Comparative study of experimental and simulation of Neem Oil Methyl Ester and Its Blends with Diesel in a Conventional DI Diesel Engine

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***Abstract*:- Neem oil methyl ester and its blends with diesel as an alternative fuel are considered suitable and the most promising fuel for Diesel engine. The properties of NOME are found to be that of similar to Diesel engine. Many researchers have evaluated the performance, combustion and emissions of conventional diesel engine using bio-diesel and its blends experimentally. However, experiments require enormous effort, money and time. Hence a simulation model incorporating a thermo dynamic based single zone combustion model is developed. A comprehensive computer code using C++ language was developed for CI engine. Performance characteristics such as BTE and BSEC and combustion characteristics such as flame temperature, cylinder pressure and heat release rate and emission on NOx were analyzed. On the basis of first law of thermodynamics the properties at each crank angle was calculated. The simulated combustion,. Performance and emission characteristics are found satisfactory with the experimental results.**

Key words: Bio-diesel, BTE, BSEC, NOME, B25 and flame temperature.

1. INTRODUCTION

Modeling compression ignition engine depends on characteristics of fuel. It is a process of designing a model of real system and conducting experiment with it for the purpose of understanding the behavior of the system. The numerical model of a Diesel engine can be regarded as an explanation of a real engine operation, which combines mathematical relation between the relative components, can be used to simulate the dynamic process of Diesel engine. A clear overview of engine operation is helpful to understand the modeling of real diesel engine [1]. It serves as a tool for better understanding of the combustion and its effort on engine, so as to buildup more strong real systems.

Computer simulation has contributed enormously towards new evaluation in the field of internal combustion engines. Mathematical tool have become very popular in recent years owing to the continuously increasing improvement in computational power. Diesel engines occupy a prominent role in the present transportation and power generation sectors. There have been many methods tried and are used to reduce pollutant emissions from a Diesel engine [2]. The main options to reduce pollutants are the usage of bio-fuels and adopting some modifications to the combustion process. Diesel engine simulation models can be used to understand the combustion, performance and emissions, these models reduce the number of experiments.

From the point of view of protecting the global environment and the concern for long term supplies of conventional diesel fuel, It becomes a necessary to develop alternative fuel that give engine performance at par with Diesel. Among the alternative fuels, bio-diesel folds good promises as an eco-friendly alternative fuel. Vegetable oils obtained from non-edible sources are considered promising alternative fuel for compression ignition engine compared to their edible counterpart due to food vs fuel controversy. 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 [3]. The model predicts CI engine in in terms of flame temperature, cylinder temperature, cylinder pressure, Heat release rate, brake thermal efficiency, Brake specific energy consumption and NOx for all tested fuel such as NOME, B25 and Diesel.

2. NEED FOR ALTERNATIVE FUELS

The crude oil and petroleum products will become very scarce and costly to find and produce. The fuel economy of engines is greatly improved from the past. It will probably continue to be improved. Increase in number of automobiles in the recent times dictates that there will be a great demand for fuel in the near future [5]. Gasoline and Diesel will become scarce and most costly. Alternative fuel availability and use will become more common in the coming decades. All these years there have been some, IC engines fueled with non-gasoline or Diesel oil fuels.

3. OBJECTIVES

The objective of the present work is to study through experiments and simulation the use of Diesel, Neem oil methyl ester and its blends with Diesel (B25) in a conventional DI Diesel engine for achieving high efficiency and reducing the emission levels.

4. METHODOLOGY OF RESEARCH WORK

The following methodology was adopted in the present work:

- Selection of vegetable oil: Raw neem oil is non-edible oil used as an alternative fuel for transportation, stationary engines and for agricultural units.
- Conversion of raw neem oil into neem oil methyl ester using the materials such as raw neem oil, methanol, sodium hydroxide and acetone to remove all the fatty acids present in the raw neem oil and reduce the viscosity by transesterification process [7].
- Study of fuel properties of Diesel, neem oil methyl ester and its blends with Diesel B25 such as kinematic viscosity, density, flash point, fire point, and calorific value of fuel.
- Selection of suitable single cylinder, four stroke, water cooled, naturally aspirated conventional Diesel engine and development of an experimental setup with necessary instruments and analyses.
- Experiments with Diesel, NOME and B25 to study the performance, emission and combustion characteristics.
- Developing C++ program for simulation of conventional Diesel engine and LHR engine.
- Validation of the simulation results with that of the experimental results.

5. RAW NEEM OIL

Neem oil is non-edible oil available in huge surplus quantities in south Asia. Annual production of Neem oil in India is estimated to be 30,000 tons. Traditionally, It has been used as fuel in lamps for lighting purpose in rural areas and is used on an industrial scale for manufacturing of soap, cosmetics, pharmaceuticals and other non-edible products. India has shortage of edible oils so its bio-diesel program is centred on non-edible vegetable oils like Neem. For feed stock diversification and utilization of currently available local resources, non-edible sources like Neem, karanja etc. should be scientifically investigated for efficient bio-diesel production and engine utilization. Keeping this background in consideration, production of bio-diesel from high free fatty acids Neem oil and its utilization as a potential alternative fuel for diesel engine has been investigated [11].

Neem's name is derived from Sanskrit **NIMBA** and it was known as SARVA ROGA NIVARINI or curer of all illnesses. 50 kg of fruit yields 30 kg of seed, which gives 6 kg of oil and 24 kg of seed cake. The raw Neem oil is obtained of 20% from the neem seed. Mechanical press method is the one used since antiquity [14]. Neem seed kernels are placed into a tub and either a screw or some form of press is used to squeeze the kernels under pressure until the oil is pressed out and collected.

6. VISCOSITY REDUCTION

Pre heating, pyrolysis, micro emulsification, blending and transesterification are the different methods used to reduce the viscosity of vegetable oils. The transesterification process is one of the best methods for reducing viscosity of the vegetable oils [9]. More over it is cost effective and very simple process.

7. TRANSESTERIFICATION OF RAW NEEM OIL INTO NEEM OIL METHYL ESTER (NOME)

Transesterification is the process of using an alcohol (e.g. methanol or ethanol) in the presence of catalyst, such as Sodium Hydroxide (NaOH) or Sodium Meth-oxide (NaOMe) or Potassium Hydroxide (KOH) to chemically break the molecule of the raw renewable Neem oil into Neem oil methyl ester (NOME) with glycerol as a byproduct [12].

Table: 1 Chemical structure of fatty acids of neem oil

Fatty acids	**Structure**	**Saturated/ Unsaturated**	**Formula**	**Molecular Weight**	**% by volume in the oil (Ju et al 2005)**	**Type of fatty acid and its percent**
Palmitic	16:0	Saturated	$C_{16} H_{32} O_2$	256	10	Saturated fatty acids (28%)
Stearic	18:0	Saturated	$C_{18} H_{36} O_2$	284	11	
Myristic	3:0	Saturated	$C_3 H_6 O_2$	74	7	
Oleic	18:1	Unsaturated	$C_{18} H_{34} O_2$	282	30	Mono-unsaturated fatty acids (30%)
Linoleic	18:2	Unsaturated	$C_{18} H_{32} O_2$	280	42	Poly-unsaturated fatty acids (42%)

8. NEEM OIL AND ITS PROPERTIES

In the present study, the non-edible neem oil is used as an alternate fuel for blending with Diesel after esterification. Experimental investigations were carried out on Diesel blended with NOME and compared with unblended Diesel in a Diesel engine under standard operating conditions.

9. DERIVATION OF CHEMICAL FORMULA FOR NOME AND B25

❖ Fatty acid

The main acid present in Raw Neem Oil is

i. Palmitic - $C_{14}H_{28}O_2$
ii. Stearic - $C_{17} H_{34} O_2$
iii. Linoleic - $C_{10} H_{20} O_2$

Taking into consideration of the raw of neem oil formula is General formula arrived as $C_{18}H_{35}O_2$ Fatty Acid. To show it in the form of an acid the structural formula with functional group is shown as $C_{17} H_{34}$ COOH. COOH is a functional group to indicate carboxylic acid

❖ Gylcerol

- $CH_2OH - CHOH - CH_2OH$

❖ Triglyceride

Neem Oil is a Triglycerides of Fatty acid that is composed of Glycerol in combination of Fatty acids. Since Glycerol is having 3OH Group, the molecules of Fatty Acid are always in combination with 1 molecular of Glycerol. The formula of Gylceride ester is $(C_{17}H_{34}COO)_3 C_3H_5$

❖ Methyl Ester

Conversion of Glyceride ester into Methyl ester by the addition of Methanol in the presence of catalyst sodium hydroxide (NaOH)

- $(C_{17}H_{34}COO)_3C_3H_5 + 3NaOH$ □ $3C_{17}H_{34} COONa$
- $3C_{17}H_{34}COONa+3CH_3OH$ □ $3C_{17}H_{34}COOCH_3+3NaO$

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- $C_{17}H_{34}COONa+CH_3\ OH$□ $C_{17}H_{34}\ COOCH_3+NaOH$

The Neem Oil Methyl Ester chemical formula is $C_{17}H_{34}$ $COOCH_3$

10. COMPUTATIONAL PROCEDURE

In this analysis the molecular formula for Diesel, Neem oil Methyl Ester and B25 are approximated, as $C_{10}H_{22}$, $C_{17}H_{14}COOCH_3$, and $C_{12.25}H_{25.75}O_{0.5}$ ($C_{49}H_{103}O_2$) respectively. In the present work a zero dimensional, single zone thermo-dynamic model for C.I engine cycle simulation was developed. The model was used to predict and analyze the engine combustion, performance and emission characteristics fueled with Diesel, Neem oil methyl ester (bio-diesel) and its blends with Diesel (B25). The simulation of compression ignition engine fueled and its blends with Diesel was developed using C++ program. The various equations of thermodynamic model are solved numerically [20]. The fuel parameters number of moles of carbon, hydrogen and oxygen, heating value, molecular weight of the fuel and various constant used in the model or defined in the data subroutine. Bore, stroke length, connecting rod length compression ratio, percentage of excess air, engine speed, inlet conditions and atmospheric condition are given as input parameters. The molecular formula for Diesel, NOME and B25 fuels are employed. During the cycle the program concerning the simulation model predicts cylinder pressure, ignition delay, heat release, brake thermal efficiency, brake specific energy consumption, oxides of nitrogen, flame temperature, cylinder temperature and spray penetration parameters. The results and graphs were generated as outputs to the program for the given inputs.

11. VALIDATION

Engine cycle simulations are, in general based on certain assumption, sum of which are mathematical and some are empirical. The validity of this assumption and the predicative capabilities of the model can be better judged by the comparing the theoretical prediction with the experimental data. Unless the model gives results that are adequate approximations of what would occur in the real system, simulation can lead to the wrong answers. Validation is achieving a sufficient level of confidence that the model does provide a representation of reality [19]. There is no single test to prove that a model is 100 percent valid. Statistical comparisons of the outputs of the model and the real-system under identical inputs can also be made to test the model's accuracy.

12. RESULTS AND DISCUSSION

Comparison between conventional and simulation of diesel engine (validation)

Experimental investigation and simulation of conventional Diesel engine have been compared using fuels Diesel (100%), NOME (100% bio-Diesel) and B25 (bio-diesel 25% and Diesel 75%). The cylinder pressure, heat release rate, brake thermal efficiency, brake specific energy consumption (BSEC) and oxides of nitrogen (NO_x) are compared with experimental and simulation results of conventional Diesel engine [16].

❖ Cylinder pressure

The cylinder pressure with crank angle data are measured and have been plotted along with the predicted values (simulation data) for conventional Diesel engine are shown in Fig.1 for all tested fuels at full load. The experimental data is shown in bold lines while the predicted data is shown in terms of dotted line.

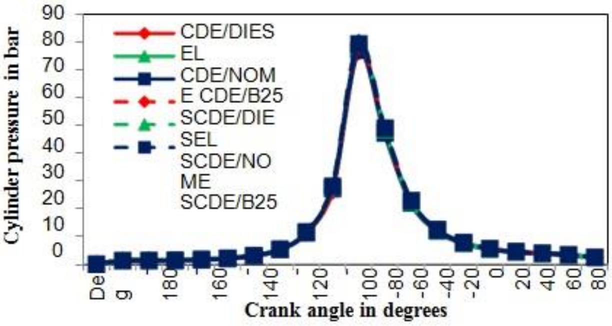

Fig.1 Variation of cylinder pressure with crank angle

The experimental data for cylinder pressures for Diesel, NOME and B25 are 76 bar, 78 bar and 77 bar respectively for conventional Diesel engine. The difference in pressure between Diesel and NOME is 2-bar and the difference in pressure between Diesel and B25 is 1 bar. The maximum cylinder pressure is increased by 2.63% and 1.3% for NOME, B25 respectively than Diesel fuel.

The predicted value of conventional Diesel engine (simulation) of the maximum cylinder pressure for NOME is 80 bar. The least cylinder pressure for Diesel is 78-bar. The cylinder pressure for B25 lies between Diesel and NOME and its value is 79-bar. The difference in pressure between Diesel and NOME is 2-bar and the difference in pressure between Diesel and B25 is 1 bar. The cylinder pressure for NOME and B25 is increased by 2.56 % and 1.3 % respectively compared to Diesel fuel.

The cylinder pressures at all the crank angles are higher for NOME and B25 compared to Diesel fuel due to higher cetane number and shorter ignition delay. Hence, combustion starts early in the case of NOME and B25 results in higher cylinder pressure. NOME is oxygenated fuel and their higher oxygen content results in better combustion and higher cylinder pressure [20]. At any power output the brake specific energy consumption is also higher for NOME and its blends compare to Diesel fuel also results in higher cylinder pressure. It is observed that the predicted cylinder pressure is marginally higher than the experimental value and it varies from 1 to 3% is within the acceptable limits for all tested fuels.

❖ Heat release rate

Fig.2 shows the variation of heat release rate with crank angle at full load for all tested fuels both for experimental and predicted values of conventional Diesel engine. The experimental data is shown in bold line while the predicted data is shown in terms of dotted line.

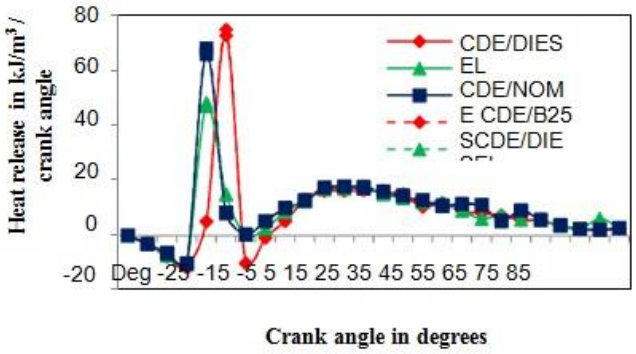

Fig.2 Variation of heat release rate with crank angle

❖ Brake thermal efficiency

The effect of break power on brake thermal efficiency for Diesel, NOME and B25 are shown in Fig.3 for both experimental and predicted values of conventional Diesel engine. There is a steady rise in brake thermal efficiency as the load increases. The brake thermal efficiency is a function of brake power. The experimental data are shown in solid lines while the predicted data is shown in terms of dotted line.

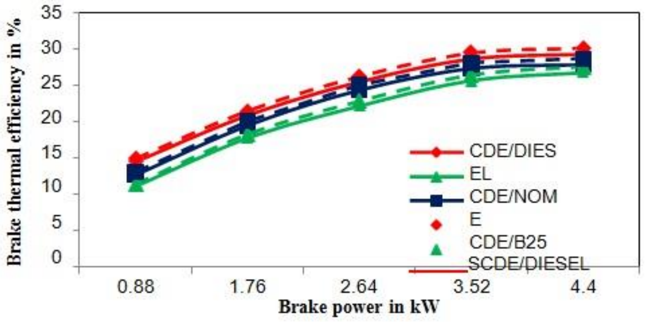

Fig.3 Brake thermal efficiency with brake power

❖ Brake specific energy consumption (BSEC)

Variations of brake specific energy consumption with brake power for all tested fuels from no load to full load are shown in Fig.4 both for experimental and predicted values of conventional Diesel engine.

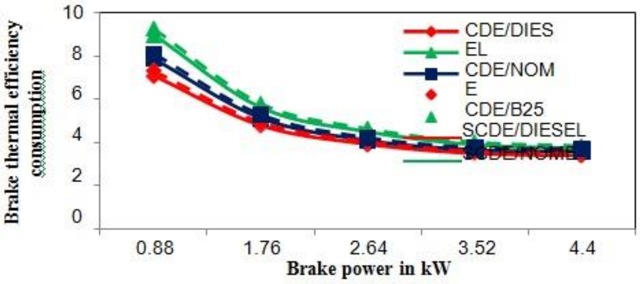

Fig.4 Brake specific energy consumption versus brake power

❖ Oxides of nitrogen (NO_X)

The variations of NO_x for Diesel, NOME and B25 from no load to full load are shown in Fig.5 both for experimental and predicted values of conventional Diesel engine. The experimental data are shown in solid lines while the predicted data is shown in terms of dotted line.

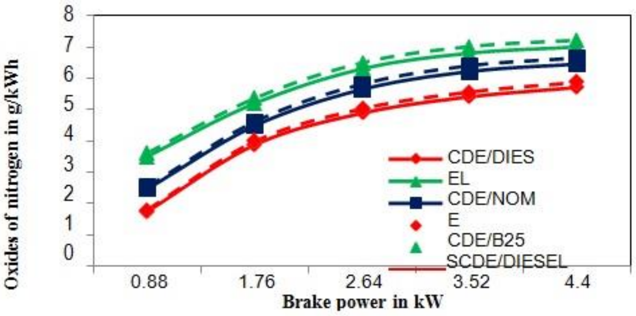

Fig.5 Variation of NO_X with brake power

❖ Ignition delay

Ignition delay of a fuel is one of the important parameters in determining the knocking characteristics of Diesel engines. Ignition delay is a period measured in milliseconds or crank angle between start of fuel injection into the combustion chamber and the start of combustion. The ignition delay depends on many factors such as compression ratio, inlet pressure, injection parameters and the properties of the fuel. Fig.6 shows the variation of delay period of NOME, B25 with brake power compared with Diesel at full load.

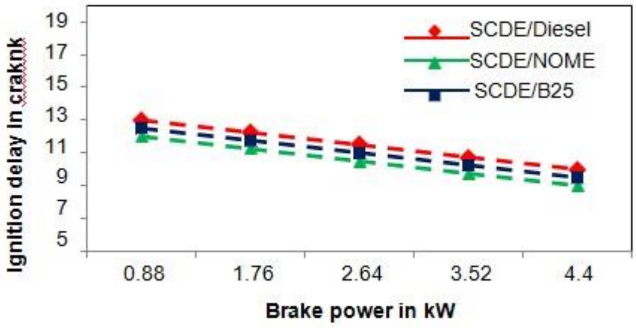

Fig.6 Ignition delay versus crank angle at full load

❖ Flame temperature

The calculation of the temperature of the products of combustion reaction is very important for the design of internal combustion engines. If no work, no heat transfer and no change in potential and kinetic energy occur, then all the thermal energy goes to raise the temperature of the products of combustion. When the combustion is complete the maximum amount of chemical energy is converted into heat energy and the temperature of the products reaches its maximum and this temperature considered to be as the upper limit for the actual combustion temperature. The maximum combustion is called Flame temperature. If the combustion is incomplete or excess air is used, the temperature of the products of compression will be less than maximum combustion temperature. Incomplete restricts the conversion of all chemical energy into thermal energy and excess will have cooling effect and hence the temperature is lower than maximum temperature in both the cases.

The Flame temperature in the combustion system depends on the fuels, chemical composition, the reactant mixture, pressure of the reactant mixture, the temperature of the reactant mixture and constraints on the system. In Diesel engine the combustion take place at constant pressure. The variations of Flame temperature for complete combustion with crank angle are shown in Fig.7 for all tested fuels at full load for conventional Diesel engine

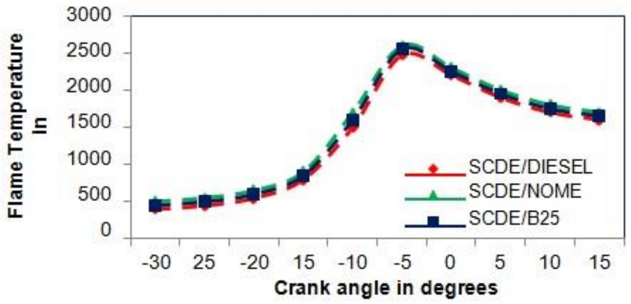

Fig.7 Flame Temperature vs Crank Angle

The maximum flame temperature for NOME is 2600 K. The least flame temperature for Diesel is 2470 K. The flame temperature of B25 is 2550K lies between NOME and Diesel. The increase in temperature for NOME and B25 are due to increase in cylinder pressure and oxygen present in the fuel and subsequently increases the oxides of nitrogen when compared to Diesel fuel.

❖ **Cylinder temperature**

The variation of cylinder temperature with crank angle is shown in Fig.8 for all tested fuels at full load for simulation of conventional Diesel engine. The maximum cylinder temperature for NOME is 2050 K. The least cylinder temperature for Diesel is 1950 K. The cylinder temperature of B25 is 2000 K lies between NOME and Diesel. High pressure of compressed mixture increases its burning rate. This increases the peak pressure inside the combustion chamber. The presence of oxygen in the bio-diesel make complete combustion of fuel thereby producing more heat is released from the gases. Thus the peak temperature of bio-diesel fueled engine is higher than that of Diesel fueled engine.

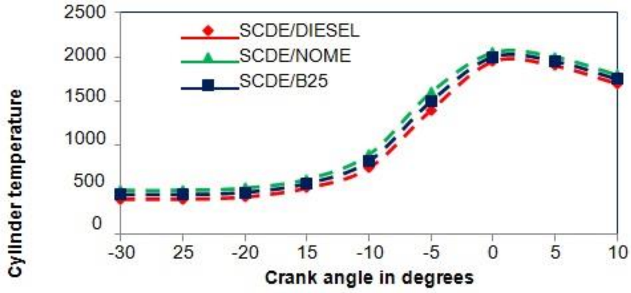

Fig.8 Variation of cylinder temperature with crank angle

The following are the summary of experimental and simulation of conventional Diesel engine to study the effect of NOME and its blends with Diesel B25.

- The cylinder pressure is increased by 2.63% and 1.5% for NOME, B25 respectively than Diesel fuel of an experimental investigation of conventional Diesel engine. The cylinder pressure for NOME and B25 is increased by 2.56 % and 1.3 % respectively compared to Diesel of a simulation of conventional Diesel engine. It has been concluded that both for predicted and simulated value of conventional Diesel engine of NOME and B25 are found to higher than Diesel due to higher cetane number and shorter ignition delay.
- The heat release rate for NOME and B25 are decrease by 36% and 10% respectively than Diesel fuel of a conventional Diesel engine. The heat release rate for NOME and B25 are decreased by 35% and 9% respectively than Diesel fuel of a simulation of conventional Diesel engine. It has been analyses that both for experimental and predicted value (simulation) of conventional Diesel engine are lower heat release rate of NOME and B25 due to shorter ignition delay results in less instance of pre-mixed combustion phase.
- The brake thermal efficiency for NOME and B25 are reduced by 2% and 1% respectively compared to Diesel of a conventional Diesel engine. The brake thermal efficiency for NOME and B25 are reduced by

○ % and 3.3 % respectively compared to Diesel of a simulation of conventional Diesel engine. It has been investigated that both for experimental and simulation of conventional engine for NOME and B25 are lower than Diesel due to higher viscosity, density, boiling point, lower calorific value of fuel, lubricity and poor volatility.

- The brake specific energy consumption for NOME and B25 are increased by 8.8% and 5.9% respectively compared to Diesel of a conventional Diesel engine. The brake specific energy consumption for NOME and B25 are increased by 8.1% and 5.4% respectively compared to Diesel of a simulation of conventional Diesel engine. It has been studied that both for experimental and predicted value of conventional Diesel engine the brake specific energy consumption for NOME and B25 are found to be higher than Diesel due to higher kinematic viscosity results in poor atomization, vaporization and dispersion of fuel in the combustion chamber.
- The oxides of nitrogen for NOME and B25 are increased by 23% and 14% respectively compared to Diesel of a conventional Diesel engine. The oxides of nitrogen for NOME and B25 are increased by 22% and 12% respectively compared to Diesel of a simulation of conventional Diesel engine. It has been concluded that both for experimental and conventional Diesel engine the NOME and B25 increases NOx emission due to higher oxygen content.
- The ignition delay of NOME and B25 are found to be shorter than Diesel fuel due to higher cetane number and higher density of the fuel. The ignition delay is decreased by 10 % and 5 % for NOME and B25 respectively than Diesel fuel.
- The Flame temperature of NOME and B25 are found to be higher than Diesel fuel.
- The cylinder temperature of NOME and B25 are found to be higher than Diesel fuel.

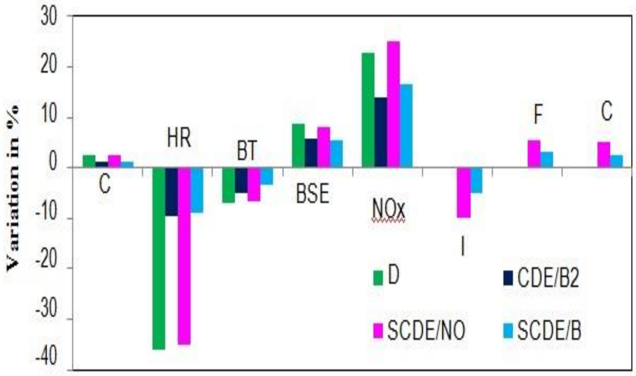

Fig.9 Comparison of NOME and B25 with Diesel at rated power output shows percentage variation of combustion, performance and emissions of both conventional and simulation of Diesel engine

13. CONCLUSION

The fuel recommended through this investigation is a Bio-diesel (NOME) derived from non-edible vegetable oil which is available in plenty. Utilizing NOME as a fuel for CI engine will not affect the food industry and will not reduce the land availability for growing food crops. In addition to the above advantages, NOME is indigenously available and utilizing it as a alternative fuel for Diesel will reduce India's dependence on oil import which is about 150 million tons per annum.

NOME and B25 produced meets the standard bio-diesel specifications. The production and consumption of NOME and B25 are inevitably rising in future due to low environmental impact, ease of handling, and possibility of use without need for major adjustments of existing engines of motor vehicles. Production and use of bio-diesel leads to saves foreign exchange, improves energy security of the nation, provides employment to rural masses, produce sustainable and relatively inexpensive fuel and start propagating the concept with village population to supplement their income with the existing tree population. Based on engine performance tests, it is concluded that bio-diesel blends used satisfactorily in the Diesel engine without any major modifications in the hardware of the system.

The predicted results are compared with experimental results of the engine fueled Diesel, NOME and B25. This model predicted the combustion, performance and emission characteristics in closer approximation to that of experimental results. The variation in experimental and theoretical results may be due to the fact that theoretical model is a homogeneous mixture with complete combustion is assumed. But in general, it is difficult to attain 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. Hence, it is believed this model is suitable for prediction of the combustion, performance and emission characteristics of CI engine fueled with any hydrocarbon fuel in conventional Diesel engine.

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LIST OF ABBREVIATIONS

NOME	–	Neem oil methyl ester
NaOH	–	Sodium hydroxide
KOH	–	Potassium hydroxide
C	–	Carbon
H	–	Hydrogen
O_2	–	Oxygen
CO_2	–	Carbon dioxide
CO	–	Carbon monoxide
N_2	–	Nitrogen
HC	–	Hydrocarbon
NO_x	–	Oxides of Nitrogen
SO_2	–	Sulphur dioxide
HSU	–	Hardridge smoke unit
TFC	–	Total Fuel Consumption
BSEC	–	Brake specific energy consumption
BTE	–	Brake Thermal Efficiency
BP	–	Brake power
CV	–	Calorific value of fuel
CDE/DIESEL	–	Conventional Diesel Engine
CDE/NOME	–	Conventional Diesel Engine Using NOME
CDE/B25	–	Conventional Diesel Engine Using B25 fuel