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Mathematical Correlation for Brake Thermal Efficiency and NO$_x$ Emission of CI Engine using Ester of Vegetable Oils

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Abstract**—**The aim of this study is to develop mathematical relationships for the performance parameter brake thermal efficiency (BTE) and emission parameter nitrogen oxides (NO$_x$) for the various esters of vegetable oils used as CI engine fuel. The BTE is an important performance parameter defining the ability of engine to utilize the energy supplied and power developed similarly it is indication of efficiency of fuels used. The esters of cottonseed oil, soybean oil, jatropha oil and hingan oil are prepared using transesterification process and characterized for their physical and main fuel properties including viscosity, density, flash point and higher heating value using standard test methods. These esters are tried as CI engine fuel to analyze the performance and emission parameters in comparison to diesel. The results of the study indicate that esters as a fuel does not differ greatly with that of diesel in properties. The CI engine performance with esters as fuel is in line with the diesel where as the emission parameters are reduced with the use of esters.

The correlation developed between BTE and brake power(BP), gross calorific value(CV), air-fuel ratio(A/F), heat carried away by cooling water(HCW). Another equation is developed between the NO$_x$ emission and CO, HC, smoke density (SD), exhaust gas temperature (EGT). The equations are verified by comparing the observed and calculated values which gives the coefficient of correlation of 0.99 and 0.96 for the BTE and NO$_x$ equations respectively.

Keywords**—**Esters, emission, performance, and vegetable oil.

I. INTRODUCTION

THE use of plant oil as fuel for CI engine is not new. Dr. Rudolf Diesel (Inventor of diesel engine) demonstrated his engine in Paris in 1900 using groundnut oil as fuel. The plant oil fuels were not accepted much at that time, as they were more expensive. It was found that all properties of plant oils were close to diesel except viscosity and volatility [1]. Various methods were adopted to overcome these problems. It included cracking of oil, blending of oils with diesel, heating of plant oils before injecting into the combustion chamber of engine and esterification of plant oils [2]. Vegetable oils present a very promising alternative to diesel since they are renewable and have similar properties as that of diesel. Many researchers have studied the use of vegetable oils in diesel engines. Vegetable oils offer almost the same power output with slightly lower thermal efficiency when used in diesel engine [3,4]. Reduction of engine emissions is a major research aspect in engine development with the increasing concern on environmental protection and the stringent exhaust gas regulation. Vegetable oils and their derivatives, especially methyl esters, commonly referred to as ‘biodiesel’, are prominent candidates as alternative diesel fuels. Biodiesel is generally made of methyl esters of fatty acids produced by the transesterification reaction of triglycerides with methanol in the presence alkali as a catalyst [5]. In India, a large variety of vegetable oils are available in huge amounts. Different vegetable oils and its derivatives are tried as a CI engine fuel. The use of cottonseed oil esters [6], soybean oil esters [7], jatropha oil esters [8] and hingan oil (*Balanites Aegyptiaca (L.) Del*) oil esters [9] have been already justified by the researchers as CI engine fuel.

In the present investigation, esters are prepared from cottonseed oil, soybean oil, jatropha oil and hingan oil by base catalyzed transesterification process. The cottonseed oil(CSO), soybean oil(SO), jatropha oil(JO) and hingan oil(HO) are extracted from their seeds. Ester properties were determined and their combustion and emission characteristics were studied on a four-stroke single-cylinder direct-injection, water cooled CI engine to check their feasibility as CI engine fuels. An attempt is made to correlate the performance and emission parameter by developing the equations.

II. MATERIALS AND METHOD

A. Transesterification of Vegetable Oils:

The formation of methyl esters by transesterification of vegetable oils requires 3 moles of alcohol stoichiometrically [3]. However, excess alcohol is required to drive the reaction close to completion and to obtain a maximum ester yield. Single step alkali/base catalyzed transesterification process as discussed in [10] is adopted for converting CSO, SO, JO and HO to methyl esters of fatty acids. The process variables that

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affect the transesterification reactions and their proportion are varied to obtain maximum ester yield from the vegetable oil. The amount of NaOH/KOH is determined using a titration process as advised in [11].

The methyl ester of CSO, SO, JO and HO obtained after transesterification are termed as cottonseed oil methyl ester (CSOME), soybean oil methyl ester (SOME), jatropha oil methyl ester (JOME) and hingan oil methyl ester (HOME).

B. Fuel Properties:

Fuel properties that are important from engine performance and emission point of view are determined. Several tests were conducted to evaluate the physico-chemical properties such as density, viscosity, calorific value, acid value and sulphur content for CSOME, SOME, JOME, HOME and commercial diesel (Diesel).

C. Engine Performance and Emission Measurement:

The performance of compression ignition (CI) engine using prepared CSOME, SOME, JOME, HOME as fuel is studied in comparison with diesel. The CI engine used for the study is Kirloskar, Single cylinder, four-stroke, water-cooled, constant Speed, direct injection (DI) diesel engine. The schematic diagram for experimental setup is given in Fig. 1. The exhaust gas temperature, cooling water temperatures are measured with thermocouples mounted on the test setup. Fuel consumption is measured with the help of a burette of 50ml volume. The smoke density is measured with the help of a Nissan-Bosch Smoke meter, nitrogen oxides (NOx), carbon monoxide (CO) and hydrocarbon (HC) emission is measured with AVL Digas 444 Analyzer. The engine is started on neat diesel fuel and warmed up, the warm up period ends when the liquid cooling water temperature is stabilized. Parameters like fuel consumption, exhaust gas temperature, speed, airflow, etc. are measured and recorded for different loads. Similar procedure is repeated for all the four esters used in the study. The test is repeated for three times. Finally, average values of the three readings were taken for calculation. The recorded data were then analyzed from the graphs recording thermal efficiency, air-fuel ratio (A/F) and brake-specific fuel consumption (BSFC) for different esters and diesel.

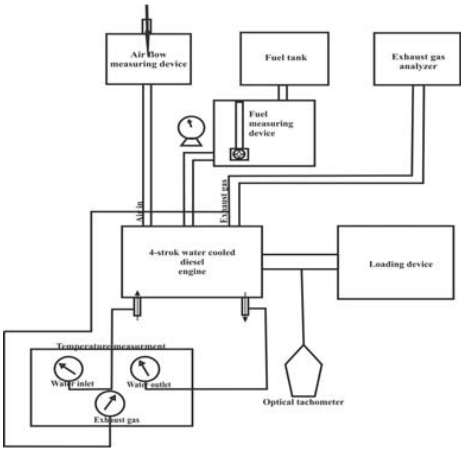

Fig. 1 Schematic diagram of the experimental setup for engine trial

III. DEVELOPMENT OF MATHEMATICAL CORRELATION

A. Correlation for BTE:

Brake thermal efficiency (BTE) of the engine is the major parameter of interest for any fuel used as far as CI engine performance is concerned. It is the ratio of work output of the engine to the heat input in general. Expressed as, enthalpy efficiency in thermodynamics. The BTE of the engine is influenced by various parameters, while using different fuels having different properties. The factors which may have significant impact on BTE are considered for formulation of mathematical model for the present study and they are namely brake power, rotational speed of engine, torque developed, mass of fuel consumed, mass of air required, calorific value of fuel, densities of fuel and air, viscosity of fuel, heat carried away by cooling water, compression ratio, length of stroke and diameter of piston and atmospheric pressure etc. In all 19 variables are identified, and by using Buckingham π theorem concept, an attempt is made to develop a mathematical model to study the effect of these parameters simultaneously on BTE.

Using Buckingham's **π** theorem [12] the model is formulated which states that "If there are 'n' variables (dependent and independent variables) in a dimensionally homogeneous equation and if these variables contain 'm' fundamental dimensions (such as M, L, T etc), then the variables are arranged into (n - m) dimensionless terms. These dimensionless terms are called as **π** – terms.

The variables which can influence the BTE (η_{th}) of an engine is arranged as follows.

$$\eta_{th} = f\left(B.P, N, T, m_f, CV, m_a, \rho_f, \rho_a, AF, Ta, Tg, Q_w, v, r, L, d, P_a, g\right)$$

Where,

$\text{B.P} = \text{Brake power(kW)} = \text{L}^2\text{MT}^{-3}$
$\text{N} = \text{Speed(rpm)} = \text{L}^0\text{M}^0\text{T}^{-1}$
$\text{T} = \text{Torque(Nm)} = \text{L}^2\text{M}^1\text{T}^{-2}$
$\text{m}_\text{f} = \text{mass of fuel(kg/s)} = \text{L}^0\text{MT}^{-1}$
$\text{Cv} = \text{Calorificvalue(kJ/kg)} = \text{L}^2\text{M}^0\text{T}^{-2}$
$\text{ma} = \text{mass of air(kg/s)} = \text{L}^0\text{MT}^{-1}$
$\rho_\text{f} = \text{Density of fuel(kg/m}^3\text{)} = \text{L}^{-3}\text{MT}^0$
$\rho_\text{a} = \text{Density of air(kg/m}^3\text{)} = \text{L}^{-3}\text{MT}^0$
$\text{AF} = \text{Airfuel ratio} = \text{L}^0\text{M}^0\text{T}^0$
$\text{Ta} = \text{Temperatue of air }^0\text{C} = \theta$
$\text{Tg} = \text{Temperatue of ExhaustGases }^0\text{C} = \theta$
$\theta\text{w} = \text{Heat carried away by coolingwater(kW)} = \text{L}^2\text{MT}^{-3}$
$\nu = \text{Viscosity(mm}^2\text{/sec)} = \text{L}^2\text{M}^0\text{T}^{-1}$
$\text{r} = \text{Compression ratio} = \text{L}^0\text{M}^0\text{T}^0$
$\text{L} = \text{Length of stroke(m)} = \text{LM}^0\text{T}^0$
$\text{d} = \text{Diameter of piston(m)} = \text{LM}^0\text{T}^0$
$\text{P}_\text{a} = \text{Atmospheric Pressure(N/m}^2\text{)} = \text{L}^{-1}\text{MT}^{-2}$
$\text{g} = \text{Accelation due toGravity(m/sec}^2\text{)} = \text{LM}^0\text{T}^{-2}$

above equation can be written as

$$f\left(\eta_{th}, B.P, N, T, m_f, Cv, ma, \rho_f, \rho_a, AF, Ta, Tg, \theta w, v, r, L, d, P_a, g\right) = 0$$

Total number of variables (dependent and independent) = 19
Therefore, number of π terms formed will be = 19 – 3 = 16

Selecting repeating variables as d, N, ρ_f, because according to Buckingham's **π** theorem, the repeating variables should be chosen in such a way that one variable contains geometric property, other variable contains flow property and the third variable contains fluid property therefore in this case,

1) Geometric property - Diameter of Piston (d)
2) Flow property - Speed of engine (N)
3) Fluid property - Density of fuel (ρ_f)

' η_{th} ' is a dependent Variable and hence should not be selected.

Now the π terms formed, solved and substituted as discussed by Buckingham ' π ' theorem.

Substituting the values of all ' π ' terms the functional relation is as given below equation 1.

$$f\left(\eta_{th}, \frac{B.P}{d^5 N^3 \rho_f}, \frac{T}{N^2 d^5 \rho_f}, \frac{CV}{d^2 N^2}, \frac{ma}{N \rho_f d^3}, \frac{m_f}{N d^3 \rho_f}, \frac{\rho a}{\rho_f}, AF, \frac{\theta w}{N^3 d^5 \rho_f}, \frac{\nu}{N d^2}, r, \frac{L}{d}, \frac{Pa}{d^2 N^2 \rho_f}, \frac{g}{N^2 d}, Ta, Tg\right) = 0 \quad (1)$$

or

$$\eta_{th} = \left[\frac{B.P}{N^3 d^5 \rho_f}, \frac{T}{d^5 N^2 \rho_f}, \frac{CV}{d^2 N^2}, \frac{ma}{N \rho_f d^3}, \frac{m_f}{N d^3 \rho_f}, \frac{\rho a}{\rho_f}, AF, \frac{\theta w}{N^3 d^5 \rho_f}, \frac{\nu}{N d^2}, r, \frac{L}{d}, \frac{Pa}{d^2 N^2 \rho_f}, \frac{g}{N^2 d}, Ta, Tg\right] \quad (2)$$

In above equation,

$\frac{\nu}{Nd^2}$ = F (Frond No.) & $\frac{g}{N^2 d}$ = Re (Reynolds No.)

$$\therefore \eta_{th} = \left[\frac{B.P}{N^3 d^5 \rho_f}, \frac{T}{d^5 N^2 \rho_f}, \frac{CV}{d^2 N^2}, \frac{ma}{N \rho_f d^3}, \frac{m_f}{N d^3 \rho_f}, \frac{\rho a}{\rho_f}, AF, \frac{\theta w}{N^3 d^5 \rho_f}, F, r, \frac{L}{d}, \frac{Pa}{d^2 N^2 \rho_f}, \mathrm{Re}, Ta, Tg\right] \quad (3)$$

Rewriting and neglecting constant and less influencing terms

$$\eta_{th} = \varphi\left[\frac{B.P}{N^3 d^5 \rho_f}, \frac{T}{d^5 N^2 \rho_f}, \frac{CV}{d^2 N^2}, AF, \frac{\theta w}{N^3 d^5 \rho_f}\right] \quad (4)$$

$$\eta_{th} = \varphi\left[X_1, X_2, X_3, X_4, X_5\right] \quad (5)$$

Substituting,

$X_1 = \frac{B.P}{N^3 d^5 \rho_f}$, $X_2 = \frac{T}{d^5 N^2 \rho_f}$, $X_3 = \frac{CV}{d^2 N^2}$, $X_4 = AF$

$X_5 = \frac{\theta w}{N^3 d^5 \rho_f}$ and $Y = \eta_{th}$

The equation becomes

$$y = \varphi\left[(x_1)^{a1} (x_2)^{a2} (x_3)^{a3} (x_4)^{a4} (x_5)^{a5}\right] \quad (6)$$

Now, by solving by linear regression analysis method for coefficients a1, a2, a3, a4 and a5, we have

$$y = 3.785\left[(x_1)^{-0.449} (x_2)^{1.328} (x_3)^{0.255} (x_4)^{0.653} (x_5)^{-0.18}\right]$$

Substituting the values of X_1, X_2, X_3, X_4, X_5 and y in the equation (6) we get,

$$\eta_{th} = 0.003\left[\left(\frac{B.P}{N^3 d^5 \rho_f}\right)^{-0.449} \left(\frac{T}{d^5 N^2 \rho_f}\right)^{1.328} \left(\frac{CV}{d^2 N^2}\right)^{0.255} (AF)^{0.653} \left(\frac{\theta w}{N^3 d^5 \rho_f}\right)^{-0.18}\right] \quad (7)$$

Finally a relationship is developed, as given by equation (7), between BTE, Brake power, Torque, Calorific value of fuel, Air-Fuel ratio and Heat carried away by the cooling water. Out of the 19 parameters considered, which may affect the BTE of the engine, only 5 emerged as the prominent influencing parameters. The mathematical correlation thus developed is validated with the data generated by the experimental observations in the laboratory.

B. Correlation for NOx Emission:

The exhaust emission parameters that are noticed in an internal combustion engine are smoke density (SD), carbon monoxide (CO), hydrocarbon (HC) and oxides of nitrogen (NO_x). The NO_x emission is major parameter of interest in case of bio-originated fuels.

Majority of exhaust gas analyzers in India are designed to measure CO, HC emission for SI engine and smoke density (SD) for CI engine. In present study an attempt is made to correlate these emission parameters. A unique correlation is developed between NO_x(ppm), SD (%), CO (%), HC (ppm) and exhaust gas temperature (EGT) in ^{0}C. The NO_x emission in ppm can be predicted with the help of equation (8).

$$NO_{x(ppm)} = 0.00075\left[\left(SD_{(\%)}\right)^{0.3} \left(CO_{(\%)}\right)^{-0.023} \left(HC_{(ppm)}\right)^{0.2} \left(EGT_{(^0C)}\right)^{2.05}\right] \quad (8)$$

The mathematical correlation thus developed is validated with the data generated by the experimental observations in the laboratory.

IV. RESULTS AND DISCUSSIONS

A. Transesterification:

The transesterification process for SO, CSO, JO and HO is presented in Table 1.

TABLE I
TRANSESTERIFICATION OF SO, JO, CSO AND HO

Oil	Alcohol	Molar ratio	Catalyst	Reaction temperature	Duration of test (Stirring)	Ester yield
SO	Methanol	6:1	NaOH 1%w/w	60 ^{0}C	85 min	97%
CSO	Methanol	6:1	NaOH 1%w/w	65 ^{0}C	75 min	95%
JO	Methanol	10:1	NaOH 1.4% w/w	60 ^{0}C	90 min	94%
HO	Methanol	8:1	KOH 1.25% w/w	60 ^{0}C	60 min	95%

The base catalyzed transesterification of SO, CSO, JO and HO gives ester yield of 97%, 94%, 94% and 95% respectively.

The amount of esters resulted during the transesterification is strongly affected by molar ratio of methanol to oil and the reaction temperature. Catalysts are used in transesterification process to enhance the speed of reaction. NaOH is preferred over KOH as catalyst due to its lower cost. The catalyst KOH is used in the present study for transesterification of HO, because use of NaOH as a catalyst resulted in thickening of the esters and very less amount of ester yield is observed.

B. Characterization of Liquid Fuels

The important properties of HOME and B20 are quiet comparable with diesel as given in Table II.

TABLE II
PHYSICO-CHEMICAL PROPERTIES OF ESTERS

Property	SOME	CSOME	JOME	HOME [ ]	Diesel
Density, Kg /m^3	885	882	879	860	840
Viscosity^a, (mm^2/s)	4.08	4.0	4.4	3.98	2.60
Calorific value, (MJ /kg)	39.76	40.32	39.85	39.65	42.5
Acid Value,(mgKOH/g)	0.15	0.32	0.38	0.34	--
Total sulphur (%)	0.02	0.03	0.04	0.03	0.05

a: measured at 40 ^{0}C.

C. Engine Performance and Emission Characteristics:

1. Engine Performance:

The engine performance calculated at different loads and the variation is plotted against the applied load in kW. The variation of BSFC with the applied load for different esters tested (i.e. SOME, CSOME, HOME and JOME) and diesel is as shown in Fig. 2.

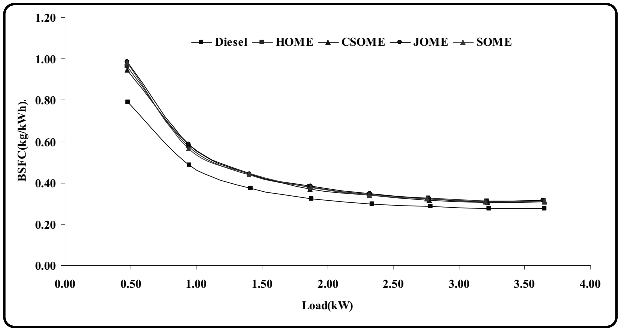

Fig. 2 Variation of BSFC with applied load for diesel and different esters

The BSFC for all the four esters tested is higher than diesel and is much close to each other. This is due to the fact that the esters have lower heating value compared to diesel; so more mass of esters is needed to maintain constant power output. Fig. 3 shows the variation of BTE with applied load for esters and diesel.

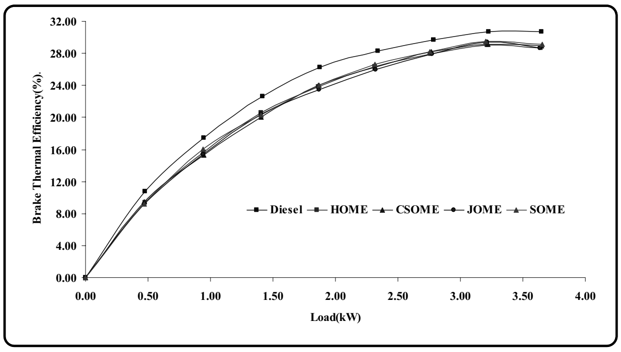

Fig. 3 Variation of BTE with applied load for diesel and different esters

It can be seen from the figure that the BTE increases with increase in applied load irrespective of the fuel used in the engine. The BTE of the esters is less than diesel this is due to the increased fuel consumption of esters due to its lower calorific value in comparison with diesel.

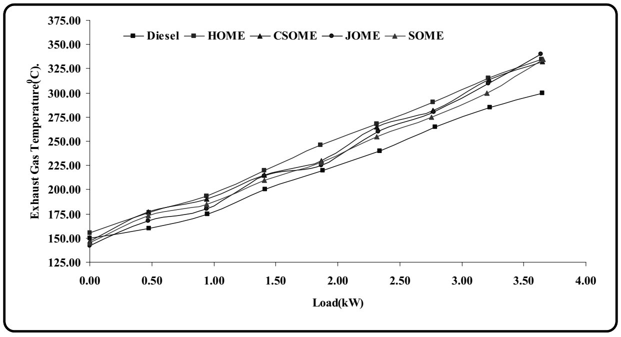

Fig. 4 Variation of EGT with applied load for diesel and different esters

From Fig. 4 it is seen that the exhaust gas temperature for esters is slightly higher as compared with diesel fuel. The ester chain contains oxygen which helps to its complete combustion resulting into higher temperature in the combustion clamber and hence increased temperature of exhaust gas.

2. Emission Characteristics:

The variation of SD, CO and HC emission with applied load is given in Fig. 5, Fig. 6 and Fig. 7 respectively. It is observed that the SD, CO and HC emission are found to be reduced with all the esters tested in comparison to diesel. This is because of the tendency of esters towards complete combustion which is enhanced by the excess oxygen present in the esters.

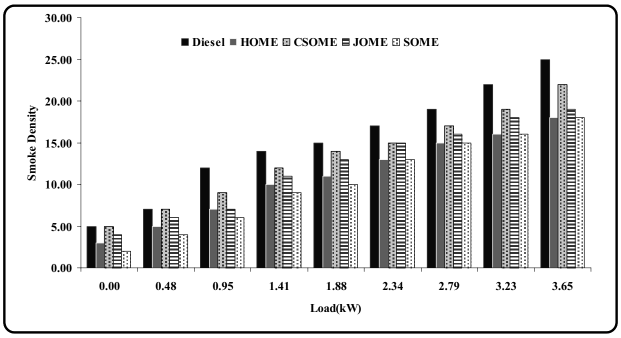

Fig. 5 Variation of smoke density (%) with applied load

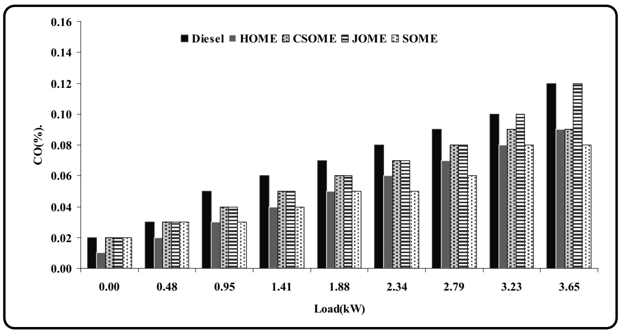

Fig. 6 Variation of CO emission with applied load

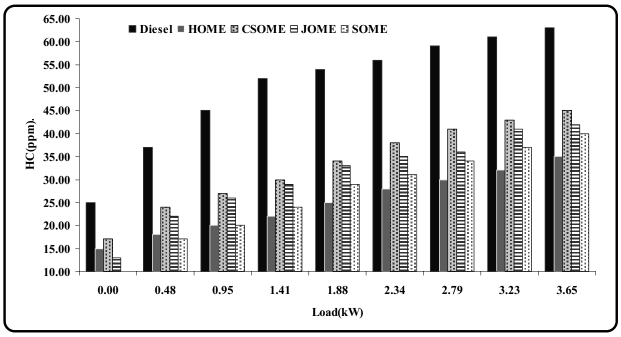

Fig. 7 Variation of HC emission with applied load

Fig. 8 represents the variation of NO_x emission with applied load for different esters and diesel. The NO_x emission depends upon combustion chamber temperature which in turn depends on the applied load. The NO_x emission in case of esters is slightly increased at full load condition. This is due to the increased combustion chamber temperature when engine is fuelled with esters and NO_x. This also cleared from the Fig. 3 which shows the increased exhaust gas temperature with esters as compared to diesel.

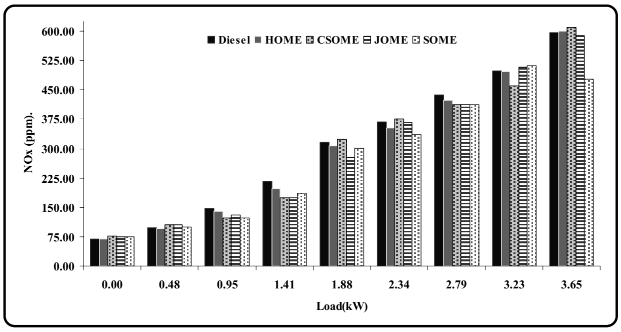

Fig. 8 Variation of NOx emission with applied load

D. Mathematical Correlation:

In the present study the attempts are made to correlate the data generated in laboratory and the data calculated using mathematical correlation developed. The correlation developed given in "(7)" can be effectively used to calculate any of the parameter mentioned in the equation when other parameters are known.

Equation(7) is validated by obtaining the plot between the observed values and the calculated values, as shown in Fig. 9. The plot thus obtained reveals that there exists a healthy relationship between the observed and calculated value, as the coefficient of correlation (R^2) yielded for above plot is 0.99.

Extensive data is generated to correlate NO_x and other emission parameters along with exhaust gas temperature. Equation (8) thus developed, predicts NO_x emission from the engine by correlating various emission characteristics and the exhaust gas temperature.

The equation is validated by comparing the observed and calculated values, as shown in Fig. 10. The plot thus obtained is having a coefficient of correlation (R^2) of 0.96. The equation is applicable for all the esters as well as its blend with diesel used as fuel in the CI engine and for any configuration of the CI engine.

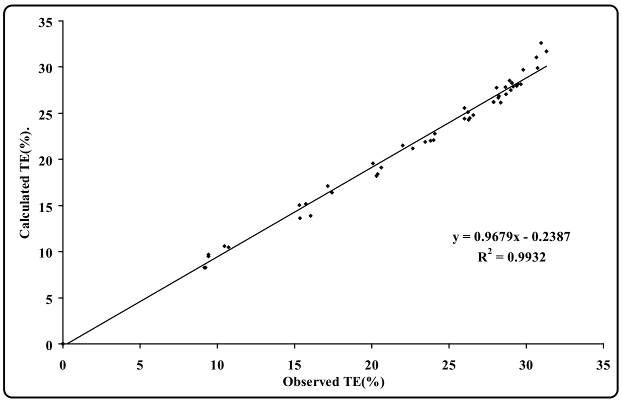

Fig. 9 Correlation between observed and calculated values of BTE for the fuels tested

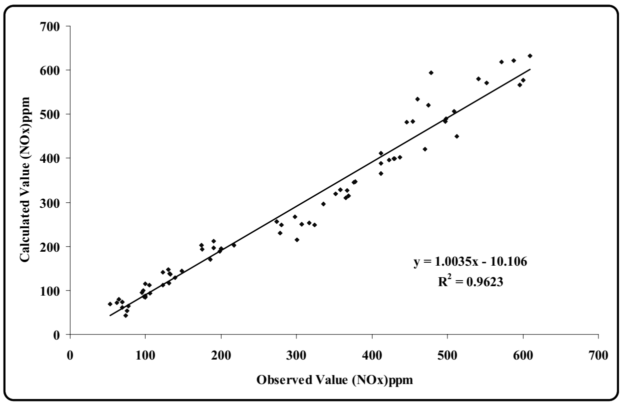

Fig. 10 Correlation between observed and calculated values of NOx emission

V. CONCLUSION

Based on the result of this study it can be said that the important properties of esters are quite closer to diesel. Engine performance test shows that SOME, CSOME, JOME and HOME as a fuel does not differ greatly from that of diesel. A slight power loss, combined with the increased fuel consumption due to lower heating value, was experienced with these esters. Considerable reduction in emission characteristics such as smoke density, carbon monoxide and hydrocarbons is achieved with the ester as compared to diesel. The trends of NO_x emission for esters are comparable with diesel at lower loads and slightly higher at full load.

The mathematical equations developed for BTE is applicable to single cylinder water-cooled, DI engines. The equation for NO_x emission prediction can be effectively used for any fuel used in CI engine and for any configuration of engine.

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