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Numerical modeling of oxides of nitrogen based on density of biodiesel fuels

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Abstract
Biodiesel is an alternative fuel derived from vegetable oils or animal fats. Research has shown that biodiesel fueled engines produce lesser carbon monoxide, unburned hydrocarbon, and particulate emissions compared to mineral based diesel fuel but emit higher oxides of nitrogen (NO_x) emissions. NOx could be strongly correlated with density or cetane number of a fuel. The objective of the present work is to predict the NO_x concentration of a neat biodiesel fueled compression ignition engine from the density of biodiesel fuels using regression model. Experiments were conducted at different engine loads and the results were given as inputs to develop the regression model. A single cylinder, four stroke, constant speed, air cooled, direct injection diesel engine was used for the experiments. Five different biodiesel fuels were used and NO_x were measured at different engine loads. The NO_x concentration was taken as response (dependent) variable and the density values were taken as explanatory (independent) variables. The regression model has yielded R2 values between 0.918 and 0.995. The maximum prediction error was found to be 3.01 %.

Keywords: Biodiesel, Density, Numerical modeling, Oxides of nitrogen, Regression.

1. Introduction

Global energy consumption has increased and, as a consequence, the carbon dioxide, sulfur dioxide and nitrogen oxides emissions from the combustion of fossil fuels have damaged the atmosphere to a significant extent. Carbon dioxide emissions have risen over the last two decades, reaching an atmospheric content of 360 ppm, estimating the world CO_2 emissions at about 26 billion metric ton per year, 80 percent of which comes from the combustion of fossil combustibles such as coal, petroleum and natural gas [1]. Therefore, the engine manufacturers have intended alternatively fueled engines and fuel systems, which offer ample power while residing within regulatory emission-limits. At the same time a huge deal of research and development on internal combustion engines has taken place not only in the design area but also in finding a suitable fuel. Many researchers have concluded that biodiesel holds vow as an alternative fuel for diesel engines, since its properties are very closer to those of diesel fuels. Therefore, biodiesel can be used in diesel engines with not many or no modifications. Biodiesel has a higher cetane number than diesel fuel, no aromatics, and contains around 10 – 11 % oxygen by weight [2]. These characteristics of biodiesel reduce the emissions of CO, HC and PM in the exhaust gas [2].

Furthermore, contribution of bio-fuels to green house effect is insignificant, since carbon dioxide emitted during combustion is recycled in the photosynthesis process in the plants [3, 4]. However NO_x emissions of biodiesel increase because of better combustion [3, 6]. Oxides of nitrogen may be treated as a strong function of density or cetane number of biodiesel.

The objective of the present work is to predict the oxides of nitrogen (NO_x) concentration of a neat biodiesel fueled compression ignition engine from the density of biodiesel fuels using regression model. To understand the impact of density of biodiesel on NO_x emissions, experiments were conducted in a direct injection diesel engine with different biodiesel fuels namely, sunflower oil methyl ester (SFOME), jatropha oil methyl ester (JOME), neem oil methyl ester (NOME), mahua oil methyl ester (MOME) and palm oil methyl ester (POME). The importance of the present work is to predict the engine's NO_x concentration instead of undertaking complex and time-consuming experimental studies.

2. Experiments

2.1 Composition of biodiesel fuels

The basic composition of any vegetable oil is triglyceride, which is of three fatty acids and one glycerol molecule. Biodiesel is defined as the mono-alkyl esters of fatty acids derived from vegetable oils or animal fats. In simple terms, biodiesel is the product obtained when a vegetable oil or animal fat is chemically reacted with an alcohol to produce fatty acid alkyl esters in the presence of a catalyst (sodium or potassium hydroxide). In the process, glycerol is obtained as a co-product. The fatty acid composition of different biodiesel fuels is given in Table 1.

Table 1. Fatty acid composition of biodiesel fuels

Fatty Acids	Chain length	Type	Fatty Acid Composition, Wt %				
			JOME	POME	MOME	SFOME	NOME
Lauric	12:0	S	–	0.9	–	–	0.83
Myristic	14:0	S	0.1	1.3	–	0.1	0.47
Palmitic	16:0	S	14.9	43.9	24.2	6.0	18.2
Stearic	18:0	S	9.5	4.9	25.8	5.9	20.1
Oleic	18:1	US	40.5	39.0	37.2	16.0	43.7
Linoleic	18:2	US	34.7	9.5	12.8	71.4	16.4
Linolenic	18:3	US	0.3	0.3	–	0.6	0.3
Others (Traces)			–	0.2	–	–	–
% of Saturated acids (S)			24.5	51.0	50.0	12.0	39.6
% of Unsaturated acids (US)			75.5	48.8	50.0	88.0	60.4

2.2 Biodiesel production

A two step "acid – base" process with acid – pretreatment followed by main base – transesterification process was done. Methonal was used as a reagent and H_2SO_4 and KOH as catalysts for acid and base reactions. Accordingly biodiesels were produced from crude sunflower, jatropha, neem, mahua and palm oils.

2.3 Fuel properties

The fuel properties were determined following the methods specified in ASTM standards as given in Table 2 for SFOME, JOME, NOME, MOME and POME.

Table 2. ASTM methods for determination of fuel properties

Property	Unit	Standard	Method
Density	g/cc	D 1298	Hydrometer
Viscosity	mm^2 / s	D 445 – 03	Redwood viscometer
Calorific Value	MJ / kg	D 240 – 02	Bomb calorimeter
Flash Point	°C	D 93 – 02a	Pensky martens open cup

2.4 Engine test
The engine used for the study was Kirloskar, single cylinder; constant speed, direct injection diesel engine and the details are given in Table 3.

Table 3. Specifications of engine used

Parameters	Specification
Make	Kirloskar
Model	TAF – 1
No. of Cylinder	Single Cylinder
Stroke	4 Stroke
Type of Cooling	Air Cooled
Ignition	Compression Ignition
Fueling	Diesel
Bore	87.5 mm
Stroke	110 mm
Compression Ratio	17.5:1
Injection Pressure	200 bar
Injection Timing	23 deg. bTDC
Speed	1500 rpm
Brake Power	4.4 kW

The engine was coupled to an electrical dynamometer and tests were performed under steady-state conditions. The engine was started on neat diesel fuel and warmed up. The biodiesel fuels were tested in random order. The tests were repeated for three times and the average value of three readings was taken to eliminate the uncertainty. QROTECH (QRO – 401) exhaust gas analyzer was used for measuring NO_x emissions.

3. Regression model to predict NO_X concentration
The relationship between NO_x and density at different engine loads was derived through regression model. To develop the regression model, densities of biodiesels and NO_x at different loads were taken as inputs. The NO_x concentrations were taken as response (dependent) variables and the density values were taken as explanatory (independent) variables. The goodness of the fit was checked by R^2 value of the regression model.

$$NO_X = A + (B \times density) \tag{1}$$

where, A = Intercept,, B = Regression constant. The intercept (A), the regression constant (B), R^2 and adj. R^2 are given in Table 4.

Table 4. Intercept, regression constant, R^2 and adj. R^2 at different engine loads

Parameter	Load (%)				
	0	25	50	75	100
A	– 1354	– 1863	– 10267	– 38364	– 18868
B	1.934	2.803	13.640	48.060	25.300
R^2	0.954	0.993	0.918	0.995	0.990
adj.R^2	0.939	0.990	0.891	0.993	0.987

4. Results and discussion
4.1 Fuel properties
The results of fuel tests on diesel and different biodiesel fuels are summarized in Table 5.

Table 5. Properties of diesel and different biodiesel fuels

Fuel	Density (kg / m^3)	Viscosity @ 40°C (mm^2 / s)	Calorific Value (MJ / kg)	Flash Point (°C)
Diesel	826	2.60	42.2	68
SFOME	841	3.91	39.4	177
JOME	836	4.26	39.7	170
NOME	832	4.53	40.1	146
MOME	830	4.66	36.9	127
POME	830	4.36	41.1	164

4.2 NO_X emissions

The NO_x values in parts per million (ppm) against the engine load for different biodiesels and diesel fuel are given in Table 6 and represented in Figure 1. From the figure, it can be observed that the NO_x concentration varies linearly with engine load. As the load increases, the overall fuel-air ratio increases resulting in an increase in the average gas temperature in the combustion chamber and hence NO_x formation, which is sensitive to temperature, increases. The amount of NO_x produced for diesel fuel varied between 233 and 2071 ppm from no load to full load. Whereas the NO_x concentration for biodiesel fuels is higher than that of the diesel fuel for a given load.

Table 6. NO_x concentration of biodiesel fuels at various loads

% of Load	NO_X (ppm)					
	Diesel	SFOME	JOME	NOME	MOME	POME
No Load	233	276	263	259	256	251
25	436	494	482	471	465	461
50	980	1203	1123	1115	1055	1055
75	1421	2058	1829	1610	1531	1525
100	2071	2404	2283	2200	2140	2100

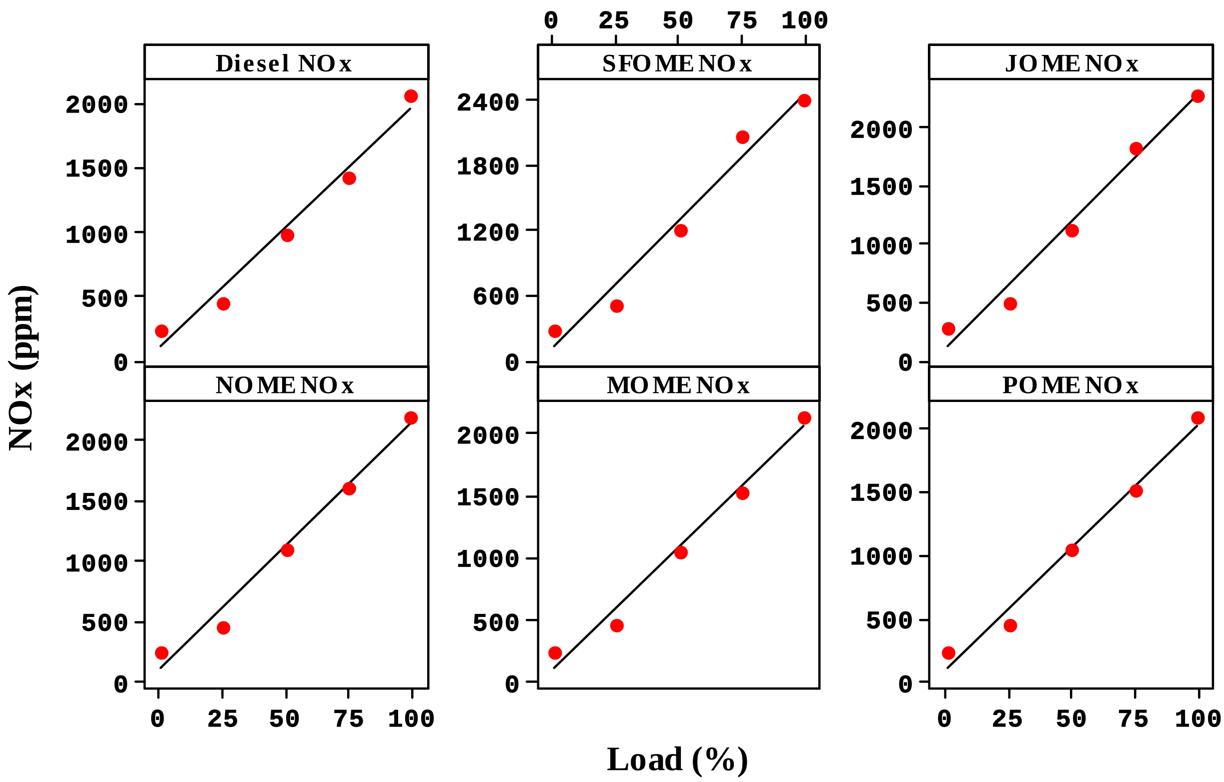

Figure 1. NO_X Vs engine load for different biodiesel fuels

The NO_x concentration for different biodiesels at different loads was investigated. At all loads SFOME gives higher NO_x (ppm) than the other biodiesel fuels. From Table 5, it can be observed that SFOME has higher density as compared to that of other biodiesel fuels. The relationship between density of biodiesel and NO_x was also investigated. For a given engine operating condition, the NO_x concentration increases with increase in biodiesel density. This can be explained as follows.

1. For the same injection pressure, the atomization of higher density fuel is poorer than that of a lower density fuel.
2. Poor atomization process may result in a larger fuel droplet diameter.
3. If the fuel droplet diameter is larger, more time is required for droplet vaporization which in turn may increase the physical delay time period.
4. Larger physical delay will increase the peak pressure rise during the initial portion of the combustion process (due to more fuel accumulation and hence rapid ignition).
5. Hence, the peak temperature also increases, which in turn increase the NO_x concentration.

Therefore, the NO_x concentration may be considered as a strong function of fuel density.

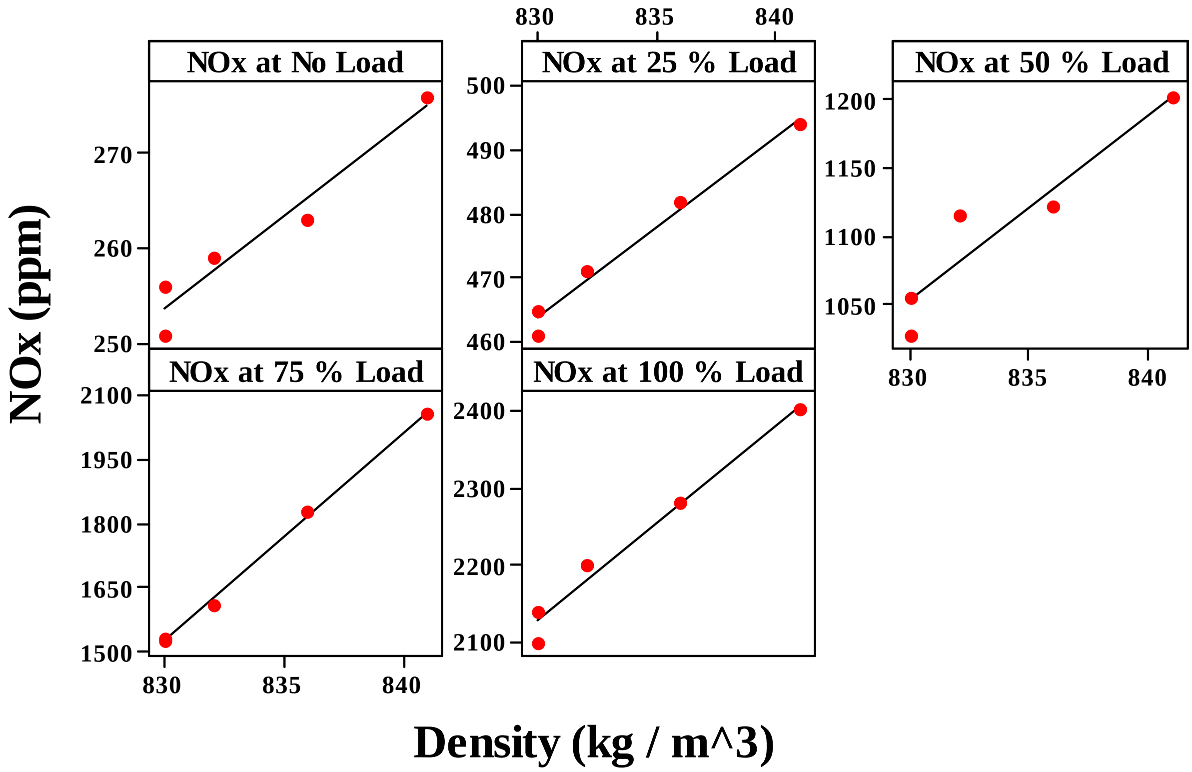

Figure 2. NO_x vs. density at different engine loads

The NO_x versus density at different loads is shown in Figure 2. Using equation (1), NO_x as a function of density can be calculated at different engine loads by substituting the corresponding intercept and regression constant. From equation (1), NO_x at different loads was predicted and listed against actual (experimental) values in Table 7. From Table 7, it can be observed that the maximum prediction error is 3.01 %.

Table 7. Comparison of regression predicted results and experimental results

Biodiesel	NO_x (ppm) at No Load		Error	
	Actual	Predicted	Absolute (ppm)	Relative (%)
SFOME	276	275	–1	– 0.36
JOME	263	265	2	0.89
NOME	259	258	– 1	– 0.55
MOME	256	254	– 2	– 0.89
POME	251	254	3	1.08
Biodiesel	NOx (ppm) at 25 % Load		Error	
	Actual	Predicted	Absolute (ppm)	Relative (%)
SFOME	494	494	0	0.07
JOME	482	480	– 2	– 0.35
NOME	471	469	– 2	– 0.40
MOME	465	463	– 2	– 0.32
POME	461	463	2	0.54
Biodiesel	NO_x (ppm) at 50 % Load		Error	
	Actual	Predicted	Absolute (ppm)	Relative (%)
SFOME	1203	1204	1	0.10
JOME	1123	1136	13	1.16
NOME	1115	1081	– 34	– 3.01
MOME	1055	1054	– 1	– 0.08
POME	1028	1054	26	2.55
Biodiesel	NO_x (ppm) at 75 % Load		Error	
	Actual	Predicted	Absolute (ppm)	Relative (%)
SFOME	2058	2054	– 4	– 0.17
JOME	1829	1814	– 15	– 0.81
NOME	1610	1622	12	0.74
MOME	1531	1526	– 5	– 0.34
POME	1525	1526	1	0.05
Biodiesel	NO_x (ppm) at 100 % Load		Error	
	Actual	Predicted	Absolute (ppm)	Relative (%)
SFOME	2404	2409	5	0.22
JOME	2283	2283	0	0
NOME	2200	2182	– 18	– 0.84
MOME	2140	2131	– 9	– 0.42
POME	2100	2131	31	1.48

where, Absolute Error = Predicted value – Actual value
Relative Error = (Absolute error / Actual value) x 100

5. Conclusion

The applicability of regression has been investigated for the NO_x values of a diesel engine fueled with neat biodiesel fuels. To develop the regression model, the densities of biodiesels and NO_x at different loads were taken as inputs. The regression model has yielded R^2 values between 0.918 and 0.995. The maximum prediction error was found to be 3.01 %.

The predicted results are within the acceptable limits. The relationship between density of biodiesel fuels and NO_x concentration for a given engine conditions can be determined for different biodiesel fuels using the regression model by substituting the corresponding constants in the regression model. Therefore, equation (1) is recommended to predict the engine's NO_x concentration instead of undertaking complex and time-consuming experimental studies.

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