. The simulated results were validated by conducting the experiments on the test engine under identical operating condition on a turbocharged D.I diesel engine. In this analysis 20% of biodiesel (derived from Jatropha oil) blended with diesel and used in both conventional and LHR engine. The simulated combustion and performance characteristics results were found satisfactory with the experimental.

T.K. Gogoi and D.C. Baruah [31], developed a cycle simulation model incorporating a thermodynamic based single zone combustion model to predict the performance of diesel engine. It is assumed that there is spatial uniformity of pressure, temperature and composition of the cylinder content at each crank angle. The fuels considered are diesel and 20% (B20), 40% (B40), 60% (B60) (by volume) blending of biodiesel from Karanja oil with diesel. The molecular formula of diesel isapproximatedas $C_{12}H_{23}$. Karanja oil is mostly oleic and linoleic. The chemical formula of pure biodiesel is considered as $C_{17.75}H_{33.43}O_{1.98}$ and this has been derived from the fatty acid composition of karanja oil. It is also assumed that the air fuel mixture is lean and this leads to temperatures at which dissociation of products does not have much effect on engine performance. Therefore, dissociation of products of combustion is neglected in order to keep the analysis simple. However, combustion products should be defined by considering dissociation in order to represent a more realistic cycle. Polynomial expressions are used for each species (O_2, N_2, CO_2, H_2O) considered in the

calculation of specific heats, internal energy and enthalpy as a function of temperature. The compression phase begins at the point of closing of the inlet valve (IVC) and continues up-to crank angle at which combustion begins.

The effect of engine speed and compression ratio on brake power and brake thermal efficiency was analyzed through the model. The fuel considered for the analysis were diesel, 20%, 40%, 60% blending of diesel and biodiesel derived from Karanja oil. Depending upon the engine design parameters, the brake power of the engine increases with speed, the peak power occurs at particular speed and any further increase in speed results in decrease of power. This has been a characteristic of diesel engine. At CR of 17.5, the engine peak power occurred at 1500 rpm for diesel, B20 and B40; however, for B60 it occurred at 1400 rpm. The model predicts a higher rate of pressure and temperature rise for the blends during combustion as compared to diesel. An increase in brake power was observed in case of the blends B40 and B60 compared to diesel. However, the model predicts slightly lower brake power for the blend B20. The blends B20, B40 and B60 present an increase in brake thermal efficiency compared to diesel. This is due to an increase in the brake power in case of the blends and their lower calorific values. However, with 60% blending, it reveals better performance in terms of brake power and brake thermal efficiency.

M. Kekez, and L. Radziszewski [32] conducted experimental research on an engine test bench were used to build analytical empirical model of engine working cycle, based on fuzzy sets theory. In order to achieve this, the new genetic-fuzzy system GFSm with advanced information encoding and adjustable number of rules, being a modification of Pittsburgh approach, was designed. Using this system, two models of cylinder pressure curves were built. The best accuracy in terms of maximum pressure error and indicated work error (less than 5% for each examined crankshaft speed) was achieved by GFS model comprising 12 rules. The model allows simulation of cylinder pressure curves with high accuracy, for all allowable crankshaft speeds. Time of computation and saving the

results to disk is 0.04s. The model can be extended (by means of scaling functions) for modeling pressure curves for the engine fueled by different fuels.

Yongfeng Li et al [33], developed a phenomenological model, the TP (Temperature Phase) model, was presented to carry out optimization calculations for turbulent diffusion combustion in a high-pressure common rail diesel engine. Since auto-ignition is the first important event of diffusion combustion under diesel conditions, we began to construct a kinetic mechanism for n-heptane ignition based on the detailed model proposed by Barths et al. However, Barths' mechanism (involving 324 chemical species and 1650 reactions) is too large to use in multidimensional turbulent diffusion computations.

Therefore, only a few lumped or equivalent intermediate species (e.g., the first and second *n-*heptyl isomers were retained to represent all the *n-*heptyl isomers) and some relevant key reactions were selected on the basis of steady state assumptions. These reactions are crucial for reproducing the auto-ignition behavior of *n-*heptane/air mixtures from the low/intermediate regime to the hightemperature regime. The high temperature oxidation of n*-*heptane proceeds from the attack on the fuel by H, OH and $HO₂$ radicals to form n-heptyl radicals and through the break-up of these into C_2H_4 , CH₃ and H radicals. These are oxidized by C_1-C_2 -chemistry reactions. The low temperature chemistry of lower aliphatic hydrocarbons is characterized by the degenerate chain branching. This low temperature mechanism is no longer valid when the temperature increases beyond about 850 K. The competition of the reverse reaction of the first and second O_2 addition with the subsequent internal H-abstraction reaction is the key to the understanding of the negative temperature dependence of the ignition delay. With increasing temperature, these reverse reactions become faster than their forward reactions, thereby stopping the reaction sequence. A transition to the high temperature mechanism must occur.

Temperature is the most important parameter in the TP model, which includes two parts: an auto-ignition and a soot model. In the auto-ignition phase, different reaction mechanisms are built for different zones. For the soot model,

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different methods are used for different temperatures. The TP model is then implemented in KIVA code instead of original model to carry out optimization. The results of cylinder pressures, the corresponding heat release rates, and soot with variation of injection time, variation of rail pressure and variation of speed among TP model, KIVA standard model and experimental data were analyzed. The results indicate that the TP model can carry out optimization and CFD (computational fluid dynamics) and can be a useful tool to study turbulent diffusion combustion.

2.4 OBJECTIVES OF THE PRESENT PROBLEM

The main objective with this thesis is to achieve a simulation model that simulates the performance and emission parameter during a compression and combustion cycle. The computer model should be implemented in E.E.S and must be able to handle varying injection pressure and fuel injection points. In this work an attempt is made to study the following**:-**

- i. Mathematical model for predicting the variation of fuel injection angle by using diesel and jatropha oil as fuel on engine performance.
- ii. Mathematical model for observing the effect of injection pressure on engine performance.
- iii. Model for analyzing the effect of fuel inlet temperature on engine performance.
- iv. Simulation of the developed model for engine performance by F-Chart Software.

2.5 NEED FOR PRESENT INVESTIGATION

In fact, there are many models developed over the years from zero- to three-dimensional computational fluid dynamic (CFD) models. In a simple zerodimensional model, a mixture throughout the cylinder is assumed to be uniform and homogeneous as time is varied independently, which is obviously a crude approximation. The combustion process in these models are simply treated equivalent to a heat addition or heat release phenomenon established usually on the basis of the first law of thermodynamics and the corresponding experimental observations.

However, CFD models, which are based on the numerical calculations of mass, momentum, energy, and species conservation equations in one, two, or three dimensions, can produce a great amount of estimated data of flow, temperature, and concentration fields in operating engines. These models are increasingly becoming successful but require very large computing resources even with a simplistic description of complex chemical reactions taking place during combustion process. The use of multidimensional CFD models, which can take complex chemical kinetics reactions into account, still remains a challenge.

Therefore, in this contribution, a relatively simple two zone model was employed to simulate the combustion process in internal combustion engines with a hydrocarbon fuel such as methane along with diluents such as carbon dioxide and nitrogen to represent biogases, generally encountered in practice. In principle, a number of modeling techniques could be used as a basis for the development of the prescribed simulation model. However, for simplicity and due to ease of availability, the simulation model modified was arbitrarily based on the combustion model presented by Ferguson and then additional aspects were added in to accommodate the presence of carbon dioxide and nitrogen as diluents.

The equilibrium combustion products were increased to 13 species instead of 10 species as developed by Ferguson. The employed modeling consists of two main modules (a) fuel-air and residual gas properties calculation module to calculate gas properties during compression and in unburned zone during

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combustion phase, and (b) equilibrium combustion product properties calculation module is used for calculating pressure and temperature fluctuations during combustion and expansion phases

CHAPTER 3 METHODOLOGY

3.1 MODELING

The processes in the cylinder of diesel engine are very complex. This is caused by naturally transient and heterogeneous character, controller mainly turbulent mixing of fuel and air .There exist many approaches towards diesel engine modeling. These approaches depends on the use of these models and their accuracy and complexity varies a great extend. The advantages of these models are especially the reasonable precision and low computational complexity. Mean value model (MVM) models neglect the discrete cycles of the engine and assume all processes and effects are spread out over the engine cycle. Another family of control oriented models is called discrete event models (DEM).

The models are useful for air/fuel ratio feed forward control and misfire detection algorithms. This assumes homogeneous conditions throughout the cylinder. This is a good approximation for the compression-ignition engines but not for the spark-ignition engines. Another important characteristic is that the air flows outside the cylinder are not modeled. Instead of this the conditions in the intake and exhaust manifold are introduced to the model as the external inputs. This significantly simplifies the structure of the model because the external parts (turbocharger, compressor, manifolds etc.) do not need to be modeled. Such approach is also called air flow chop modeling.

There are numerous ways of describing reality through a model. Some are more complex than others and the different approaches may differ in both structure and accuracy. Which one to choose therefore very much depends on the particular situation and especially the field of application. Here follows a summary of the main engine model classifications.

3.1.1 EQUATIONS AND BLACK BOX

There are a number of approaches available when deciding on the basis of a model. Physical equations theoretically describing the system is the most common method since it creates a general model working for many operating areas. Its drawback is that reality might be difficult to describe correctly in theory. Also, such a model is often resource consuming. Another common approach is to base the model entirely on measurements. The measured data is stored as a table of two or more dimensions in a so called black box and then fetched when needed depending on one or more input signals. This approach often provides an accurate result since it is based directly on empiricism; however it is only defined for a limited region. A combination of both approaches, where the main basis of the model rests on physical equations and black boxes are used to model certain complexities, is also common.

3.1.2 SINGLE ZONE AND MULTI-ZONE

The combustion process can be described with varying complexity and accuracy. Normally the degree of complexity is decided by the number of zones in which the cylinder has been divided. An engine model therefore is either single-zone or multi-zone. In a single-zone model the gas mixture within the cylinder is considered to be homogenous for each sample. It is also assumed to be made up strictly of ideal gases. In a multi-zone model, for example the two-zone model, the gases are still considered ideal. However, the homogenous approach has been replaced by a heterogenous one. Here the cylinder is also divided into two zones, one containing injected fuel and the other surrounding air. Each zone itself is homogenous and no heat transfer occurs between the two zones. The simplicity of the single-zone model is its biggest advantage. This makes it fast and therefore applicable in real time systems. The multi-zone model is more complex and more accurate compared to the single-zone model. A multi-zone model is often needed for combustion chamber design, but for most aspects of control design a two-zone model is good enough.

3.1.3 MEAN VALUE AND IN CYCLE VRIATIONS

When it comes to the cylinder, two main approaches can be found. The most common approach is to model all cylinders as one, describing the total engine torque as a mean value over one or more engine cycles. The result of this approach is called Mean Value Engine Model (MVEM). An alternative to the MVEM is a model describing the in-cycle variation torque. One such example is the Cylinder-by-Cylinder Engine Model (CCEM). Unlike the MVEM, it describes each cylinder individually and generates for example a torque signal with each individual combustion pulse present. Normally a MVEM is sufficient enough for use in processes such as control system design. However, for some aspects of power train control a model illustrating the in-cycle variations of the torque could prove useful. An example of such an aspect could be backlash caused by play between gears, thus affected by individual combustion pulses. Here the brief overall structure of methodology is as shown below Figure 3.1.

Figure 3.1. Overall structure of engine system model

In this work following fundamental assumptions have been made:-

- Cylinder charge is a homogeneous gas mixture of fuel vapor and air.
- Pressure and temperature inside the cylinder are uniform and vary with crank angle.
- Specific heats of the gaseous mixture are calculated as a function of temperature.
- Wall wetting may occur during the injection. So that the cylinder wall temperature changes.
- Model must be initialized with correct initial condition such as inlet pressure and temperatures.

3.2 IMPLEMENTATION TOOLS

There are several software tools that allow modeling and graphical representation of complex physical processes as diesel engine cycle. On the other hand there are just a few like Matlab and Modelica that are widely used in automotive industry. These two tools differ in a way how the physical processes are represented. Matlab-Simulink strictly uses causal description of the process and is more appropriate for real-time and control applications and control. Modelica uses the concept of energy transfers between different parts of the physical process without obvious direction and seems to be more suitable tool for modeling of physical processes. In the latest version of Matlab the new modeling tool called Simscape is introduced. This tool used Modelica concept of modeling and can be also easily linked with other Matlab parts as Simulink and Stateflow.The diesel engine model described below is implemented in F-chart software.

3.3 THE MODEL

Due to the complexity of the diesel engine combustion and the turbulent fuel air- mixing it is difficult to develop an effective model that does not take too long computational time. There are different approaches to implement a diesel combustion model i.e. single-zone or multi-zone. To develop model that is

accurate enough, has an acceptable simulation time and has a complexity level that reflects the timeframe of this work, a two-zone model has been selected. The model includes only those processes occurring during closed cycle, when all valves are closed. The compression phase begins at the point of closing of the inlet valve (IVC) and continues up to crank angle at which combustion begins. The period from the end of combustion to the exhaust valve opening (EVO) is the expansion phase. The compression and expansion phases are considered as polytrophic.

3.3.1 ENERGY BALANCE EQUATION

The energy balance equations for the present model can be expressed in differential form. Then the first law of thermodynamics for compression phase, considering only one zone (pure air) is given as:

$$
\frac{dQ}{d\theta} = \frac{dU}{d\theta} + p\frac{dV}{d\theta} \tag{3.1}
$$

Where $\frac{dQ}{dQ}$ $\left(\frac{dQ}{d\theta}\right)$ is the rate of heat loss to the combustion chamber walls, $\left(\frac{dU}{d\theta}\right)$ is the rate of change of internal energy, and $\int p \frac{dV}{dx}$ $\left(p\frac{dV}{d\theta}\right)$ is the rate of work done on the system.

During the combustion and expansion phases, at the start of combustion the entire volume is assumed to be the unburned region and at the end of combustion the entire volume is assumed to be the burned region. Therefore, the energy balance equation, using the two zone model in the combustion chamber is given [34]-[35] and can be expressed by:

$$
m\frac{du}{d\theta} + u\frac{dm}{d\theta} = \left(\frac{dQ}{d\theta}\right) - \left(p\frac{dV}{d\theta}\right) - \left(\frac{30mh_i}{\pi N}\right)
$$
(3.2)

The various term of the equation are elaborated below as:

$$
\left(\frac{du}{d\theta}\right)
$$
, is the rate of change of internal energy of mixture of mass m.
\n $\left(\frac{dm}{d\theta}\right)$, is the rate of change of mixture mass m.
\n $\left(\frac{dQ}{d\theta}\right)$, is the net heat release rate which is the difference between the rate of

heat release during the combustion period and rate of heat transfer from combustion chamber gases to the combustion chamber walls .

$$
\left(p\frac{dV}{d\theta}\right)
$$
, is the rate of work done by the system.

Where m is the mass of the mixture (air $+$ fuel) contained in the combustion chamber (kgs), m_l is the mixture mass loss through piston rings (kg/s), h₁ is the enthalpy loss (J/ kg), N is the engine speed (rpm), θ is the crank angle (degrees), V is the instantaneous cylinder volume $(m³)$, P is the cylinder pressure (Pa) and *Q* is the heat energy (Joule).

3.3.2 VOLUME AT ANY CRANK ANGLE

The instantaneous cylinder volume V_{θ} is given by:

$$
V_{\theta} = V_{c} + \left\{ \pi \frac{d^{2}}{4} \frac{l}{2} \right\} \left\{ 1 + m - \left(m^{2} - \sin^{2} \theta \right)^{0.5} - \cos \theta \right\}
$$
 (3.3)

Where $m = (2.L)I^{-1}$, d is Cylinder bore (m), L is connecting rod length (m), l is stroke length (m), V_{θ} is the volume at any crank angle (m³), V_c is the clearance volume (m^3) and θ is the crank angle.

3.3.3 GAS PROPERTIES CALCULATION

The gas properties are functions of pressure, temperature and its composition. The higher temperature can be achieved for that system where the combustion is completed and the system became adiabatic. It depends on the chemical composition of the reactant mixture, pressure and temperature of the mixture and combustion process. A hydrocarbon fuel can be represented by $C_xH_yO_z$. The chemically suitable amount of oxygen (O_{cc}) required for combustion per mole of fuel can be written as:

$$
O_{cc} = m_c + 0.25m_h - 0.5m_o \tag{3.4}
$$

The minimum amount of oxygen required (O_{min}) for combustion in the reactants per mole of fuel (to convert H_2 to H_2O and C to CO) can be expressed as:

$$
O_{\text{min}} = O_{cc} - 0.5 m_c \tag{3.5}
$$

Here m_c , m_h and m_o are respectively the number of moles of carbon, hydrogen and oxygen atoms in one mole of fuel. From these mole fraction calculations, mixture properties such as enthalpy, internal energy, specific volume and specific heat at constant pressure are calculated.

3.3.4 INTERNAL ENERGY

The internal energy (u) can be written in terms of the internal energy of unburned zone Uu and burned zone U_b with (x) as a mass fraction burned as:

$$
u = \frac{U}{m} = xU_b + (1 - x)U_u
$$
\n(3.6)

Similarly the specific volume can be written in terms of the specific volume of the unburned zone (u) and the burned zone (b) as:

$$
v = \frac{V}{m} = xv_b + (1 - x)v_u
$$
 (3.7)

Differentiating Eqn. (3.6) and (3.7) with respect to crank angle and replacing the partial derivative terms with the logarithmic forms gives the internal energy and specific volumes for burnt and unburnt zone as:

$$
\left(\frac{d\nu_{\scriptscriptstyle b}}{d\theta}\right) = \left(\frac{\nu_{\scriptscriptstyle b}\partial\left(\ln\nu_{\scriptscriptstyle b}\right)dT_{\scriptscriptstyle b}}{T_{\scriptscriptstyle b}\partial\left(\ln T_{\scriptscriptstyle b}\right)d\theta}\right) + \left(\frac{\nu_{\scriptscriptstyle b}\partial\left(\ln\nu_{\scriptscriptstyle b}\right)dP}{P\partial\left(\ln P\right)d\theta}\right) \tag{3.8}
$$

$$
\left(\frac{dv_u}{d\theta}\right) = \left(\frac{v_u \partial (\ln v_u) dT_u}{T_u \partial (\ln T_u) d\theta}\right) + \left(\frac{v_u \partial (\ln v_u) dP}{P \partial (\ln P) d\theta}\right)
$$
\n(3.9)

$$
\left(\frac{du_{\scriptscriptstyle b}}{d\theta}\right) = \left(C_{\scriptscriptstyle p_{\scriptscriptstyle b}} - \frac{Pv_{\scriptscriptstyle b}\partial\left(\ln v_{\scriptscriptstyle b}\right)}{T_{\scriptscriptstyle b}\partial\left(\ln T_{\scriptscriptstyle b}\right)}\right)\frac{dT_{\scriptscriptstyle b}}{d\theta} - v_{\scriptscriptstyle b}\left(\frac{\partial\left(\ln v_{\scriptscriptstyle b}\right)}{\partial\left(\ln T_{\scriptscriptstyle b}\right)} + \frac{\partial\left(\ln v_{\scriptscriptstyle b}\right)}{\partial\left(\ln P\right)}\right)\frac{dP}{d\theta} \tag{3.10}
$$

$$
\left(\frac{du_{\nu}}{d\theta}\right) = \left(C_{\nu_{u}} - \frac{Pv_{u}\partial\left(\ln v_{u}\right)}{T_{u}\partial\left(\ln T_{u}\right)}\right)\frac{dT_{u}}{d\theta} - v_{u}\left(\frac{\partial\left(\ln v_{u}\right)}{\partial\left(\ln T_{u}\right)} + \frac{\partial\left(\ln v_{u}\right)}{\partial\left(\ln P\right)}\right)\frac{dP}{d\theta} \tag{3.11}
$$

Where Cp_b and Cp_u are the specific heat capacity at constant pressure for the burned and unburned zones. Further the first term in Eqn. (2) can be written as follows:

$$
\left(m\frac{du}{d\theta}\right) = \left(x\frac{du_{b}}{d\theta} + (1-x)\frac{du_{u}}{d\theta} + (u_{b} - u_{u})\frac{dx}{d\theta}\right)m\tag{3.12}
$$

Where x is the mass burned fraction can be calculated by Weibe function by using following expression:

$$
x = 1 - \exp\left[-a\left(\frac{\theta - \theta_0}{\Delta \theta}\right)^{c+1}\right]
$$
 (3.13)

Where θ_0 is the start of combustion and $\Delta\theta$ is the combustion duration and 'a' is an adjustable parameter that characterizes the completeness of combustion process. The parameter c represents the rate of combustion. The value of 'c' for all fuels is taken as 2.0 and 'a' as 5.0.

3.3.5 HEAT LOSS FROM COMBUSTION CHAMBER

The heat loss from the combustion chamber can also be expressed by using both burned and unburned zones as follows:

$$
\left(\frac{dQ}{d\theta}\right) = \left(\frac{30(Q_b + Q_u)}{\pi N}\right) \tag{3.14}
$$

Where

$$
Q_b = hA_b(T_b - T_w) \tag{3.15}
$$

$$
Q_u = h A_u (T_u - T_w) \tag{3.16}
$$

The surface areas of the two different zones are given by A*^u* and A*b*. These areas can be related to a mass fraction burned *x* by using an empirical formula [36]:

$$
A_{b} = \left(\frac{\pi d^2}{2} + \frac{4V}{d}\right) x^{0.5}
$$
 (3.17)

$$
A_{\mathcal{U}} = \left[\left(\frac{\pi d^2}{2} + \frac{4V}{d} \right) (1 - x^{0.5}) \right] \tag{3.18}
$$

Where d is the bore of the cylinder (m). The convective heat transfer coefficient h for Eqn. (3.15) and (3.16) is given by [30] as follows:

3.3.6 HEAT TRANSFER COEFFICIENT

Heat transfer coefficient of gas for each degree crank angle is calculated from the following equation as:

$$
h = 0.26(k/d) \text{Re}^{0.6} \tag{3.19}
$$

Where k is the thermal conductivity for each change in viscosity $(W/m-k)$ and Re is the Reynolds number for each time step is calculated as follows:

$$
Re = \frac{\rho dV_p}{\mu}
$$
 (3.20)

Where ρ is the density of gas mixture (kg/m³), μ is the dynamic viscosity (kg/m-s) and V_p is the mean piston speed (m/s).

3.3.7 INSTANTANEOUS PRESSURE AND TEMPERATURE OF THE COMBUSTION CHAMBER

The instantaneous pressure and temperature for different zones at any crank angle can be found out as:

$$
\left(\frac{dP}{d\theta}\right) = \left(\frac{A+B+C}{D+E}\right) \tag{3.21}
$$

Where terms A, B, C, D and E can be explained as:

$$
A = \frac{1}{m} \left(\frac{dV}{d\theta} + \frac{30VC_b}{\pi N} \right)
$$
 (3.21a)

$$
B = h \left(\frac{30 \left(\frac{\pi d^2}{2} + \frac{4V}{d} \right)}{\pi N m} \right) \left(\frac{v_b \partial \ln v_b}{C_{\rho b} \partial \ln T_b} x^{1/2} \frac{T_b - T_w}{T_b} + \frac{v_u \partial \ln v_u}{C_{\rho a} \partial \ln T_u} (1 - x^{1/2}) \frac{T_u - T_w}{T_u} \right) (3.21b)
$$

$$
C = -\left(v_{\scriptscriptstyle b} - v_{\scriptscriptstyle u}\right) \frac{dx}{d\theta} - v_{\scriptscriptstyle b} \frac{\partial \ln v_{\scriptscriptstyle b}}{\partial \ln T_{\scriptscriptstyle b}} \frac{h_{\scriptscriptstyle u} - h_{\scriptscriptstyle b}}{C_{\scriptscriptstyle p\scriptscriptstyle b} T_{\scriptscriptstyle b}} \left[\frac{dx}{d\theta} - \frac{(x - x^2) C_{\scriptscriptstyle b} 30}{\pi N} \right]
$$
(3.21c)

$$
D = x \left(\frac{v_b^2}{C_{p b} T_b} \left(\frac{\partial \ln v_b}{\partial \ln T_b} \right)^2 + \frac{v_b \partial \ln v_b}{P \partial \ln P} \right)
$$
(3.21d)

$$
E = (1 - x) \left(\frac{v_u^2}{C_{\text{pu}} T_u} \left(\frac{\partial \ln v_u}{\partial \ln T_u} \right) 2 + \frac{v_u}{P} \frac{\partial \ln v_u}{\partial \ln P} \right)
$$
(3.21e)

$$
\left(\frac{dT_b}{d\theta}\right) = \frac{-h\left(\frac{\pi d^2}{2} + \frac{4V}{d}\right)x^{1/2}\left(T_s - T_w\right)30}{\pi N m C_{\rho b} x} + \left[\frac{v_b}{C_{\rho b}}\frac{\partial \ln v_b}{\partial \ln T_b}\left(\frac{A+B+C}{D+E}\right)\right] + \frac{h_a - h_b}{C_{\rho b} x} \left[\frac{dx}{d\theta} - \frac{(x-x^2)C_b 30}{\pi N}\right]
$$
\n(3.22)

$$
\left(\frac{dT_u}{d\theta}\right) = \frac{-30h\left(\frac{\pi d^2}{2} + \frac{4V}{d}\right)\left(1 - x^{1/2}\right)\left(T_u - T_w\right)}{\pi N m C_{\rho u}\left(1 - x\right)} + \left[\frac{v_u}{C_{\rho u}} \frac{\partial \ln v_u}{\partial \ln T_u}\left(\frac{A + B + C}{D + E}\right)\right]
$$
(3.23)

Where C_b is the blow by constant and h_l is the enthalpy loss which can be determined as:

$$
h_{\iota} = (1 - x^2) h_{\iota} + x^2 h_{\iota}
$$
 (3.24)

3.3.8 IGNITION DELAY

The ignition delay is the time duration between start of fuel injection and start of combustion. Many expressions for ignition delay are found in literature as a function of mixture pressure, temperature, fuel cetane number [37]-[38]. The following empirical correlation is used to obtain the value of ignition delay [39]:

$$
t_{d} = \frac{2.64}{P^{0.8} \phi^{0.2}} \exp\left(\frac{1650 - 20CN}{RT}\right)
$$
 (3.25)

Where R is universal gas constant, CN is fuel cetane number and \varnothing is fuel air equivalence ratio. However, the constants and exponents in the above correlation are to be better calibrated against experimental results and conclusion.

3.3.9 MASS OF FUEL INJECTED

Considering that nozzle open area is constant during the injection period, total mass of the fuel injected for each crank angle is calculated as follows:

$$
m_f = C_d A_n \sqrt{2\rho_f \Delta P} \left(\frac{\Delta \theta_f}{360N}\right) n \tag{3.26}
$$

Where n is the number of injector nozzle holes, C_d is the coefficient of discharge of injector nozzle, A_n is the cross sectional area of nozzle (m²), ΔP is the pressure drop in the nozzle (Pa), N is the engine speed and $\Delta\theta_f$ is the fuel injection period.

3.3.10 PRESSURE DROP IN THE NOZZLE

The pressure drop in the nozzle is calculated as follows [40]:

$$
\Delta P = 0.5 \rho_f \left(\frac{u_{inj}}{C_d}\right)^2 \tag{3.27}
$$

Where u_{inj} the spray velocity from nozzle hole is given as:

$$
u_{inj} = \left(\frac{dm_f}{d\theta}\right) \left(\frac{6N}{\rho_f A_n}\right) \tag{3.28}
$$

Where
$$
\left(\frac{dm_f}{d\theta}\right)
$$
 is the fuel injection rate $(\text{kg}/^0\text{CA})$

$$
\left(\frac{dm_f}{d\theta}\right) = \left(\frac{m_f}{n\Delta\theta_f}\right) \tag{3.29}
$$

3.3.11 SAUTER MEAN DIAMETER (SMD)

It is the ratio of mean volume to the mean surface area of the fuel droplets and has an important role in defining the fuel atomization characteristics. Smaller SMD results better fuel atomization and ultimately the fuel combustion efficiency.

$$
SMD = 3.08v^{0.335}(\sigma\rho_f)^{0.737}\rho_a^{0.06}(\Delta P)^{-0.54}
$$
 (3.30)

Where v is the kinematic viscosity (m²/s, σ is surface tension of fuel(N/m), ρ_f is the density of fuel(kg/m³), ρ_a is the density of air(kg/m³) and ΔP is the pressure drop across the nozzle(Pa).

3.3.12 NET WORK DONE

Work done in each crank angle is calculated from [34]:

$$
dW = \left(\frac{P_1 + P_2}{2}\right) (V_2 - V_1) \tag{3.31}
$$

Where P_1 and P_2 are the change in pressure for each crank angle inside the combustion chamber, and V_1 and V_2 are the changes in volume inside the combustion chamber for the same crank angle.

3.3.13 NITRIC OXIDE FORMATION

As the consideration of chemical equilibrium cannot predict the actual NO concentration. The general accepted kinetics formation scheme proposed by [41] is used. The equations which describe the model together with their forward reaction rate constants k_{if} ($m^3/kmol/s$) are as follows:
(a)
$$
N+NO \leftrightarrow N_2+O
$$
 $k_{if=3.1x10^{10}exp^{(-160/T)}}$

(b) N+O₂
$$
\leftrightarrow
$$
 NO+O k_{2f}=6.4x10⁶exp^(-3125/T)

(c) N+OH
$$
\leftrightarrow
$$
 NO+H k_{3f}=4.2x10¹⁰

The change of NO concentration (in $kmol/m³$) is expressed as follows:

$$
\frac{1}{V} \left(\frac{d((NO)V)}{dt} \right) = 2(1 - \alpha^2) \left(\frac{R_1}{1 + \alpha R_1 / (R_2 + R_3)} \right)
$$
(3.32)

Where R_i is the one way equilibrium rate for reaction i, defined as:

 $R_1=$ k _{1f} (N)_e(NO)_e, R₂=k _{2f} (N)_e (O₂)_e, R₃=k _{3f} (N)_e(OH)_e with index e denoting equilibrium concentration and term $\alpha = (NO)/(NO)_e$

3.3.14 Soot concentration

Soot is a fine dispersion of black carbon particles in a vapor carrier. The main source of soot is from the incomplete hydrocarbon combustion. Soot particles form, grow, and oxidize as a result of chemical reactions that occur during combustion. The detailed of soot modeling are mentioned by Razleytsev [42]. Exhaust gas soot concentration related to normal conditions are as follows:

$$
\left[C\right]_{e} = \int_{\theta}^{480} \frac{d\left[C\right]}{dt} \frac{d\theta}{6\eta} \left(\frac{0.1}{p}\right)^{\frac{1}{\gamma}}
$$
(3.33)

Where γ =1.33 is an exhaust gas adiabatic exponent, p is the cylinder pressure, [C] is the current soot concentration in the cylinder and θ is the crank angle.

In brief overall structure of existing and modified model can be written as below:

3.4 EXISTING MODEL

The existing model can be written on the basis of single zone in the form of input variables, major governing equations and output variables. The detailed of the existing model is presented in Fig 3.2.

Figure 3.2. Structure of the existing model

3.5 MODIFIED MODEL

The same way as above modified model can also be written, on the basis of two zones in the form of input variables, major governing equations and output variables. Parameters such as two zones, mixture mass loss through piston rings were taken in to consideration for the model and presented in Fig.3.3.

Figure 3.3. Structure of the modified model

3.6 PARAMETERS MODIFIED

There are various parameters which are modified in the existing model to convert in the modified model. These are presented in Table 3.1.

Table 3.1 Comparison between existing and modified model

CHAPTER 4 SIMULATION

The equations of the model adopted in the chapter 3 are suitable for any hydrocarbon fuel as diesel, vegetable oil and biodiesel. These equations are solved numerically using with time step size of $0.5⁰$ crank angle. The engine geometrical parameters, molecular weight of gaseous products and various constants used in the model are defined. The input parameters used in model are injection pressure, crank angle and the molecular formula of the diesel and jatropha oil. The several physical, chemical and thermal properties are also measured and calculated as input parameters as shown in Table 2.1 [43].The properties of gaseous constituents such as enthalpy, internal energy and specific heats are calculated as a function of temperature. The pressure and temperature of the gases in the combustion chamber are calculated for every half degree crank angle. From the typical design of the engine, the combustion chamber volume at every degree crank angle is calculated with the help of above stated equation.

Before start of calculations, the design characteristics of the engine in hand are provided, as well as the operating data at the start of the cycle, i.e. at the IVC event. The calculations stop at the EVO event. The outputs of the modeling program are instantaneous pressure, temperature, volume and the performance and emission parameters that include brake thermal efficiency, brake specific fuel consumption, NOx and soot density. The performance and emission characteristics of the engine fueled with jatropha oil (preheated and unheated) and diesel are analysed by this model .The engine model is analysed for the variation in fuel injection pressure for different fuels. An engineering equation solver program, developed by F-Chart software is used for simulation [44].

4.1 NUMERICAL SOLUTION STAGES

In brief, the numerical solution stages consist of calculation of compression phase, calculations of combustion and expansion phases and calculation of the air (unburned) and burning phase.

4.1.1 COMPUTATION OF COMPRESSION PHASE

- i. Introduce the data at the IVC event, i.e. P_1 , T_1 , trapped composition (air with no fuel) and compute V_1 from engine geometry. Select the crank angle step size $\Delta\theta$, here, to 0.5⁰.
- ii. The initial internal energy E_1 was calculated using its T_1 relation and similarly for the heat capacities Cp and Cv.
- iii. For the new crank angle $\theta_2 = \theta_1 + \Delta\theta$, compute V_2 from the engine geometry.
- iv. Temperature T_2 was estimated by assuming an isentropic change:

 $T_2 = T_1 * (V_1/V_2)$ ^(R/Cv*T1)

Then, find pressure P_2 from perfect gas state equation:

 $P_2 = (V_1/V_2)^*(T_2/T_1)^*P_1$

- v. The internal energy E_2 was calculated using its T_2 relation.
- vi. Calculate the work in the step:

 $dW = (P_1+P_2)/2(V_2-V_1)$

- vii. Calculate dQ from heat loss model
- viii. Apply the first law of thermodynamics for a closed system:

f (E)= $E_2-E_1+dW-dQ=0$

Solve the equation with respect to T_2 using the Newton–Rapson numerical method so that a better estimate of T_2 is found.

- ix. Calculate P_2 for the revised value of T_2 using the gas state equation at the time moments 1 and 2.
- x. Repeat steps v-ix until the error $f(E)$ in the first law equation is negligible.
- xi. Continue this way, until θ_2 equals the value at the start of fuel injection.

4.1.2 COMPUTATION OF COMBUSTION AND EXPANSION PHASE

- i. Connect the forming two-zone system with the previous single zone one.
- ii. Set the conditions at the end of the previous time step (old state) as initial conditions for the current time step (new state) for both zones.
- iii. For crank angle $\theta_2 = \theta_1 + \Delta \theta$, compute V_2 from engine geometry.
- iv. Estimate pressure p_2 at the end of the time step, to be checked later on, by assuming isentropic change (with $\gamma = 1.35$), $P_2 = P_1 (V_1/V_2)^{\gamma}$.
- v. Check the temperatures of all zones.
- vi. Check the volumes of the zones and change pressure P_2 if necessary.
- vii. Calculate various useful quantities, such as the gross and net heat release rates as well as their cumulative values at each step
- viii. Repeat steps (i-vii) and continue this way until $Δ θ$ reaches the EVO event, i.e. the end of the closed cycle.

4.1.3 CALCULATIONS FOR UNBURNED ZONE

The calculations in this zone were similar to the ones during the compression phase.

- i. The initial internal energy E_1 was calculated using its T_{1u} relation and similarly for the enthalpy h_1 and heat capacity $C_v(T_{1u})$ of air.
- ii. V_{1u} was calculated from the gas state equation, $V_{1u} = (m R \text{mol} \ T_{1u})/$ P_1 where m was the total kmol in the air zone at state 1 per kmol.
- iii. Make a first estimate of T_{2u} considering an isentropic change.
- iv. The internal energy E_2 was calculated using its T_{2u} relation and similarly for the heat capacity C_v (T_{2u}) of air.
- v. V_{2u} was calculated from the gas state equation, V_{2u} =m Rmol T_{2u}/P_2 .
- vi. Calculate the work in the step, $dW = 0.5(P_1 + P_2) (V_{2u} V_{1u})$.
- vii. Apply the first law of thermodynamics for an open system. Solve the equation with respect to T_{2u} using the Newton– Rap son numerical method, so that a better estimate of T_{2u} is found.
- viii. Repeat steps iv-vii until the error $f(E)$ in the first law equation is negligible.

4.1.4 CALCULATIONS FOR BURNING ZONES

- i. The internal energy of burning zone was calculated at state $1 E_{1b}$, from its T_{1b} relation.
- ii. Estimate the temperature T_{2b} at the end of the time step (state 2), i.e. after combustion, considering an isentropic change:
- iii. Estimate the volume of the burning zone using the gas state equation:
- iv. The internal energy E_{2b} was calculated using its T_{2b} relation and similarly for the heat capacity $C_v(T_{2b})$ in state 2.
- v. The volume in state 2 was calculated using the gas state equation:
- vi. Calculate the work dW_1 in the time step, for a change from state 1 after mixing to state 2, $dW_1 = 0.5(P_1 + P_2)(V_{2b} - V_{1b})$.
- vii. Apply the first law of thermodynamics for a change from state 1 to state 2 (a closed system is considered, since the addition of air has already been taken into account). Solve the equation with respect to T_{2b} using the Newton–Rap son numerical method, so that a better estimate of T_{2b} is found.
- viii. Repeat steps iv-vii until the error $f(E)$ in the first law equation is negligible.
	- ix. Compute the quantity of NO in burning zone through by solving the relevant differential equation.
	- x. Compute the net soot formed in burning zone through the relevant differential equations.

xi. Finally, calculate the work for the total change from state 1 (unburned) to state 2, since this is the real work produced: $dW = 0.5(P_1 + P_2) (V_{2b} - V_{1b})$.

4.2 VARIATIONS OF CYLINDER VOLUME IN COMPRESSION STROKE WITH CRANK ANGLE

The cylinder volume variations with crank angle is shown in Figure 4.1. As piston moves from BDC to TDC cylinder volume is decreasing, which verify the programmed out. The value at near 350° crank angle shows the value of clearance volume.

Figure 4.1. Variation of cylinder volume vs crank angle

4.3 EFFECT OF DENSITY OF AIR ON HEAT TRANSFER PER CRANK ANGLE

The variations of heat transfer per crank angle with respect to density of air are shown in the Figure 4.2. As density of air increases in the combustion chamber, heat transfer also increases. So such types of variations of heat transfer and air density verify the program developed.

Figure 4.2. Variation of heat transfer per crank angle vs density of air

4.4 NET WORK DONE OUT PUT WITH CRANK ANGLE

The net work done with crank angle variations is shown in Figure 4.3.The negative work done in the figure shows that the work is done on the system in the compression phase, which is from 225° to 345° . After the fuel injection in the combustion chamber, burning takes place and expansion phase starts which shows the positive work done.

Figure 4.3. Variation of work done vs crank angle

CHAPTER 5 RESULTS AND DISCUSSION

5.1 INTRODUCTION

In the combustion modeling the molecular formula of diesel fuel is taken as $C_{17}H_{32}$. From the fatty acid composition, jatropha classifies it as linoleic or oleic acid types, which are unsaturated fatty acids [16]. So based on these properties, the molecular formula of jatropha oil is approximated as $C_{18}H_{32}O_2$ [45]-[46]. In general, this combustion model, developed for C.I engine analysis is suitable for any hydrocarbon fuel. This includes diesel, biodiesel or their blends as well as vegetables oil. The engine model is analyzed for the variation in fuel injection pressure, point of fuel injection and fuel inlet temperature for the diesel as well as jatropha oil.

5.2 ENGINE PERFORMANCE AND EMISSIONS

5.2.1 EFFECT OF FUEL INJECTION POINT ON BRAKE THERMAL EFFICIENCY

The fuel injection point is taken for analysis because the time duration between the point of fuel injection and the start of combustion process has been felt to be one factor which is not sufficient to allow the fuel particles to get atomized properly. The increase in time delay provides more time available for this pre combustion. It is stated that the jatropha oil demands ignition timing to be more for better combustion and hence improves the engine performance and emission characteristics. Advancing the fuel injection point by 1^0 results in increase in ignition delay of 0.07s. This results in better fuel atomization

characteristics and enhanced the combustion efficiency. The increase in delay period is achieved by advancing the fuel injection point. In present model the reference or static point of fuel injection is taken 20° BTDC for diesel fuel. The fuel injection point used for the analysis of model is 20^0 BTDC to 26^0 BTDC in 2^0 steps. Advancing the fuel injection point is limited because increased delay period increases the possibility of engine detonation and affects efficiency. The possible reason for detonation and reduction in engine performance is due to the fact that advanced ignition timing results in an increased peak pressure and temperature before and around the TDC.

Figure 5.1 Brake thermal efficiency vs. crank angle (BTDC) for jatropha at speed 1000 rpm, 80% of full load and static17.5 MPa injection pressure

Figure 5.2 Brake thermal efficiency vs. crank angle (BTDC) for diesel at speed 1000 rpm, 80% of full load and static17.5 MPa injection pressure

Figure 5.1 and 5.2 represents the predicted trend of BTE as a function of crank angle at speed 1000 rpm and 80% of full load (7.35 kW). BTE decreases with advancing crank angle for diesel fuel. But in case of jatropha oil, it first increases up to 24^0 and then started decreasing. Due to increased brake power and less fuel energy input with jatropha oil, the BTE trend is increasing in case of jatropha oil. But it starts decreasing as injection timing is more advanced, as cylinder pressure and temperature during the delay period become lower. Therefore, the ignition delay period becomes longer [47]. This phenomena results in more fuel being burnt during premixed combustion phase following ignition delay period.

5.2.2 EFFECT OF FUEL INJECTION PRESSURE ON BRAKE THERMAL EFFICIENCY

The effect of varying fuel injection pressure at a constant fuel injection point has been investigated in the model at different pressures from17.5 MPa to

20.5 MPa in 1.0 MPa step variation. The investigation has been carried out with objective that the fuel atomization characteristics which indirectly depend upon fuel droplets size injected into the combustion chamber gets improved as the fuel droplets reduce at high fuel injection pressures. The sauter mean diameter has an important role in defining the fuel atomization characteristics. Smaller SMD results better fuel atomization and ultimately the fuel combustion efficiency. The SMD of diesel at room temperature and injection pressure 17.5 MPa is found 3.82×10^{-5} m. The SMD of diesel can be reduced from 3.82×10^{-5} m to 3.5×10^{-5} m as the pressure increases from 17.5 MPa to 20.5 MPa. The SMD of jatropha oil at room temperature and 17.5 MPa is obtained as $12.56x10^{-5}$ m. It reduces from $12.56x10^{-5}$ m to $11.53x10^{-5}$ m as pressure is increased from 17.5 MPa to 20.5 MPa. As Jatropha oil is heated up to 90° C, the SMD at 17.5 MPa can be reduced from 12.56 $\times 10^{-5}$ m to 4.33 $\times 10^{-5}$ m. This is a substantial reduction in SMD by preheating. Preheating the fuel has lowered the viscosity from 48.7×10^{-6} m²/s to 3.68×10^{-6} m²/s. The comparison of SMD for jatropha oil and diesel at room temperature showed that the difference between them is very high 8.74×10^{-5} m. This difference can be reduced to a good extent $(0.5x10^{-5}m)$ as the jatropha oil is preheated. This appreciable improvement is due to the fact that the viscosity and surface tension reduces to sufficiently high extent. Figure 5.3 and 5.4 represents the predicted trend of BTE as a function of fuel injection pressure at constant speed, load and point of injection.BTE decreases as fuel injection pressure either decreases or increases from 19.5 MPa.

Figure 5.3 Brake thermal efficiency vs. injection pressure for jatropha at speed 1000 rpm, 80% 0f full load and $20⁰$ static injection point (BTDC)

Figure 5.4 Brake thermal efficiency vs. injection pressure for diesel at speed 1000 rpm, 80% Of full load and 20^0 static injection point (BTDC)

5.2.3 EFFECT OF FUEL INJECTION POINT ON BRAKE SPECIFIC FUEL CONSUMPTION

The predicted variation of BSFC keeping fuel injection pressure constant with varying fuel injection point is shown in Figure 5.5 and 5.6. It has been noticed that the brake specific fuel consumption for diesel is lower than the Jatropha oil operation. However with the advantages of high operating temperature due to presence of oxygen molecule in the Jatropha oil lowers the calorific value, also having low viscosity, low cetane number, and higher surface tensions resulting in all together effect combustion characteristics. It can also be seen that the BSFC of engine with diesel fuel started increasing whenever operating point advances. But in the case of jatropha oil as the fuel injection angle advances from 20^0 BTDC to 24^0 BTDC it shows a decreasing pattern. When we further advance from 24^0 it shows a rising trend. This is in correlation with BTE trends with change in fuel injection point.

Figure 5.5 Brake specific fuel consumption vs. crank angle (BTDC) for diesel at speed 1000 rpm, 80% of full load and static 17.5 MPa injection pressure

Figure 5.6 Brake specific fuel consumption vs. crank angle (BTDC) for jatropha at speed 1000 rpm, 80% of full load and static 17.5 MPa injection pressure

5.2.4 EFFECT OF FUEL INJECTION PRESSURE ON BRAKE SPECIFIC FUEL CONSUMPTION

 The effect of fuel injection pressure keeping the angle constant has been plotted in Figure 5.7 and 5.8.The engine BSFC with diesel fuel get increases continuously when fuel injection pressure increases above 17.5 MPa. But in case of jatropha oil which is higher than diesel at 17.5 MPa initially started decreasing up to 19.5 MPa but further increase in pressure its goes up. Lower viscous fuel breaks in to lighter fuel particle at the end of fuel injection which increases the atomization and better combustion. In contrast higher viscous fuels increase the mixture momentum due to heavier fuel particle size. This reduces the combustion efficiency for jatropha oil than diesel. But in contrast higher combustion efficiency can be obtained for jatropha oil than diesel engine [16]. The increased mixture momentum and penetration depth is responsible for this improvement, which can be achieved by increasing the fuel injection pressure.

Figure 5.7 Brake specific fuel consumption vs. injection pressure for diesel at speed 1000 rpm, 80% of full load and 20^0 static injection point BTDC

Figure 5.8 Brake specific fuel consumption vs. injection pressure for jatropha at speed 1000 rpm, 80% of full load and 20^0 static injection point BTDC

5.2.5 EFFECT OF FUEL INJECTION POINT ON NOx EMISSION

It is important to consider NO_x as one of the major pollutant and emission concerns. When the combustion temperature is decreased the emission of NOx is reduced but the smoke and particulate emission increases. By retarding the injection timing the temperature inside the combustion chamber decreases and therefore a reduction in the NO_x emission can obtained. Figure 5.9 and 5.10 represents the predicted trend of fuel injection point variation on NO_x emission keeping fuel injection pressure constant. This trend show the continuous increasing the NOx with diesel fuel as the angle of fuel injection advances from 20^0 BTDC. This increased NO_x emission is due to the increase in peak cylinder pressure and temperature as the combustion occurs earlier in the cycle and more heat is released before and around the top dead centre. The charge elements which burns early in the cycle are subjected to higher temperature and pressure with advance in peak timing and remain at high temperatures for the longer period.

These early burn elements contribute most to NOx formation and hence higher NOx formation rates result with advanced ignition timing. The NO_x emission for jatropha oil decreases with advance angle of fuel injection up to $24⁰$ BTDC but it started increasing for further increase. This reverse behavior of diesel and jatropha oil in NO_x emission on varying the point of fuel injection may be because the established combustion process in jatropha oil might be still later than diesel fuel. This consequence of late combustion could be having been due to low temperature even little beyond the TDC point. This indicates that combustion efficiency may improve in case of jatropha oil as fuel injection angle advances. The inverse result beyond 24° BTDC may be due to possibility of engine knocking and erratic behavior. Predicted trend by this model is very close to experimental analysis done by previous researcher [48].

Figure 5.9 NOx emissions vs. crank angle (BTDC) for diesel at speed 1000 rpm, 80% of full load and static17.5 MPa injection pressure

Figure 5.10 NOx emissions vs. crank angle (BTDC) for jatropha at speed 1000 rpm, 80% of full load and static17.5 MPa injection pressure

5.2.6 EFFECT OF FUEL INJECTION PRESSURE ON NOx EMISSION

 From the Figure 5.11 and 5.12 it can be predicted that the NOx emission in case of diesel fuel increases as the fuel injection pressure increases from 17.5 MPa keeping constant point of fuel injection. But this trend was reversed when the pressure further increases from 19.5 MPa. This may be due to the fact that peak pressure and temperature is very close to TDC or even in some cases after TDC which result in exposing the NOx for very small time period to the excess air available for the formation of NOx .The reverse effect on engine beyond the injection pressure 19.5 MPa might be due to the possibility of engine knocking and erratic behavior of engine. In case of jatropha oil it is much more than diesel fuel at 17.5 MPa. But it reduces up to 19.5 MPa and then started increasing for further rise in pressure.

Figure 5.11 NOx emissions vs. injection pressure for diesel at speed 1000 rpm, 80% of full load and 20^0 static injection point BTDC

Figure 5.12 NOx emissions vs. injection pressure for jatropha at speed 1000 rpm, 80% of full load and 20^0 static injection point BTDC

5.2.7 EFFECT OF VARYING FUEL INJECTION PRESSURE ON PERFORMANCE AND EMISSION OF ENGINE

Brake thermal efficiency, Brake specific fuel consumption and smoke opacity were calculated at different fuel injection pressures for diesel as well as pre heated Jatropha oil. For diesel fueled engine, BSFC decreases as the fuel injection pressure increases from 17.5 MPa to 195 MPa Figure 5.14. Further increase in fuel injection pressure results in increased BSFC. BTE was found to increase with increasing fuel injection pressure from 17.5 MPa to 19.5 MPa Figure 5.13. However, increase in fuel injection pressure from 19.5 MPa to 20.5 MPa showed decrease in thermal efficiency. Maximum thermal efficiency (30.8%) was found at fuel injection pressure of 19.5 MPa. It can be seen from Figure 5.15 that increase in fuel injection pressure from 17.5 MPa to 19.5 MPa resulted in decreased smoke opacity. However, further increase in fuel injection pressure from 195 bars to 205 bars showed increased smoke opacity. Therefore, smoke opacity was lowest at a fuel injection pressure of 19.5 MPa. Based on BSFC, BTE and smoke opacity, 19.5 MPa was found optimum fuel injection pressure for diesel. BTE, BSFC, and smoke opacity were calculated at different fuel injection pressure for preheated Jatropha oil. BSFC decreases as the load increases as shown in figure 5.16. But, at higher loads, BSFC increases. Lowest BSFC (0.31 kg/kWh) was found at 19.5 MPa. Maximum thermal efficiency (30.3%) was found at 19.5 MPa at 7.35 kW rated load as shown in figure 5.17. Thermal efficiency decreases when fuel injection pressure either decreases or increases from 19.5 MPa. Smoke opacity was also lowest at 19.5 MPa. Smoke opacity was 33% at 195 bar and at 75% of rated load as shown in figure 5.18. Based on BSFC, BTE, and smoke opacity, 19.5 MPa was also found optimum fuel injection pressure for preheated Jatropha oil. Heating the oil reduces the viscosity of Jatropha oil and for pre-heated Jatropha oil also, same optimum fuel injection pressure as that for diesel was found.

Figure 5.13 Effect of fuel injection pressure on brake thermal efficiency of diesel fueled engine

Figure 5.14.Effect of fuel injection pressure on brake specific fuel consumption of diesel fueled engine

Figure 5.15. Effect of fuel injection pressure on smoke opacity of diesel fueled

engine

Figure 5.16. Effect of fuel injection pressure on brake thermal efficiency of jatropha oil (preheated) fueled engine

Figure 5.17. Effect of fuel injection pressure on brake specific fuel consumption of jatropha oil (preheated) fueled engine

Figure 5.18. Effect of fuel injection pressure on smoke opacity of jatropha oil (preheated) fueled engine

5.2.8 EFFECT OF VARYING FUEL INLET TEMPERATURE ON PERFORMANCE AND EMISSION OF ENGINE

The model was evaluated for performance and emission using unheated Jatropha oil and preheated Jatropha oil. The baseline data was generated using diesel. Diesel fuel operation shows lowest BSFC as shown in figure 5.20. Higher BSFC was observed when running the engine with Jatropha oil. Lower calorific value of Jatropha oil leads to increased volumetric fuel consumption in order to maintain similar energy input to the engine. Figure 5.19 show that the BTE of preheated Jatropha oil was found slightly lower than diesel. The possible reason may be higher fuel viscosity. Higher fuel viscosity results in poor atomization and larger fuel droplets followed by inadequate mixing of vegetable oil droplets and heated air. However, BTE for preheated Jatropha oil was higher than unheated Jatropha oil. The reason for this behavior may be improved fuel atomization because of reduced fuel viscosity. Figure 5.21 shows that the smoke opacity for Jatropha oil operation was greater than that of diesel. Heating the Jatropha oil result in lower smoke opacity compared to unheated oil but it is still higher than diesel.

Figure 5.19. Brake thermal efficiency of diesel, jatropha oil (preheated) and jatropha oil (unheated) fueled engine

Figure 5.20. Brake specific fuel consumption of diesel, jatropha oil (preheated) and jatropha oil (unheated) fueled engine

Figure 5.21. Smoke opacity of diesel, jatropha oil (preheated) and jatropha oil (unheated) fueled engine

5.3 CORRECTION FACTOR FOR VARIOUS PERFORMANCE AND EMISSION PARAMETERS

5.3.1 BRAKE THERMAL EFFICIENCY

Correction factor for brake thermal efficiency is explained in two variable conditions .Firstly with varying the crank angle and secondly with fuel injection pressure. Figure 5.22 and 5.23 shows the value of correction factor in the form of governing equation. The values of correction factor in both conditions are finding out by putting the crank angle and fuel injection pressure as input variable in the respectively governing equations.

Figure 5.22 Brake thermal efficiency correction factor with crank angle

Figure 5.23 Brake thermal efficiency correction factor with fuel injection pressure

5.3.2 BRAKE SPECIFIC FUEL CONSUMPTION

Figure 5.24 and 5.25 shows the correction factor for brake specific fuel consumption variations with crank angle and fuel injection pressure. Between the crank angle from 20^0 to 22^0 the value of correction factor is negative. This is due to that we taking some assumptions in modeling with respect to actual conditions. Same trends also continue from 25° onwards. But in the case of varying fuel injection pressure all the value of correction factor are in negative side. These are all due to setting the conditions at the end of the previous time step (old state) as initial conditions for the current time step (new state) for both zones. And estimating pressure p_2 at the end of the time step, to be checked later on, by assuming isentropic change (with $\gamma = 1.35$), $P_2 = P_1 (V_1/V_2)^{\gamma}$. But in actual conditions these are not isentropic changes.

Figure 5.24 Brake specific fuel consumption correction factor with crank angle

Figure 5.25 Brake specific fuel consumption correction factor with fuel injection pressure

5.3.3 NO^x EMISSION

 NO_x correction factor variations with fuel injection pressure and crank angle shows in Figure 5.26 and 5.27.In both the conditions the value of correction factor are negative as well as major differ from the trends line. These are due to not correctly calculating the numbers of moles of each constituent which are taking part in combustions, which effects the gas properties calculations.

Figure 5.26 NO_x correction factor with crank angle

Figure 5.27 NO_x correction factor with fuel injection pressure

5.4 COMPARISION OF THEORETICAL AND EXPERIMENTAL RESULTS

The brake thermal efficiency of compression ignition engine fueled by diesel, jatropha oil (preheated) and jatropha oil (unheated) is compared with that obtained from the theoretical model as shown in Figure 5.19. The brake thermal efficiency of diesel engine is slightly higher with preheated jatropha oil fueled engine. The brake thermal efficiency of the engine decreases with using unheated jatropha oil. The calorific value of jatropha oil is lower than (about 14%) that of diesel because of the presence of oxygen in its molecule. Hence, the brake thermal efficiency of jatropha oil (unheated) fueled engine is lower as compared to that of diesel fueled engine. The variation in experimental and theoretical results may be due to the fact that in theoretical model homogeneous mixture with complete combustion is assumed. But in general, it is difficult to attain complete combustion. Despite the simplification resulting from the assumed hypothesis and empirical relations, the developed simulation proved to be reliable and adequate for the proposed objectives.

Figure 5.28. Comparison of brake thermal efficiency

5.5 VALIDATION OF THE MODEL

To validate the model, a comparison is given in the present work between the results obtained from the simulation model and the ones obtained from an experimental investigation conducted in the U.P.E.S.Dehradun. The comparison between the calculated and experimental value determined for 1000 rpm engine speed and 7.35 kW load examined, is given in Fig. 5.16. The coincidence between calculated and experimental values is good, verifying the accuracy of the simulation model. The values obtained from the proposed model and the detailed one are practically the same for all test conditions examined. The basic data of the engine are given in Table 5.1. Furthermore, in order to validate the model against existing sophisticated models and to find the level of significance in case of diesel fuel BTE, a chi-square test is performed which as shown below.

5.5.1 CHI-SQUARE TEST

 χ^2 test enables us to ascertain how well the theoretical distribution fit in to empirical distribution. If the calculated value of χ^2 is less than the tabular value at a specified level (generally 5%) of significance, the fit is considered to be good. If

the calculated value of χ^2 is greater than the tabular value, the fit is considered to be poor.

Observed value (O_i) $\frac{0}{0}$	30.7	29.8	27.5	28.3	26.2
Expected value(E_i) %	31.7	28.5	30.8	27.5	27.5
(O_i-E_i)	-1	1.3	-3.3	0.8	-1.3
$(O_i-E_i)^2$	1	1.69	10.89	0.64	1.69
$(Oi-Ei)^2/Ei$	0.03	0.059	0.35	0.023	0.061

Table 5.1 Calculation for the value of χ^2

χ $^{2} = \Sigma \left[(\text{O}_{\text{i}} - \text{E}_{\text{i}})^{2} / \text{E}_{\text{i}} \right] = 0.523$

Tabular value of χ^2 at 5% level of significance for n-1 =4 is 7.815.

So χ^2 0.05 = 7.815 . Since the calculated value of χ^2 is less than that of the tabulated value. So theoretical results support the experimental results.

Table 5.2 Engine specifications

Manufacturer	Field Marshal Engine Ltd., India			
Model	$FM-4$			
Engine type	Vertical, 4-stroke, singlecylinder, compression- ignition			
	engine			
Rated power	7.35 kW at 1000 rpm			
Bore/stroke	$120/139.7$ (mm)			
Compression ratio	17:1			
Nozzle	DL30S12002MICO			
Nozzle holder	9430031264MICO			
Fuel pump plunger	9x03/323MICO			
Nozzle opening pressure	145 bar			
Sump capacity	4.5 litre			

CHAPTER 6 CONCLUSIONS

A two zone thermodynamic model is modified for analyzing the performance characteristics of the compression ignition engine. The model is modified in such a way that it can be used for characterizing any hydrocarbonfueled engines, as diesel or biodiesel. The modeling results showed that,

- With advancing the crank angle and increasing the fuel injection pressure the break thermal efficiency decreases and break specific fuel consumption increases for diesel fuel and reverse behaviour has been observed in case of jatropha oil up to a limit.
- The efficiency of engine with jatropha oil was improved from 31.0% to 34.8% which is 1.8 % higher than the diesel fuel. The BSFC was reduced from 0.30 kg/kWh to 0.26 kg/kWh.
- The performance characteristics of the engine follow the same trend for all fuels as diesel, preheated jatropha and unheated jatropha oil.
- The predicted results are compared with the experimental results of the engine fueled by diesel, jatropha (PH) and jatropha (UH). This model predicted the engine performance characteristics in closer approximation to that of experimental results.

Hence, it is concluded that this modified model can be used for the prediction of the performance characteristics of the compression ignition engine fueled by any type of hydrocarbon fuel.

SCOPE OF FUTURE WORK

The existing model that has been presented in this thesis can be further modified and improve in the following items:

- **Advanced model of fuel spray:** Another step to increase accuracy in the model is to divide the fuel spray into several zones and consider droplet distribution. This is a more advanced fuel spray model.
- **Swirl model:** To get a more accurate model of the fuel spray distribution it should be considered to model the swirl factor. The swirl factor is a measurement of how turbulent the airflow is in the combustion chamber.
- **Cylinder wall temperature**: Examine how the changes in the in-cylinder wall temperature effects the combustion process.
- **Wall wetting:** There may occur injections where the injected fuel hits the in-cylinder wall and cools down which prevents the evaporization process to happen.
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ANNEXURE

A1. PROGRAM FOR EXISTING MODEL

\$Unit System SI MASS DEG KPA C KJ

Input variables

Governing equations

T2=T1*(V1/V2)^ (R/Cv) T2=T1*(V1/V2)^ (R/Cv) E2=mair*Cv*T2 The Contract of the Contract of Texas variable values with the "Final internal energy" rhoair=P2/(Rair*T2) "Density of air" Re=rhoair*d*Up/muair "Reynolds number" Tg=(T1+T2)/2 "Air temperature"

kair=Cp*muair/0.7 "Thermal conductivity of air" Tw=T1 **The Table 10 and Table 10** and Table 10 and Ta

Output variables

A2. PROGRAM FOR MODIFIED MODEL

\$Unit System SI MASS DEG KPA C KJ

Input variables

Governing equations

dVb*dtheta=(Vb*del*(lnVb)*dTb)/(Tb*del*(lnTb)*dtheta)+(Vb*del*(lnVb)*dP)/(P*del*lnP)*dt heta Vb=integral(dVb*dtheta,theta,theta1,theta2) "Specific volume for burned zone" dVu*dtheta=(Vu*del*(lnVu)*dTu)/(Tu*del*(lnTu)*dtheta)+(Vu*del*(lnVu)*dP)/(P*del*lnP)*dt heta Vu=integral(dVu*dtheta,theta,theta1,theta2) "Specific volume for unburnt zone" dUb*dtheta=(Cpb-(P*Vb*del*(lnVb))/(Tb*del*(lnTb)))*dTb*dtheta - Vb*((del*(lnVb))/(del*(lnTb))+(del*(lnVb))/(del*(lnP)))*dP*dtheta Ub=integral(dUb*dtheta,theta,theta1,theta2) "Internal energy for burnt zone" dUu*dtheta=(Cpu-(P*Vu*del*(lnVu))/(Tu*del*(lnTu)))*dTu*dtheta - Vu*((del*(lnVu))/(del*(lnTu))+(del*(lnVu))/(del*(lnP)))*dP*dtheta Uu=integral(dUu*dtheta,theta,theta1,theta2) "Internal energy for unburnt zone"

Output variables

```
dw=((P+P2)/2)*(V2-V1) "Work done in each crank angle "
dNO*dt=2*(1-alpha^2)*(R1)/(1+(alpha*R1)/(R2+R3))
```
NO=integral(dNO*dt,time,time1,time2) "Change of NO concentration" dC*dt=dtheta/(6*n)*(0.1/P)^(1/1.3) C=integral(dC*dtheta,theta,theta1,theta2) "Current soot concentration"

A3. PROGRAM RESULTS

CURRICULUM VITAE

B.P Singh obtained B.Tech with honors in Mechanical Engineering from H.B.T.I Kanpur and M Tech. in Mechanical Engineering from U.P.T.U Luck now, Uttar Pradesh, India.

Presently serving as Associate Professor at Moradabad Institute of Technology, Moradabad, U.P, India. Also having eight years industrial experience. His research interest is in energy and thermal engineering with main emphasis on alternative fuels for internal combustion engines, renewable energy.

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PAPER STATUS FROM THE WORK