Renewable Energy 34 (2009) 1806–1811

Contents lists available at ScienceDirect

Renewable Energy

journal homepage: www.elsevier.com/locate/renene

Theoretical modeling of iodine value and saponification value of biodiesel fuels from their fatty acid composition

A. Gopinath, Sukumar Puhan*, G. Nagarajan

Internal Combustion Engineering Division, Department of Mechanical Engineering, Anna University, Chennai 600 025, Tamil Nadu, India

ARTICLE INFO

Article history:
Received 18 October 2007
Accepted 25 November 2008
Available online 4 January 2009

Keywords:
Biodiesel
Fatty acid composition
Iodine value
Saponification value
Regression model

ABSTRACT

Biodiesel is an alternative fuel consisting of alkyl esters of fatty acids from vegetable oils or animal fats. The properties of biodiesel depend on the type of vegetable oil used for the transesterification process. The objective of the present work is to theoretically predict the iodine value and the saponification value of different biodiesels from their fatty acid methyl ester composition. The fatty acid ester compositions and the above values of different biodiesels were taken from the available published data. A multiple linear regression model was developed to predict the iodine value and saponification value of different biodiesels. The predicted results showed that the prediction errors were less than 3.4% compared to the available published data. The predicted values were also verified by substituting in the available published model which was developed to predict the higher heating values of biodiesel fuels from their iodine value and the saponification value. The resulting heating values of biodiesels were then compared with the published heating values and reported.

1. Introduction

The use of biodiesel derived from vegetable oils or animal fats as a substitute for conventional petroleum fuel in diesel engines has received increased attention. For the combustion analysis of biodiesels, the chemical properties of the biodiesels are to be studied to a greater extent. The chemical properties of biodiesel fuels include chemical structure, iodine value (IV), saponification value (SV), heating value, peroxide value, etc. Therefore predicting biodiesel properties is the first and foremost stimulating task for the studies of biodiesel in diesel engines. In the present work the IV and the SV of ten biodiesels were predicted using their fatty acid methyl esters composition by the regression model and compared with the reported data.

The objective of this work is to predict the iodine value and the saponification value of any given biodiesel from their fatty acid ester composition, so that there may be no need for testing programmes to determine these properties.

2. Method

2.1. Fatty acid methyl ester composition for different biodiesels

Fatty acid methyl esters present in various biodiesel fuels used for predicting the IV and SV obtained from Ayhan Demirbas [1], Graboski and McCormick [2], Senthil Kumar et al. [3] and Ghadge and Raheman [4] are presented in Table 1.

2.2. Data for iodine value and saponification value for different biodiesels

IV and SV of ten biodiesel fuels obtained from Ayhan Demirbas [1], Graboski and McCormick [2], Senthil Kumar et al. [3] and Ghadge and Raheman [4] are presented in Table 2.

2.3. Correlation analysis

To evaluate the degree of linear association between the iodine value and FAMEs and between saponification value and FAMEs, correlation analysis was conducted and the Pearson coefficient of correlation between the properties (iodine value and saponification value) and FAMEs were found out as listed in Table 3.The scatter plot of iodine value vs FAMEs and of saponification vs FAMEs with fitted regression line are shown in Fig. 1 and Fig. 2, respectively.

2.3.1. Pearson product moment correlation coefficient (r)

It is the measure of degree of linear relationship between two variables. The correlation coefficient lies between −1 and +1. If one variable tends to increase as the other decreases, the correlation coefficient is negative. Conversely, if the two variables tend to increase together the correlation coefficient is positive [5].

* Corresponding author. Tel.: +91 9444489013.
E-mail addresses: gopinathmeice@yahoo.co.in (A. Gopinath), sp_anna2006@yahoo.co.in (S. Puhan), nagarajan@annauniv.edu (G. Nagarajan).

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doi:10.1016/j.renene.2008.11.023

Table 1
Fatty acid methyl esters in different biodiesels.

S.No.	Biodiesel	Fatty acid methyl esters, wt%						
		Palmitic 16:0	Stearic 18:0	Oleic 18:1	Linoleic 18:2	Linolenic 18:3	Erucic 22:1	Others
1	Ailanthus	31.0	0.0	8.1	51.1	7.3	0.0	2.0
2	Corn	11.8	2.0	24.8	61.3	0.0	0.0	0.0
3	Poppy seed	12.6	4.0	22.3	60.2	0.5	0.0	0.3
4	Rapeseed	3.5	0.9	64.1	22.3	8.2	0.0	0.0
5	Safflower seed	7.3	1.9	13.6	77.2	0.0	0.0	0.0
6	Soybean	13.9	2.1	23.2	56.2	4.3	0.0	0.0
7	Palm	43.6	4.5	40.5	10.1	0.2	0.1	0
8	Sunflower	6.0	5.9	16.0	71.4	0.6	0.0	0
9	Mahua	24.2	25.8	37.2	12.8	0	0	0
10	Jatropha	14.9	9.5	40.5	34.7	0.3	0	0.1

Table 2
Iodine value and saponification value for different biodiesels.

S.No.	Biodiesel	Iodine value (g iodine/100 g oil)	Saponification value (mg KOH/g oil)
1	Ailanthus	107.18	206.34
2	Corn	119.41	194.14
3	Poppy seed	116.83	196.82
4	Rapeseed	108.05	197.07
5	Safflower seed	139.83	190.23
6	Soybean	120.52	194.61
7	Palm	59	205
8	Sunflower	136	193
9	Mahua	80	187
10	Jatropha	105	198.85

$$r = \frac{S(X-\overline{X})(Y-\overline{Y})}{(X-\overline{X})^2(Y-\overline{Y})^2}$$ where X and Y are the two variables.

From the correlation analysis (Table 3), it can be observed that the palmitic and stearic fatty acids has a low degree of negative correlation with iodine value and the oleic acid has a high degree of negative correlation with iodine value. The linoleic acid has a high degree of positive correlation and the linolenic acid has a moderate degree of positive correlation with the iodine value. Fig. 1 shows the scatter plot of iodine value and FAMEs with the fitted regression line. On the other hand, the correlation analysis between the saponification value and FAMEs shows that stearic fatty acid is moderately positively correlated with the saponification value. The oleic acid is highly positively correlated and the linoleic acid is highly negatively correlated with the saponification value. Fig. 2 shows the scatter plot of saponification value and FAMEs with the fitted regression line.

Table 3
Pearson product moment correlation coefficient (r) between "iodine value vs FAMEs" and "saponification value vs FAMEs".

S.No.	FAMEs	Pearson product moment correlation coefficient (r)	
		Iodine value vs FAME	Saponification value vs FAME
1.	Palmitic	−0.126	0.202
2.	Stearic	−0.232	0.401
3.	Oleic	−0.827	0.887
4.	Linoleic	0.884	−0.893
5.	Linolenic	0.413	−0.363

2.4. Regression model

After evaluating the Pearson correlation coefficient, two regression models as given by Eqs. (1) and (2) were developed to predict the iodine value and the saponification value of biodiesels.

$$\text{Iodine value (IV)} = 35.9 - (0.212 \times \text{P}) + (0.660 \times \text{S}) + (0.448 \times \text{O}) + (1.23 \times \text{L}) + (1.73 \times \text{LL}) \quad (1)$$

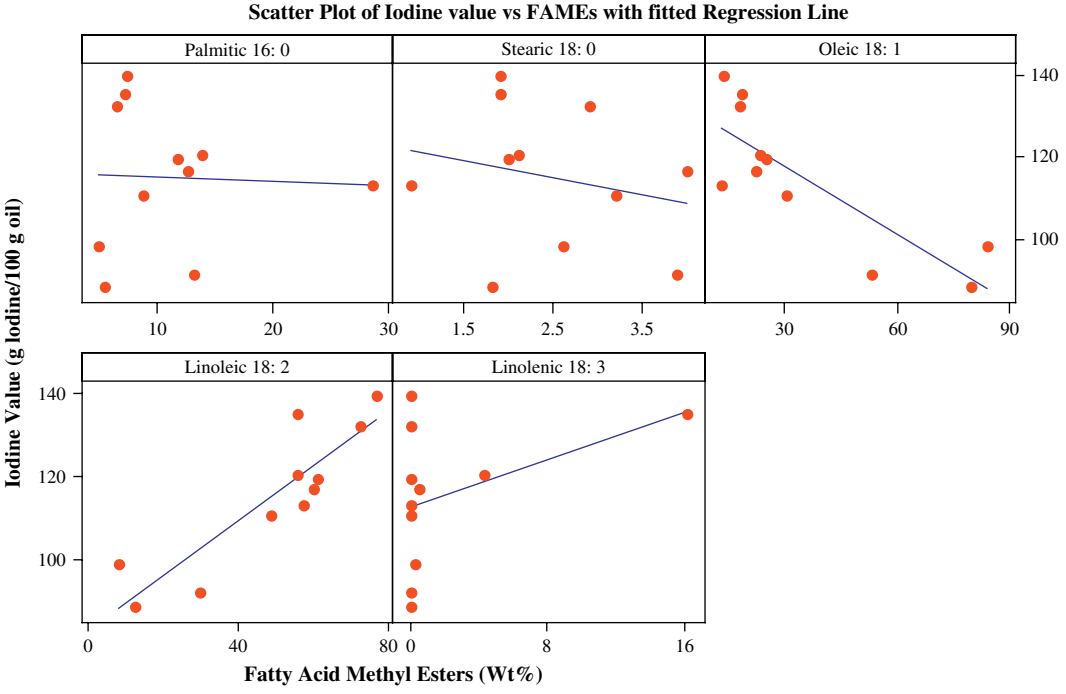

Fig. 1. Scatter plot of iodine value vs FAMEs with fitted regression line.