Journal of Engineering and Applied Sciences
MEDWELL PUBLICATIONS

Application of Multiple Linear Regression for the Prediction of Some Properties of Biodiesel using Fatty Acid Compositions

Awogbemi Omojola, Inambao Freddie and Onuh Emmanuel Idoko
Green Energy Solutions Research Group, Department of Mechanical Engineering, Howard College, University of Kwa Zulu-Natal, 4041 Durban, South Africa

Key words: FAME, fatty acid compositions, linear correlations, property prediction, biodiesel

Corresponding Author:
Awogbemi Omojola
Green Energy Solutions Research Group, Department of Mechanical Engineering, Howard College, University of Kwa Zulu-Natal, 4041 Durban, South Africa

Page No.: 1951-1961
Volume: 15, Issue 8, 2020
ISSN: 1816-949X
Journal of Engineering and Applied Sciences

Abstract: The quest for renewable, cost-effective, environmentally friendly and sustainable alternative fuels to run Compression Ignition (CI) engines has escalated the tempo of research in biodiesel in recent decades. Investigations aimed at improving combustion, engine performance and emission characteristics of CI engines fuelled with Fatty Acid Methyl Esters (FAME) have increased substantially in recent years. Properties of biodiesel are key parameters in relation to engine performance, emission characteristics and its suitability as CI engine fuel; these properties are influenced by the Fatty Acid (FA) composition of the biodiesel. In order to overcome the complexities related to real-time experimental determination of biodiesel properties, various prediction techniques have been used. This current effort explores multiple linear regression to formulate linear correlations for the prediction of the density, Cetane Number (CN), Calorific Value (CV) and Kinematic Viscosity (KV) of biodiesel using the five commonest FAs (palmitic, stearic, oleic, linoleic and linolenic acids). Input data were sourced from literature to formulate linear relations for these FAME fingerprints and the outcome subjected to statistical analysis. The predictive capabilities of the models were verified using other experimental data mined from various sources. The outcomes of analysis shows that the adjusted R^2 and maximum absolute errors are 83 and 0.35% for density, 84.3 and 1.72% for CN, 43 and 0.98% for CV and 68.3 and 4.33% for KV. It is evident that linear correlations established from five FAs are highly successful in predicting density, CN, CV and KV of biodiesel from a wide range of feedstocks.

INTRODUCTION

As a result of the global population explosion, rapidly expanding urbanization, industrial revolution and economic development, global energy demand and consumption has continued to increase with a huge chunk of the energy being sourced from nonrenewable sources. Fossil fuel contributed 86.9, 82.67 and 85% to global

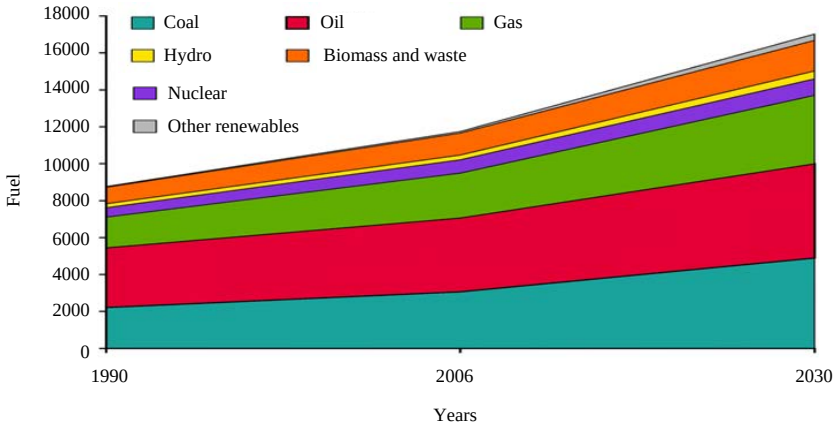

Fig. 1: Global total primary energy consumption by fuel

energy consumption in 2010, 2013 and 2016, respectively. Similarly, in 2013, crude oil and coal contributed 30.92 and 28.95% to global energy consumption while this increased to33% for crude oil and 28% for coal in 2016 (BP., 2019). Over the past 15 years oil has contributed a third of the global energy consumption, closely followed by coal and natural gas (Schiffer, 2016). Products of refined fossil fuels are used to power internal combustion engines, particularly Compression Ignition (CI) engines which continue to contribute significantly to industrial growth, economic and commercial growth, agricultural sector development, social and household needs as well as transportation of goods and services. Generally, global primary energy consumption has continued to increase and is projected to continue increasing (Fig. 1) (EEA., 2012).

The transport sector consumed about 28% of total global energy and contributed 24% of global carbon dioxide (CO_2) emissions in the year 2016 (Statista, 2018). According to the United States EPA. (2017), transport vehicles contributed 71% of total greenhouse gas emissions globally in 2010. The solution to this disturbing trend is to develop clean and affordable alternative fuels to reduce dependence on fossil fuels, guaranteeing an amicable coexistence of humans and the environment and ensuring sustainable economic growth. Reducing the use of fossil-based fuel will ensure that air quality, particularly around high-density traffic residential areas, is maintained within World Health Organization (2006) standards to safeguard human and environmental health.

Biodiesel, a renewable fuel, comprises mono-alkyl/ methyl esters of long chain fatty acids obtained from various feedstocks including neat vegetable oils, used vegetable oils, microalgae, animal fats, etc., biodiesel, also known as Fatty Acid Methyl Esters (FAME) are generated by various techniques including pyrolysis, dilution or blending of oils, micro-emulsification and transesterification and are dried to ensure compliance with standards. Internationally acceptable specifications for FAME are well documented in the American Standard for Testing and Materials (ASTM) and European Union (EN) documents such as ASTM D6751 and EN 14214, respectively. Different countries set up their own standards based on these two standards and other international protocols to suit their particular geographical locations (Jaaskelainen, 2009; ACEA., 2013). According to Index Mundi (2019), based on reports by the United States Energy Information Administration, global biodiesel production grew from 25.46 thousand barrels per day (mbpd) in 2002-123.9 mbpd in 2006 and to 432.9 mbpd in 2012. Consumption was reported to be 22.26, 118.1 and 419.9 mbpd in 2002, 2006 and 2012, respectively and is still increasing. Replacement of Petroleum-Based Diesel (PBD) fuel with biodiesel offers technical, economic, sanitation and economic benefits, notably a simpler refining process, cheaper feedstock, verifiable means of waste disposal, better engine performance and reduction in the emission of greenhouse gases and other hazardous gases. FAME is considered to be the most widely used liquid renewable fuel in Europe, accounting for about 80% of biofuel market share, owing to its non-toxicity, biodegradability and renewability (Zhu *et al*., 2017).

There is near consensus among fuel refiners and engine researchers regarding the importance of fuel properties in determining fuel quality, fuel mixing, ease of ignition, fuel combustion and other activities in the combustion chambers. Properties such as oxygen content, density, Cetane Number (CN), Kinematic Viscosity (KV), Flash Point (FP), Cold Filter Plugging Point (CFPP), Cloud Point (CP), Heating Values (HV) and Pour Point (PP) have been found to influence fuel quality, handling, safety, transportation, combustion, engine performance and emission characteristics (Imdadul *et al*., 2016; Zaharin *et al*., 2017). Fatty Acid (FA) compositions of FAME have been an important factor in the determination of its fingerprint properties, quality, storage capacity, engine performance, and emission characteristics. Thus, FA composition determines the major properties of FAME.

Experimental, numerical, simulation and statistical investigations have been used to exploit the nexus between FA composition of biodiesel and some of its properties to predict these important properties. Specifically, cold flow properties, KV, CN and other biodiesel fingerprints are significantly influenced by FA composition, branching, chain length, number and position of double bonds. Samavi *et al*. (2016) predicted the KV and FP of FAME as a function of its FA composition and verified the outcome with experimental data. Giakoumis and Sarakatsanis (2018) estimated the CN, KV and density of biodiesels from their FA compositions. Multiple Linear Regression (MLR) analysis has been employed to develop compositional-based models to predict biodiesel properties from various feedstocks with considerable accuracy because the derived correlations possess a sound theoretical basis (Bamgboye and Hansen, 2008; Gopinath *et al*., 2009; Piloto-Rodriguez *et al*., 2013; Giakoumis, 2013). Statistical investigations were successfully carried out to predict the density, CN, KV, FP, CFPP, CP and PP of FAME based on the degree of saturation and FA composition (Giakoumis, 2013). MLR, Artificial Neural Network (ANN) and other machine learning techniques were used to forecast the properties of FAME based on their FA compositions. The outcome of the investigations shows that these techniques are able to predict some important properties of the FAME samples (Piloto-Rodriguez *et al*., 2013; Filho *et al*., 2015; Saldana *et al*., 2012; Balabin *et al*., 2011).

In determining the most occurring FAs in biodiesel, FA composition of 123 samples of biodiesel found as a result of a literature search were studied and found to comprise 13 methyl esters, namely: palmitic acid (C16:0), stearic (C18:0), oleic acid (C18:1), linoleic acid (C18:2), linolenic acid (C18:3), arachidic acid (C20:0), palmitoleic acid (C16:1), lauric acid (C12:0), myristic acid (C14:0), eicosenic acid (C20:1), behenic acid (C22:0), erucic acid (C22:1) and lignoceric acid (C24:0). Available information shows that C16:0, C18:0, C18:1, C18:2 and C18:3 are the most common FAs in biodiesels (Filho *et al*., 2015; Hoekman *et al*., 2012; Meng *et al*., 2014; Moradi-Kheibari *et al*., 2019).

With the increased use of compositional-based models for the prediction of major FAME properties, the question to be answered and which serves as the motivation for this effort is whether biodiesel properties can be accurately predicted using linear correlations developed from the five most common methyl esters. The aim of this investigation, therefore, wasto use MLR techniques to formulate predictive correlations based these methyl esters to predict density, CN, KV and CV. The predictive capability of MLR-derived correlations for fingerprint prediction using compositional-based models using five methyl esters as inputs was tested and verified from data mined from literature. This current effort was limited to the application of MLR to predict the density, CN, KV and CVof unblended FAME derived from various feedstocks based on C16:0, C18:0, C18:1, C18:2 and C18:3.

MATERIALS AND METHODS

Inputs for the formulation of a reliable correlation for the prediction of biodiesel properties based on weight composition of five methyl esters requires a large and widely spread experimental data base as reported in the literature for the correlations to have a broad-based effect, irrespective of the type of feedstock, location, production technique and purification methods (Giakoumis and Sarakatsanis, 2018; Giakoumis, 2018; Jeeva and Rajashekar, 2018). The chosen five fatty acids have been found to occur in most of the Gas chromatography-mass spectrometry analyses of biodiesels, cutting across saturated, monounsaturated and polyunsaturated fatty acids. The general equation adopted for the MLR analysis is given by Eq. 1. The predicted data for each property are plotted against the experimental data to appraise the predictive capability of the model using statistical indices. The correlations are used to predict the outcome of another set of data from the literature, different from the data used to formulate the correlation and the absolute errors calculated:

$$y = A + a_1 + X_1 + a_2 + X_2 + a_3 + X_3 + a_4 + X_4 + a_5 + X_5$$

Where:

y = The dependent variable to be predicted
A = The intercept
a_1-a_5 = The coefficients of each independent variable
X_1-X_5 = The percentage composition of each FA in the sample

For this analysis, 1-5 represent C16:0, C18:0, C18:1, C18:2 and C18:3, respectively which are the independent variables.

RESULTS AND DISCUSSION

Density: The density of a material, measured in kg m^{-3} is expressed as the mass per unit volume of the material. The quantity of fuel admitted into the combustion chamber is influenced by the density of the fuel, an indication that density has a direct impact on the fuel injection process, combustion, engine performance and emission characteristics of FAME. Density also has strong correlations with KV, CN and HV which affect the air-fuel ratio and energy content of fuel injected into the engine, degree of saturation, number of double bonds, molecular weight and chain length (Sakthivel and Ilangkumaran, 2017; Knothe *et al*., 2015).

Table 1: Data for density prediction

Source	C16:0	C18:0	C18:1	C18:2	C18:3	Exp. Density	Pred. Density
Beef tallow	24.39	19.08	41.65	5.91	0.72	874.3	875.0
Canola	4.51	2	60.33	21.24	9.49	881.6	883.3
Chicken fat	24.06	6.42	41.43	18.83	1.06	876.3	878.9
Corn	11.81	2.13	27.35	57.74	0.63	882.2	882.8
Cottonseed	25.93	1.74	15.98	55.12	0.16	879.0	880.2
Croton	7.25	3.43	10.80	77.25	5.4	883.2	884.6
Hazenut	6.36	3.71	79.17	10.67	0.15	877.9	879.0
Jatropha	14.42	5.82	42.81	35.38	0.23	878.7	879.8
Karanja	10.89	7.89	53.56	21.34	2.09	882.9	880.1
Linseed	5.18	3.26	19.04	16.12	54.54	891.5	891.1
Mahua	22.23	22.49	39.01	14.87	0.1	874.5	873.0
Neem	17.57	16.6	45.83	17.79	0.72	876.2	875.5
Olive	11.47	2.83	74.52	9.54	0.51	881.2	878.6
Palm	42.39	4.2	40.91	9.70	0.29	874.7	873.1
Peanut	10.33	2.79	47.63	31.52	0.64	882.9	882.8
Rapeseed	4.07	1.55	62.24	20.61	8.72	882.2	883.4
Rice barn	18.12	2.17	42.35	34.84	0.93	880.9	880.0
Rubber seed	9.39	9.41	24.22	38.12	17.54	882.3	883.6
Safflower	7.42	2.38	14.41	75.31	0.09	883.8	885.1
Soybean	11.44	4.14	23.47	53.46	6.64	882.8	883.4
Sunflower	6.26	3.93	20.77	67.75	0.15	882.9	884.5
Soybean	15.69	6.14	42.84	29.36	2.03	880.6	880.2
Sunflower	25.1	13.23	44.36	12.06	1.18	873.0	875.3
Karanja	10.74	6.8	50.24	17.21	3.47	880.5	882.7
Karanja	8.38	5.32	40.54	14.91	2.84	890.6	888.7
Ibicellalutea	9.1	2.33	52.36	35.88	0.33	882.4	881.1
Onopordum nervosum	9.08	2.57	27.02	60.34	10.23	885.4	882.1
Peganum harmala	4.02	2.57	26.93	53.62	2.44	890.1	887.5
Smymium olusatrum	5.26	1.07	74.14	14.10	0.48	880.3	881.8
Solanum elaeagnifolium	9.86	4.24	20.92	63.32	1.07	885.9	883.4

Table 2: Statistical indices of the MLR Model for density

Regression statistics	Values
Multiple R	0.927
R^2	0.859
Adjusted R^2	0.83
SE	1.9
Observations	30

The data for the generation of the model were sourced from various literature (Giakoumis and Sarakatsanis, 2018; Jeeva and Rajashekar, 2018; Houachri *et al*., 2018). The MLR Model equation is as represented by Eq. 2 while Table 1 shows the independent variables, the experimental dependent variables and the predicted density. The predicted data is generated by the linear correlations using the FA compositions:

$$\text{Density} = 914 - 0.52X_1 - 0.54X_2 - 0.34X_3 - 0.25X_4 - 0.14X_5$$

The intercept value of 914 achieved by this effort is comparably higher than the 869 reported by Giakoumis (2013) but lower than the 923 established by Giakoumis and Sarakatsanis (2018) for comparable investigations. The statistical indices show that the R = 0.927 while the R^2 of 0.859 shows that the predicted dependent variable can be attributed to 85.9% of the independent variables in 30 observations (Table 2). A standard error of 1.9 is suggestive of a satisfactory correlation between the model equation and the experimental data, confirming the capability of the model equation to adequately predict the dependent variable.

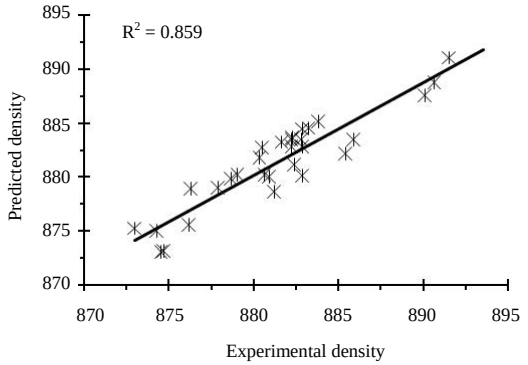

Fig. 2: The predictive capability of the density model

The model was tested on a new set of experimental values, different from those used in Table 1 in order to ascertain the predictive reliability of the model using Eq. 2. As shown in Table 3, a negligible error was established with a maximum of 0.35%. The predictive capability of the model is shown by plotting the experimental data with the predicted data (Fig. 2). The predictive capability of this model gave a higher R^2-value than the outcome of a similar prediction by Pratas *et al*. (2011).

Table 3: Density model verification

Biodiesel	Researchers	Exp. values	Pred. values	Error (%)
RME	Zhang *et al*. (2018)	882.00	882.81	0.09
SFME	Zhang *et al*. (2018)	885.00	884.82	0.02
SME	Zhang *et al*. (2018)	886.00	883.40	0.29
CSME	Zhang *et al*. (2018)	882.00	879.06	0.33
HME	Gulum and Bilgin (2017)	874.07	877.11	0.35
PBME	Ruhul *et al*. (2016)	869.50	867.96	0.18
JBME	Ruhul *et al*. (2016)	880.30	879.19	0.13
ALBME	Ruhul *et al*. (2016)	875.70	877.04	0.15

Table 4: Measured and predicted data for cetane number

Source	C16:0	C18:0	C18:1	C18:2	C18:3	Exp. CN	Pred. CN
Aphanamixis polystachya Park	23.1	12.8	21.5	29	13.6	48.52	49.50
Azadirachta indica	14.9	14.4	61.9	7.5	0	57.83	58.68
Moringa oleifera Lam	9.1	2.7	79.4	0.7	0.2	56.66	58.67
Mesua ferrea Linn	10.8	12.4	60	15	0	55.1	56.80
Corylus avellana	3.1	2.6	88	2.9	0	54.5	57.44
Basella rubra Linn	19.7	6.5	50.3	21.6	1.1	54.0	55.83
Ervatamia coronaria Stapf	24.4	7.2	50.5	15.8	0.6	56.33	57.70
Aleurites moluccana wild	5.5	6.7	10.5	48.5	28.5	34.18	36.75
Vallaria solanacea Kuntzc	7.2	14.4	35.3	40.4	0	50.26	52.15
Holoptelia integrifolia	35.1	4.5	53.3	0	0	61.22	62.08
Mappia foetida Milers	7.1	17.7	38.4	36.8	0	50.7	52.83
Swietenia mahagoni Jacq	9.5	18.4	56	0	16.1	52.26	52.02
Madhuca indicai JF Gmel	17.8	14	46.3	17.9	0	56.61	57.34
Anamirta cocculus Wight and Hrn	6.1	47.5	46.4	0	0	64.26	60.80
Broussanetia papyrifera Vent	4	6.1	14.8	71	1	41.25	45.56
Beef tallow	24.39	19.02	41.65	5.91	0.72	60.9	60.35
Canola	4.51	2	60.33	21.24	9.49	54.8	49.97
Chicken fat	24.06	6.42	41.43	18.83	1.06	57.0	57.18
Coconut	9.69	0	2.83	6.83	0	61.0	60.95
Corn	11.81	2.13	27.35	57.74	0.63	52.5	48.60
Cottonseed	25.93	1.74	15.98	55.12	0.16	53.3	50.98
Hazelnut	6.32	3.71	79.17	10.67	0.15	53.8	56.33
Jatropha	14.42	5.82	42.81	35.38	0.23	55.7	53.21
Karanja	10.89	7.89	53.56	21.34	2.09	55.4	54.59
Mahua	22.23	22.49	39.01	14.87	0.1	56.9	58.72
Olive	11.47	2.83	74.52	9.54	0.51	58.9	56.98
Palm	42.39	4.2	40.91	9.7	0.29	61.2	60.93
Peanut	10.33	2.79	47.63	31.52	0.64	54.9	53.27
Rapeseed	4.07	1.55	62.24	20.61	8.72	54.1	50.38
Waste cooking	15.69	6.14	42.84	29.36	2.03	56.2	53.70

Cetane Number (CN) is a dimensionless parameter and one of the most important properties of fuel that relates to its self-ignitability and ignition delay characteristics in a CI engine. FAME structure, FA composition, number and position of double bonds, chain length, degree of saturation/unsaturation, boiling point, the heat of vaporization, the heat of combustion, etc. have been reported to substantially affect CN. Engine combustion noise level, vibration, heat release rate, engine performance and generation of pollutants are influenced by the CN of FAME. Higher CN is believed to be a precursor for less ignition delay time, lower combustion noise, higher power as well as less emission of soot, NOx, CO and SO_2 (Sajjadi *et al*., 2016; Mishra *et al*., 2016).

Bamigboye and Hansen (2008), Tong *et al*. (2011), Ramadhas *et al*. (2006), Knothe (2005) and Piloto-Rodriguez *et al*. (2013), among other researchers have estimated CN using a percentage of FA compositions as inputs by MLR/ANN or both but with a higher number of methyl esters (>5 methyl esters). This present effort is limited to the use of the five most common FAs as inputs. The general linear regression equation (Eq. 1) is transformed into Eq. 3 through MLR for the prediction of the CN. The intercept value of 61.84 is comparable with values of 61.1 predicted by Bamigboye and Hansen and 62.2 predicted by Gopinath *et al*. (2009):

Table 5: Statistical indices of the MLR Model for cetane number

Regression statistics	Values
Multiple R	0.918
R^2	0.843
Adjusted R^2	0.810
SE	2.550
Observations	30.000

$$\text{Cetane number} = 61.84+0.07X_1+0.01X_2 - 0.05X_3 - 0.22X_4 - 0.51X_5 \quad (3)$$

Table 4 shows the FA and CN measured from experimental data sourced from literature (Giakoumis, 2013; Tong *et al*., 2011) and the dependent output predicted by the model (Table 5). A total of 30 input data were used to generate the model. The source of the data

Table 6: Cetane number model verification

Sources	Researchers	Exp. values	Pred. values	Error (%)
HME	Gulum and Bilgin (2017)	55.66	55.79	0.23
JBME	Ruhul *et al*. (2016)	53.50	53.67	0.32
ALBME	Ruhul *et al*. (2016)	55.50	55.11	0.72
Madhuca butyracea Mac	Tong *et al*. (2011)	65.27	64.46	1.26
Basella rubra Linn	Tong *et al*. (2011)	56.33	56.99	1.15
Ervatamia coronaria Stapf	Tong *et al*. (2011)	56.33	57.31	1.72

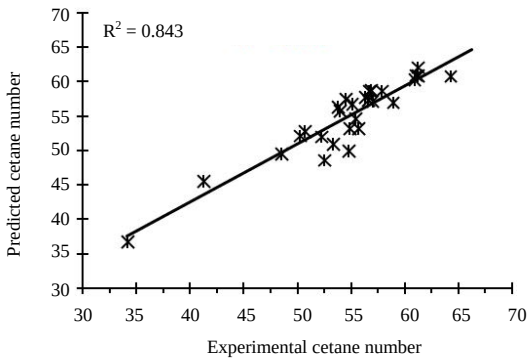

Fig. 3: The predictive capability of the cetane number model

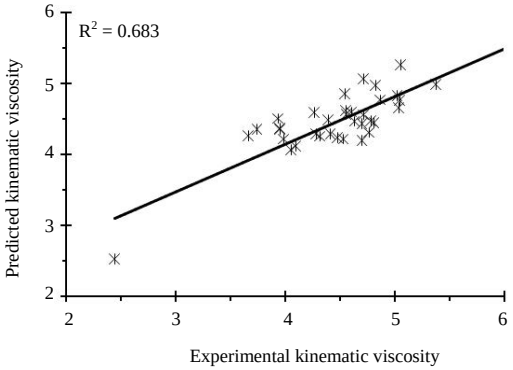

Fig. 4: The predictive capability of the kinematic viscosity model

covered a wide range of feedstock type to ensure that the model would have a wide range of applications in view of the variability of CN with feedstock type. Table 6 illustrates the statistical indices of the model. The developed model was found to be significant and competent to adequately predict the dependent variable. The R-value of 0.918 and R^2 value of 0.843 indicates that 84.3% of the independent variable determined the outcome of the model. A standard error of 2.55 displays a good statistical correlation between the model equation and the experimental data.

The model was tested to predict the CN of other reported experimental data available in the literature apart from those used in Table 4 as a way of verifying the predictive capability of the model. As shown in Table 6, the highest error obtained was 1.72% which can be adjudged a good result considering the wide variability of the feedstock. Figure 3 shows the plot of experimental data against predicted data to show the predictive capability of the model.

Kinematic viscosity: Kinematic Viscosity (KV) is the degree of the resistance of fluid flow as a result of the internal friction of a layer of fluid flowing over another layer and has been found to affect fuel injection and fuel atomization among other critical fuel behavior properties. The high value of KV predisposes the fuel to produce a large droplet size, enhanced polymerization reaction, more carbon deposits, poorer vaporization, small injection spray angle and better in-cylinder penetration of the fuel spray. Increased KV often leads to weaker fuel combustion, higher oil dilution, and increased emission of smoke and other pollutants. KV is closely related to density, specific gravity, degree of unsaturation, location of double bonds and molecular weight (Hong *et al*., 2014; Saxena *et al*., 2013). At low temperatures fuels with high KV pose critical challenges while too low KV can cause insufficient lubrication in fuel pumps, increased leakage and wear (Joshi and Pegg, 2007).

The model correlation as shown in Eq. 4 is arrived at from the general format stated in Eq. 1. The model is significant and sufficient to predict the dependent variable within an acceptable standard. Table 7 depicts the FA composition, the experimentally measured KV sourced from literature and the MLR predicted data. With the R^2 of 0.683 as shown in Fig. 4, 68.3% of the independent variable contributed to the prediction of the dependent variable. The R-value of 0.83 and standard error of 0.33 with five methyl esters is comparable to the outcome of similar research by Giakoumis and Sarakatsanis (2018) with eight methyl esters:

$$\text{Kinematic viscosity} = 1.22 + 0.03X_1 + 0.07X_2 + 0.04X_3 + 0.03X_4 + 0.02X_5 \quad (4)$$

Compared to the capability of MLR to predict CN, the model was not as accurate in predicting KV but was significant enough to predict the dependent variable within reasonable error. The predictive capability of the model was tested with experimental data, apart from the data used in Table 7 and 8 and the outcome of the verification of the predictive capability model is shown in Table 9. The model verification presented a maximum error of 4.33%. Although, this is a higher error value compared with absolute error for density and CN in the preceding sections, it is however, lower than similar results found in the literature.

Table 7: Experimental and predicted data for kinematic viscosity

Source	C16:0	C18:0	C18:1	C18:2	C18:3	Exp. KV	Pred. KV
Beef tallow	24.39	19.08	41.65	5.91	0.72	4.83	4.96
Canola	4.51	2	60.33	21.24	9.49	4.4	4.48
Chicken fat	24.06	6.42	41.43	18.83	1.06	4.81	4.44
Corn	11.81	2.13	27.35	57.74	0.63	4.32	4.26
Cottonseed	25.93	1.74	15.98	55.12	0.16	4.7	4.19
Croton	7.25	3.43	10.8	77.25	5.4	4.48	4.23
Hazenut	6.36	3.71	79.17	10.67	0.15	4.55	4.84
Jatropha	14.42	5.82	42.81	35.38	0.23	4.72	4.56
Karanja	10.89	7.89	53.56	21.34	2.09	5.04	4.65
Linseed	5.18	3.26	19.04	16.12	54.54	4.06	4.06
mahua	22.23	22.49	39.01	14.87	0.1	5.06	5.25
Neem	17.57	16.6	45.83	17.79	0.72	4.72	5.05
Olive	11.47	2.83	74.52	9.54	0.51	5.05	4.75
Palm	42.39	4.2	40.91	9.7	0.29	4.61	4.60
Peanut	10.33	2.79	47.63	31.52	0.64	4.77	4.31
Rapeseed	4.07	1.55	62.24	20.61	8.72	4.63	4.47
Rice barn	18.12	2.17	42.35	34.84	0.93	4.7	4.42
Rubber seed	9.39	9.41	24.22	38.12	17.54	4.79	4.46
Safflower	7.42	2.38	14.41	75.31	0.09	4.1	4.11
Soybean	11.44	4.14	23.47	53.46	6.64	4.29	4.28
Sunflower	6.26	3.93	20.77	67.75	0.15	4.53	4.22
RME	3.57	0.87	65.18	22.27	8.11	4.556	4.55
SMEA	10.49	4.27	24.2	51.36	7.48	3.67	4.25
SMEB	10.81	4.54	24.96	50.66	7.27	4.41	4.28
GMSME	3.97	2.99	82.54	4.98	3.7	4.87	4.77
YGME	17.44	12.38	54.67	7.96	0.69	5.02	4.82
GP	10.57	2.66	41.05	36.67	7.1	3.96	4.36
PBME	38.1	4.1	44.2	11	0.3	4.56	4.61
JBME	17.1	6.4	41.8	32.9	0.2	4.27	4.58
Coconut	13.83	3.94	14.3	4.73	0	2.45	2.52
Cottonseed	24.09	2.56	15.74	56.99	0	3.99	4.22
ALBME	14.8	16	41.3	26.6	0.2	5.38	4.97
Soy A	16.18	3.82	28.2	50.46	0	3.74	4.34
Rapeseed	5.26	1.63	62.94	20.94	6.99	3.942	4.51
Soy B	10.18	3.82	28.5	35.46	0	3.96	4.34

Table 8: Statistical indices of the MLR Model for kinematic viscosity

Regression statistics	Values
Multiple R	0.830
R^2	0.683
Adjusted R^2	0.629
SE	0.330
Observations	35.000

Calorific value: The Calorific Value (CV) of a fuel is a measure of or degree of, its heating capacity. A CV is measured in kilojoules per kg (kJ kg^{-1}) and is commonly defined as the quantity of energy generated by the complete combustion of a known volume of fuel under stipulated conditions. The gross CV, also known as the Higher Heating Value (HHV) is a measure of the fuel's heat of combustion when the water's heat of combustion is completely condensed and the heat contained in the water vapor is fully retrieved (Kaisan *et al*., 2017). The net CV, also known as the Lower Heating Value (LHV), is measured when the product of the fuel's combustion includes water vapor and the heat in the water vapor is not retrieved. The difference between the HHV and LHV is termed the heat of vaporization of water. FAME is reputed to contain higher oxygen content than Petroleum-Based Diesel Fuel (PBDF); it follows, therefore, that FAME has a LHV compared to PBDF. This fact accounts for the higher quantity of FAME injected for combustion to achieve the required engine power (Atabani and da Silva Cesar, 2014). An increment in the chain length of fuel molecules and the carbon/nitrogen to nitrogen/oxygen ratio of FAME results in a higher CV (Ramirez-Verduzco *et al*., 2012; Sanli *et al*., 2014).

Without a doubt, a higher CV is needed for effective combustion of FAME in an unmodified CI engine because of its desirable effects on combustion of IC engines. The lowest recommended value for the CV of biodiesel fuel for heating purposes as specified by EN 14213 is 35 mJ kg^{-1} (Muralidharan *et al*., 2011; Rashid *et al*., 2009). Apart from oxygen content, other factors that influence the HV of FAME include the degree of saturation, number of double bonds, C:O ratio, C:H ratio, and feedstock (Hoekman *et al*., 2012). Some properties like CP, density, FP and KV have been found to have strong correlations with HVs. In terms of emission, the higher quantity of FAME that needs to be injected into the combustion chamber to meet the required engine power has been found to affect PM and NOx emissions, particularly within an exhaust gas recirculation system (Rakopoulos and Giakoumis, 2009; Giakoumis *et al*., 2012).

Table 9: Kinematic viscosity model verification

Source	Researchers	Exp. values	Pred. values	Error (%)
Rapeseed	Geacai *et al*. (2015)	4.67	4.84	3.57
POME	Ali *et al*. (2016)	4.61	4.79	3.72
Soybean	Martinez *et al*. (2014)	4.04	4.2	3.86
Sunflower	Martinez *et al*. (2014)	4.55	4.61	1.24
Jatrop acurcas	Martinez *et al*. (2014)	4.46	4.28	4.33

Table 10: Experimental and predicted data for calorific value

Source	C16:0	C18:0	C18:1	C18:2	C18:3	Exp. CV	Pred. CV
Corn	11.81	2.13	27.35	57.74	0.63	40.19	40.163
Cottonseed	25.93	1.74	15.98	55.12	0.16	40.48	39.879
Croton	7.25	3.43	10.8	77.25	5.4	40.28	40.401
Hazelnut	6.32	3.71	79.17	10.67	0.15	39.8	40.04
Jatropha	14.42	5.82	42.82	35.38	0.23	40.38	40.062
Karanja	10.89	7.89	53.56	21.34	2.09	40.275	40.106
Peanut	10.33	2.79	47.63	31.52	0.64	39.93	40.071
Rapeseed	4.07	1.55	62.24	20.61	8.72	40.335	40.154
Rice bran	18.12	2.17	42.35	34.84	0.93	40.475	39.929
Rubber seed	9.39	9.41	24.22	38.12	17.54	40.35	40.349
Beef tallow	24.39	19.08	41.65	5.91	0.72	40.04	39.976
Canola	4.51	2	60.33	21.24	9.49	39.975	40.162
Chicken fat	24.06	6.42	41.43	18.83	1.06	39.89	39.821
Lard	25.1	13.23	44.36	12.06	1.18	39.95	39.887
Olive	11.47	2.83	74.52	9.54	0.51	40.28	39.926
Neem	17.57	16.6	45.83	17.79	0.72	39.96	40.112
Mahua	22.23	22.49	39.01	14.87	0.1	40.18	40.114
Safflower	7.42	2.38	14.41	75.31	0.09	40.155	40.339
Waste frying oil	25.043	4.283	37.942	30.032	0.19	39.223	39.811
Waste frying oil	25.95	3.899	43.574	23.637	0.265	39.833	39.754
Waste frying oil	27.614	3.93	42.754	22.805	0.281	39.312	39.719
Waste frying oil	29.117	4.375	37.455	26.233	0.21	39.259	39.717
Waste frying oil	25.645	3.863	43.228	24.306	0.271	39.441	39.762
Waste frying oil	41.438	4.775	40.636	10.293	0.182	39.741	39.413
Waste frying oil	40.637	3.369	42.104	9.958	0.173	39.336	39.401

It is believed that HVs can be predicted using the FA composition of FAME. Only a few citations are available in the literature to establish a linear correlation to link HVs with FA composition as far as the researchers know. Specifically, Sanli *et al*. (2014), Giakoumis (2013) and Giakoumis and Sarakatsanis (2018) have predicted the HVs using a percentage of FA compositions as inputs although they used more than five methyl esters. This present effort is limited to the use of the five most common FAs as input, using the MLR approach. Input data was sourced from the data sets available in the literature (Giakoumis and Sarakatsanis, 2018; Sanli *et al*., 2014).

The model correlation, shown in Eq. 5 is arrived at from the general format (Eq. 1). The model wasfound to be significant and adequate to predict the CV within an acceptable standard. Table 7 shows the five FA compositions, the experimentally determined CV (mJ/kg) sourced from literature and the MLR predicted data. Equation 5 was arrived at by generating a linear correlation between the experimentally measured CV and the MLD predicted CV (Table 10). The intercept was found to be 40.144 while C16:0 and C18:1 had a very minimal but negative effect on the output data. The predictive capability of the model is shown in Fig. 5:

Table 11: Statistical indices of the MLR Model for calorific value

Regression statistics	Values
Multiple R	0.66
R^2	0.43
Adjusted R^2	0.28
SE	0.33
Observations	25.00

$$\text{Calorific Value} = 40.144 - 0.02X_1 + 0.017X_2 - 0.001X_3 + 0.004X_4 + 0.005X_5 \quad (5)$$

The statistical analysis (Table 11) shows that the model is significant with the R^2 of 0.43. This implies that 43% of the independent variable (input) contributed to the prediction of the dependent variable (output). The R-value of 0.66 and standard error of 0.33, using only five methyl esters is comparable to the outcome of similar research (Giakoumis and Sarakatsanis, 2018; Hong *et al*., 2014; Sanli *et al*., 2014). The model was verified with different sets of data sourced from the literature and was found to satisfactorily predict the CV despite the diverse nature of the FAME sources. The difference between the measured and the predicted CV was negligible and within acceptable standards (Table 12).

Table 12: Calorific value model verification

Source	Researchers	Exp. values	Pred. values	Error (%)
Jatropha	Mofijur *et al*. (2013)	40.536	40.501	0.09
Palm	Atabani *et al*. (2012)	39.907	39.863	0.11
Corn	Gulum and Bilgin (2015)	39.93	39.538	0.98
Canola	Hong *et al*. (2014)	39.64	39.615	0.06
Soybean oil	Hong *et al*. (2014)	40.04	39.907	0.33
Grape Seed	Hong *et al*. (2014)	39.82	39.968	0.37
Karanja	Jose and Anand (2016)	39.66	39.542	0.3

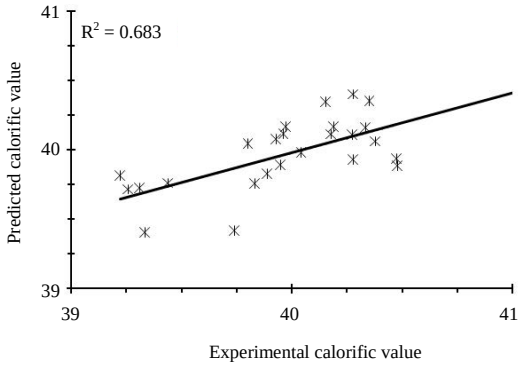

Fig. 5: The predictive capability of the Calorific Value model

CONCLUSION

One of the motivations for the use of FAME as CI engine fuel is safer handling, improved engine performance, and mitigated emissions. Experimental determination of FAME fingerprint, which is a key determinant for the behavior, handling, storage, transportation, performance and emissions of the fuel is onerous and laborious and requires costly laboratory architecture and highly trained technical personnel. Appropriately developed models and prediction correlations are considered to be a faster, cheaper and easier method of determining these properties based on certain criteria and conditions. The degree of saturation, chain length, branching, number and position of double bonds are key parameters in the performance of biodiesel. FA compositions of biodiesel are dependent on the type of feedstock, and to some extent on its production parameters and techniques which greatly influence the properties of FAME based on the proportion of the methyl esters present in the biodiesel.

This current effort employed the five most common methyl esters, namely palmitic acid (C16:0), stearic acid (C18:0), oleic acid (C18:1), linoleic acid (C18:2), and linolenic acid (C18:3) to predict density, KV, CN and CV of FAME using the MLR approach. A linear correlation was generated for the individual fingerprints and employed to predict the output using data extracted from the literature. The model was analyzed statistically to determine the standard error and other statistical indices. Predictive capability and model verification were carried out to test the competency and accuracy of the model within acceptable limits. In conclusion, the following points can be deduced: Some FAME properties can be predicted by the proportion of methyl esters as a solution for difficulties in the experimental determination of the properties. Five FAs are enough to generate a linear correlation using MLR to accurately predict the density, KV, CN and CV of FAME.

The outcome of the model verification shows that the correlation generated by this methodology can be relied upon to correctly predict the dependent outcomes being sought.

Going forward, even more accurate prediction correlations and models should be developed for predicting properties, performance, fuel mixing, combustion and emission characteristics with linear and nonlinear relations. This will eliminate the cumbersome experimental determinations of these parameters with a view to advancing capacities in engine research.

REFERENCES

ACEA., 2013. Worldwide fuel charter. European Automobile Manufacturers Association, Brussels, Belgium. http://www.oica.net/wp-content/uploads//WWFC5-2013-Final-single-page-correction2.pdf

Ali, O.M., R. Mamat, N.R. Abdullah and A.A. Abdullah, 2016. Analysis of blended fuel properties and engine performance with palm biodiesel-diesel blended fuel. Renewable Energy, 86: 59-67.

Atabani, A.E. and A.D.S. Cesar, 2014. *Calophyllum inophyllum* L.-A prospective non-edible biodiesel feedstock. Study of biodiesel production, properties, fatty acid composition, blending and engine performance. Renewable Sustainable Energy Rev., 37: 644-655.

Atabani, A.E., A.S. Silitonga, I.A. Badruddin, T.M.I. Mahlia, H.H. Masjuki ad S. Mekhilef, 2012. A Comprehensive Review on Biodiesel As An Alternative Energy Resource and its Characteristics. Renewable Sustainable Energy Rev., 16: 2070-2093.

BP., 2019. Statistical review of world energy. BP Plc., London. https://www.bp.com/en/global/corporate/energy-economics/statistical-review-of-world-energy.html

Balabin, R.M., E.I. Lomakina and R.Z. Safieva, 2011. Neural network (ANN) approach to biodiesel analysis: Analysis of biodiesel density, kinematic viscosity, methanol and water contents using near infrared (NIR) spectroscopy. Fuel, 90: 2007-2015.

Bamgboye, A.I. and A.C. Hansen, 2008. Prediction of cetane number of biodiesel fuel from the Fatty Acid Methyl Ester (FAME) composition. Int. Agrophys., 22: 21-29.

EEA., 2012. Global total primary energy consumption by fuel. European Environment Agency, Kobenhavn, Denmark, Europe.

EPA., 2017. Climate change indicators: Global greenhouse gas emissions. US Environmental Protection Agency, Washington DC., USA. https://www.epa.gov/climate-indicators/climate-change-indicators-global-greenhouse-gas-emissions

Filho, A.O. B., A.K.D. Barros, S. Labidi, I.M.A. Viegas and D.B. Marques *et al*., 2015. Application of artificial neural networks to predict viscosity, iodine value and induction period of biodiesel focused on the study of oxidative stability. Fuel, 145: 127-135.

Geacai, S., O. Iulian and I. Nita, 2015. Measurement, correlation and prediction of biodiesel blends viscosity. Fuel, 143: 268-274.

Giakoumis, E.G. and C.K. Sarakatsanis, 2018. Estimation of biodiesel cetane number, density, kinematic viscosity and heating values from its fatty acid weight composition. Fuel, 222: 574-585.

Giakoumis, E.G., 2013. A statistical investigation of biodiesel physical and chemical properties and their correlation with the degree of unsaturation. Renewable Energy, 50: 858-878.

Giakoumis, E.G., 2018. Analysis of 22 vegetable oil's physico-chemical properties and fatty acid composition on a statistical basis, and correlation with the degree of unsaturation. Renewable Energy, 126: 403-419.

Giakoumis, E.G., C.D. Rakopoulos, A.M. Dimaratos and D.C. Rakopoulos, 2012. Exhaust emissions of diesel engines operating under transient conditions with biodiesel fuel blends. Progress Energy Combust. Sci., 38: 691-715.

Gopinath, A., S. Puhan and G. Nagarajan, 2009. Theoretical modeling of iodine value and saponification value of biodiesel fuels from their fatty acid composition. Renewable Energy, 34: 1806-1811.

Gulum, M. and A. Bilgin, 2015. Density, flash point and heating value variations of corn oil biodiesel-diesel fuel blends. Fuel Process. Technol., 134: 456-464.

Gulum, M. and A. Bilgin, 2017. Measurements and empirical correlations in predicting biodiesel-diesel blends viscosity and density. Fuel, 199: 567-577.

Hoekman, S.K., A. Broch, C. Robbins, E. Ceniceros and M. Natarajan, 2012. Review of biodiesel composition, properties and specifications. Renewable Sustainable Energy Rev., 16: 143-169.

Hong, I.K., G.S. Jeon and S.B. Lee, 2014. Prediction of biodiesel fuel properties from fatty acid alkyl ester. J. Ind. Eng. Chem., 20: 2348-2353.

Houachri, T., D. Bolonio, A. Llamas, J. Rodriguez-Fernandez and M. El Gazza *et al*., 2018. Fatty Acid Methyl Esters (FAME) from oleaginous seeds grown in arid lands. Part II: Ibicella lutea, Onopordum nervosum, Peganum harmala, Smyrnium olusatrum and Solanum elaeagnifolium. Energy Sources Part A. Recovery Util. Environ. Effects, 40: 1434-1441.

Imdadul, H.K., H.H. Masjuki, M.A. Kalam, N.W.M. Zulkifli and A. Alabdulkarem *et al*., 2016. Higher alcohol-biodiesel-diesel blends: An approach for improving the performance, emission and combustion of a light-duty diesel engine. Energy Convers. Manage., 111: 174-185.

IndexMundi, 2019. World biodiesel production and consumption by year. Index Mundi, USA. https://www.indexmundi.com/energy/?product=biodiesel&graph=production+consumption

Jaaskelainen, H., 2009. Biodiesel standards & properties. Ecopoint Inc., Canada. https://www.dieselnet.com/tech/fuel_biodiesel_std.php

Jeeva, B. and C.R. Rajashekar, 2018. Investigating the role of fatty acid methyl ester composition on engine performance and emission characteristics. Int. J. Veh. Struct. Syst. (IJVSS.), 10: 257-259.

Jose, T.K. and K. Anand, 2016. Effects of biodiesel composition on its long term storage stability. Fuel, 177: 190-196.

Joshi, R.M. and M.J. Pegg, 2007. Flow properties of biodiesel fuel blends at low temperatures. Fuel, 86: 143-151.

Kaisan, M.U., F.O. Anafi, J. Nuszkowski, D.M. Kulla and S. Umaru, 2017. Calorific value, flash point and cetane number of biodiesel from cotton, jatropha and neem binary and multi-blends with diesel. Biofuels, 8: 1-7.

Knothe, G., 2005. Dependence of biodiesel fuel properties on the structure of fatty acid alkyl esters. Fuel Process. Tech., 86: 1059-1070.

Knothe, G., J. Krahl and J.V. Gerpen, 2015. The Biodiesel Handbook. 2nd Edn., Elsevier, Amsterdam, Netherlands, ISBN: 9780983507260, Pages: 494.

Martinez, G., N. Sanchez, J.M. Encinar and J.F. Gonzalez, 2014. Fuel properties of biodiesel from vegetable oils and oil mixtures. Influence methyl esters distribution. Biomass Bioenergy, 63: 22-32.

Meng, X., M. Jia and T. Wang, 2014. Neural network prediction of biodiesel kinematic viscosity at 313 K. Fuel, 121: 133-140.

Mishra, S., K. Anand and P.S. Mehta, 2016. Predicting the cetane number of biodiesel fuels from their fatty acid methyl ester composition. Energy Fuels, 30: 10425-10434.

Mofijur, M., H.H. Masjuki, M.A. Kalam and A.E. Atabani, 2013. Evaluation of biodiesel blending, engine performance and emissions characteristics of Jatropha curcas methyl ester: Malaysian perspective. Energy, 55: 879-887.

Moradi-Kheibari, N., H. Ahmadzadeh, M.A. Murry, H.Y. Liang and M. Hosseini, 2019. Fatty Acid Profiling of Biofuels Produced From Microalgae, Vegetable Oil and Waste Vegetable Oil. In: Advances in Feedstock Conversion Technologies for Alternative Fuels and Bioproducts, Hosseini, M. (Ed.). Woodhead Publishing, Cambridge, England, UK., ISBN: 9780128179376, pp: 239-254.

Muralidharan, K., D. Vasudevan and K.N. Sheeba, 2011. Performance, emission and combustion characteristics of biodiesel fuelled variable compression ratio engine. Energy, 36: 5385-5393.

Piloto-Rodriguez, R., Y. Sanchez-Borroto, M. Lapuerta, L. Goyos-Perez and S. Verhelst, 2013. Prediction of the cetane number of biodiesel using artificial neural networks and multiple linear regression. Energy Convers. Manage., 65: 255-261.

Pratas, M.J., S.V.D. Freitas, M.B. Oliveira, S.C. Monteiro, A.S. Lima and J.A.P. Coutinho, 2011. Biodiesel density: Experimental measurements and prediction models. Energy Fuels, 25: 2333-2340.

Rakopoulos, C.D. and E.G. Giakoumis, 2009. Diesel Engine Transient Operation: Principles of Operation and Simulation Analysis. Springer Science & Business Media, London, ISBN: 978-1-84882-374-7, Pages: 390.

Ramadhas, A.S., S. Jayaraj, C. Muraleedharan and K. Padmakumari, 2006. Artificial neural networks used for the prediction of the cetane number of biodiesel. J. Renewable Energy, 31: 2524-2533.

Ramirez-Verduzco, L.F., J.E. Rodriguez-Rodriguez and A.D.R. Jaramillo-Jacob, 2012. Predicting cetane number, kinematic viscosity, density and higher heating value of biodiesel from its fatty acid methyl ester composition. Fuel, 91: 102-111.

Rashid, U., F. Anwar and G. Knothe, 2009. Evaluation of biodiesel obtained from cottonseed oil. Fuel Processing Technol., 90: 1157-1163.

Ruhul, M.A., M.J. Abedin, S.A. Rahman, B.H.H. Masjuki, A. Alabdulkarem, M.A. Kalam and I. Shancita, 2016. Impact of fatty acid composition and hysicochemical properties of Jatropha and Alexandrian laurel biodiesel blends: An analysis of performance and emission characteristics. J. Cleaner Prod., 133: 1181-1189.

Sajjadi, B., A.A.A. Raman and H. Arandiyan, 2016. A comprehensive review on properties of edible and non-edible vegetable oil-based biodiesel: Composition, specifications and prediction models. Renewable Sustainable Energy Rev., 63: 62-92.

Sakthivel, G. and M. Ilangkumaran, 2017. Optimisation of compression ignition engine performance with fishoil biodiesel using taguchi-fuzzy approach. Int. J. Ambient Energy, 38: 146-160.

Saldana, D.A., L. Starck, P. Mougin, B. Rousseau, N. Ferrando and B. Creton, 2012. Prediction of density and viscosity of biofuel compounds using machine learning methods. Energy Fuels, 26: 2416-2426.

Samavi, M., B. Ghobadian, M. Ardjmand and A. Seyfkordi, 2016. Prediction of biodiesel properties and its characterization using fatty acid profiles. Korean J. Chem. Eng., 33: 2042-2049.

Sanli, H., M. Canakci and E. Alptekin, 2014. Predicting the higher heating values of waste frying oils as potential biodiesel feedstock. Fuel, 115: 850-854.

Saxena, P., S. Jawale and M.H. Joshipura, 2013. A review on prediction of properties of biodiesel and blends of biodiesel. Procedia Eng., 51: 395-402.

Schiffer, H.W., 2016. World energy resources. World Energy Council, London, UK. https://www.worldenergy.org/assets/images/imported/2016/10/World-Energy-Resources-Full-report-2016.10.03.pdf

Statista, 2018. Global CO2 emissions share from fuel combustion by sector 2016. Statista, Hamburg, Germany.

Tong, D., C. Hu, K. Jiang and Y. Li, 2011. Cetane number prediction of biodiesel from the composition of the fatty acid methyl esters. J. Am. Oil Chem. Soc., 88: 415-423.

World Health Organization, 2006. Air Quality Guidelines-Global Update-2005. WHO, ISBN-13: 92-890-2192-6, pp: 484,.

Zaharin, M.S.M., N.R. Abdullah, G. Najafi, H. Sharudin and T. Yusaf, 2017. Effects of physicochemical properties of biodiesel fuel blends with alcohol on diesel engine performance and exhaust emissions: A review. Renewable Sustainable Energy Rev., 79: 475-493.

Zhang, Z., E. Jiaqiang, Y. Deng, M. Pham, W. Zuo, Q. Peng and Z. Yin, 2018. Effects of fatty acid methyl esters proportion on combustion and emission characteristics of a biodiesel fueled marine diesel engine. Energy Convers. Manage., 159: 244-253.

Zhu, L., Y.K. Nugroho, S.R. Shakeel, Z. Li, B. Martinkauppi and E. Hiltunen, 2017. Using microalgae to produce liquid transportation biodiesel: What is next?. Renewable Sustainable Energy Rev., 78: 391-400.