Korean J. Chem. Eng., 33(7), 2042-2049 (2016)
DOI: 10.1007/s11814-016-0057-y

pISSN: 0256-1115
eISSN: 1975-7220

Prediction of biodiesel properties and its characterization using fatty acid profiles

Mahdieh Samavi*, Barat Ghobadian, Mehdi Ardjmand***,†, and Aliakbar Seyfkordi***

*Department of Chemical Engineering, Islamic Azad University, Science and Research Branch, Tehran, Iran
**Department of Biosystem Engineering, Tarbiat Modares University, Tehran, Iran
***Department of Chemical Engineering, Islamic Azad University, South Tehran Branch, Tehran, Iran
(*Received 6 August 2015 • accepted 22 February 2016*)

Abstract−Biodiesel, the mono-alkyl esters of vegetable oils or animal fats, is an eco-friendly alternative to petrodiesel. The molecular structures of biodiesels, fatty acid methyl esters were applied to predict the characteristics of biodiesel fuels. Based on the structural similarity of biodiesel and petroleum fractions, molecular weight of biodiesel was correlated with other characteristics including boiling point, viscosity and specific-gravity in the form of three equations. For 24 different kinds of biodiesel, the minimum average relative deviation (ARD) of these correlations was calculated to be 0.68%. Moreover, two correlations were developed to predict viscosity and flash point of biodiesel as a function of weighted-average number of carbon atoms (N_C) and weighted-average number of double bonds (N_{DB}) with ARD 3.72% and 4.24% respectively. Also, a high degree of correlation was shown by the logarithmic function with ARD 0.30% between specific gravity and viscosity of biodiesel. Proposed predictive models were verified by experimental data.

Keywords: Biodiesel, Characterization, Prediction, Biodiesel Property, Fatty Acid Profile

INTRODUCTION

Biodiesel is a mixture of alkyl esters of fatty acids, generally produced by the transesterification of vegetable oils or animal fats with short chain alcohols, such as methanol and ethanol. Commercial availability of biodiesel in many parts of the world shows the increasing research and investment on this fuel. This is the result of the competitive advantages of biodiesel fuels including bio-degradability, non-toxicity, renewability, carbon neutrality and having fewer engine exhaust emissions [1]. The availability of a reliable and accurate data set of fuel properties serves an important role in the simulation process and design of biodiesel. In many cases it is very difficult to provide experimental data, hence the importance of predictive methods in determining characterizations of the biodiesel [2]. The properties of biodiesel as a fuel are strongly defined by the molecular structure of its constituent species (saturated, unsaturated and hydroxylated fatty acid alkyl esters). Biodiesel fuels from different sources can have significantly varying fatty acid (FA) profiles and properties. This variation can be explained by investigating the biodiesel FA profiles [3]. Viscosity and flash point are important fuel properties. Viscosity affects the fuel quality. The first step of combustion, atomization, is substantially controlled by fuel viscosity. Higher viscosity leads to poorer fuel combustion [4].

Different methods have been applied to predict the viscosity of biodiesel. Allen et al. used the Grunberg-Nissan equation to predict the viscosity of biodiesel. They assumed the biodiesel components, fatty acid methyl esters (FAME), act like an ideal solution. Therefore, they neglected the interaction term in the equation [5]. Numerous correlations based on temperature have been reported to predict the viscosity of biodiesel. One of these correlations was presented by Ceriani et al. [6], who developed a group contribution model as a function of temperature and chemical compound formula. Later, Ceriani modified the coefficients and some terms of the reported model [7]. Chang and Liu established a linear correlation to predict the viscosity of FAME by regression on viscosity of pure FAME [8]. Su and coworkers proposed two correlations to predict viscosity and flash point of biodiesel based on weighted-average number of carbon atoms (N_c) and weighted-average number of double bonds (N_{DB}) [9]. In another investigation, empirical equations were developed to estimate four physical properties of pure methyl esters including cetane number, viscosity and higher heating value [10]. Recently, related studies using artificial neural network models have been reported in the literature. Meng et al. obtained a correlation coefficient of 0.9772 on the prediction of biodiesel viscosity [11]. In another study, models of artificial neural networks were developed to predict the density, dynamic viscosity, and cetane number of biodiesel from the composition of methyl esters and temperature [12].

Flash point is another key property of biodiesels and is practically important in safety considerations, which are highlighted for handling and transportation of fuels [3]. Different methods have been proposed in the literature to predict the flash point. Zhokhova et al. presented quantitative structure-property relationship (QSPR) methods to predict flash point [13]. A group contribution method has been proposed to predict the flash point of organic compounds by Stefani et al. [14]. Also, a correlation between flash point and boiling point has been suggested in another work [15].

On one hand, the proposed predictive methods in the literature have mainly focused on estimating the properties of pure FAME [16]. There is a paucity of work estimating characterizations of biodiesel based on FA profile. On the other hand, knowing the FA profile of biodiesel is of great importance since it controls its key

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†To whom correspondence should be addressed.
E-mail: m_arjmand@azad.ac.ir

properties. Also, the FA profile is essential both in production and evaluation of the produced biodiesels. Therefore, it can be considered as the practical tool to predict biodiesel properties. In other words, it would be possible to estimate biodiesel characteristics, which could avoid experimental work that is costly and time consuming.

This study was conducted to present new correlations to predict properties of biodiesels based on the FA content, the basic molecular structure of biodiesel. Moreover, the relationships between characteristics of biodiesel like molecular weight, boiling point, viscosity and specific gravity were investigated.

In the experimental part, biodiesels from various raw materials including vegetable oil, animal fats and waste cooking oil are produced and their FA profiles are analyzed. Viscosity, density and flash point of produced biodiesels are measured as well. Data is applied to verify the proposed predictive models.

MATERIALS AND METHODS

1. Material

Methanol 99.7%, potassium hydroxide 99% (Merck Company) were used for the synthesis procedure and n-heptane 95%, nonadecanoate (C19) were used as a solvent and internal standard for GC analysis, respectively. Sunflower, soybean, rapeseed and olive oil (Oila Company) were purchased from a local supermarket in Tehran (the capital of Iran, at 35°412 463 N latitude and N 51°252 233 E longitude). Chicken fat and tallow were supplied from a local butcher shop and waste cooking oil from a local restaurant in Tehran.

2. Biodiesel Production

Feedstocks containing high free fatty acid (FFA) cause foaming during transesterification. The FFA level of the feedstock should be reduced to less than 1% before using an alkaline catalyst [17]. Since the free fatty acid level of tallow and waste cooking oil was calculated to be 6.43% and 1.85%, the reduction of FFA to less than 1% was carried out using methanol and sulfuric acid as catalyst. The pre-esterification stage conditions were: 0.5 weight percentage (wt%) H_2SO_4, 6 : 1 methanol/fats molar ratio, at 65 °C and 4 hours as described by Encinar et al. [18].

The most preferred alcohol used in biodiesel production is methanol because of its low price, physical and chemical advantages [19]. Therefore, in the transesterification reaction methanol and KOH were selected as desired alcohol and catalyst, respectively. 6 : 1 molar ratio of alcohol/oil was utilized and the catalyst was equal to one weight percent (1% wt) of oil. The reaction took place using ultrasound instrument, UP400S (Hielscher Co., Germany) with 400 watt power for seven minutes.

In the next step, the final solution was poured into the separator and cooled overnight. The glycerol formed through the reaction gathered at the bottom, because it has a higher density. Then glycerol was separated from the top phase. Water washing removed the remaining glycerol and soap from the biodiesel using warm water (40-50 °C) three times. Finally, biodiesels were inserted in the oven and heated to 70-90 °C for approximately 5-6 hours through which the remaining water was removed.

3. Analysis of Biodiesel Properties

Density and viscosity were measured at 40 °C using a Stanbinger viscometer, model SVM3000 (Anton Paar Company, Austria) under ASTM D445 and ASTM D7042-04 standard.

Flash points were measured by a closed-up analyzer, model Mini Flash FLPH (Grabner Company, Austria), under ASTM D93 standard.

4. Analysis of Biodiesel Fatty Acid Profile

Gas chromatography (GC) set, Perkin Elmer Clarus-580 based on BS-EN 14103 standard with biodiesel column CP90 (0.25 μm×0.23 mm×30 mm) and FID as a detector was used to determine biodiesel FA profile.

RESULTS AND DISCUSSION

1. Boiling Point

The boiling point of a pure compound at a given pressure is the temperature at which vapor and liquid exist together at equilibrium. The normal boiling point (the boiling point at 1 atm) is one of the major physicochemical properties that characterizes the physical state and volatility of compound [20]. Moreover, the normal boiling point is a key parameter for the prediction of critical properties including critical temperature (Tc), critical pressure (Pc), critical volume (Vc), and other properties such as vapor pressure, density, latent heat of vaporization and viscosity. That is significant for providing predictive models as well as simulation of a system's behavior [21]. There are different methods to estimate the boiling point. Three of them are discussed below.

1-1. Group Contribution

Group contribution is one of the estimation methods requiring only the molecular structure as input. It is based on the fact that the values of properties are the sum of the contributions of individual constitutions [22].

The Joback and Reid method, Eq. (1), is an extension of the Lydersen method, one of the most traditional group contribution methods. In the Joback correlation ΔT_b is calculated according to contributions of methyl, alkyl and ester groups in the molecular structure. Constantinou and Gani developed an advanced group contribution method, Eq. (2), based on the UNIQUAC[1] functional-group activity coefficient (UNIFAC) groups that first-order groups are shown by k and second-order groups by j. The numbers of first- and second-order groups are introduced by N and M, respectively. W is zero for first-order and one for second-order groups [22].

$$T_b = 198 + \Delta T_b \tag{1}$$

$$T_b = 204.359\ln\left[\sum_k N_k(T_{b1k}) + W\sum_j M_j(T_{b2j})\right] \tag{2}$$

1-2. Yuan Correlation

An analysis of the boiling point of aliphatic hydrocarbons in the petroleum based diesel industry showed that the normal boiling points of unbranched alkanes were logarithmically correlated to the carbon number [23]. Based on the trends from unbranched alkanes Yuan et al. [23] established Eq. (3) to estimate normal boiling point (°K) of FAMEs:

$$T_b = 218.49\ \ln(\mathrm{CN}) - 6.933 \tag{3}$$

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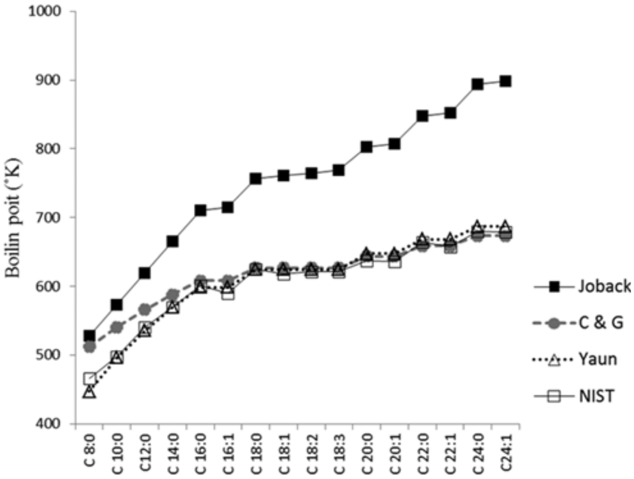

Fig. 1. Comparison of estimated and experimental data through correlations for calculating normal boiling point.

where CN is the number of carbons in the FA. They obtained correlation (3) from the data of C10-C18 and it was applied up to C24. It was reported that the correlation had an R^2 of 0.9996, and the maximum prediction error was less than 1.5 °K.

A comparison of estimated and experimental normal boiling points using these correlations is shown in Fig. 1.

Fig. 1. shows that the Constantinou and Gani method provides better prediction of boiling point compared to the Joback method for methyl esters. The Joback correlation considers the contribution of functional groups like CH_3 and CH_2. The Constantinou and Gani correlation considers the combined effect of different functional groups, as well as elements such as C, H and O present in the methyl esters. Note that the Constantinou and Gani method overestimates the boiling point of short chain fatty acids. Although the Yuan correlation does not distinguish between saturated and unsaturated fatty acids, it makes a closer prediction compared with the other two methods.

1-3. Mixing Rule

Biodiesel is a mixture of fatty acid methyl esters (FAME). The structures of different FAMEs are very similar and it can be assumed that the components in biodiesel interact with each other as an ideal solution [5]. Therefore, the mixing rule, Eq. (4), can be applied for such a system [24]. In the current study, boiling point and molecular weight are calculated through mixing rule:

$$M=\sum_i x_i M_i \tag{4}$$

where M is the biodiesel property. X_i and M_i are mole fraction and property of the i^{th} FAME, respectively. The average relative deviation (ARD) was applied to verify the predictive models which can be calculated according to Eq. (5), where N is the number of experimental data points, $X_{exp,\,i}$ is experimental data and $X_{prd,\,i}$ is the calculated properties of data point i.

$$\mathrm{ARD}=\frac{\Sigma_i^N \frac{\Sigma_i^n |x_{exp,\,i}-x_{prd,\,i}|}{X_{exp,\,i}}}{N}\times 100 \tag{5}$$

2. Molecular Weight

Molecular weight or molar mass shown by M is defined as 1 mol of any substance which has equivalent mass of M g. In the SI system the units of M are Kg/Kmol. Riazi and Daubert [20] presented a simple equation to predict physical properties of pure and mixtures of hydrocarbons, Eq. (6). Later, they improved the accuracy of the proposed equation by adding new terms to Eq. (6) and developed Eq. (7):

$$\theta=a\,\theta_1^b\theta_2^c \tag{6}$$

$$\theta=a\,\theta_1^b\theta_2^c\exp\,(d\theta_1+e\theta_2+f\theta_1\theta_2) \tag{7}$$

In the above equations θ is any physical property. θ_1 and θ_2 are

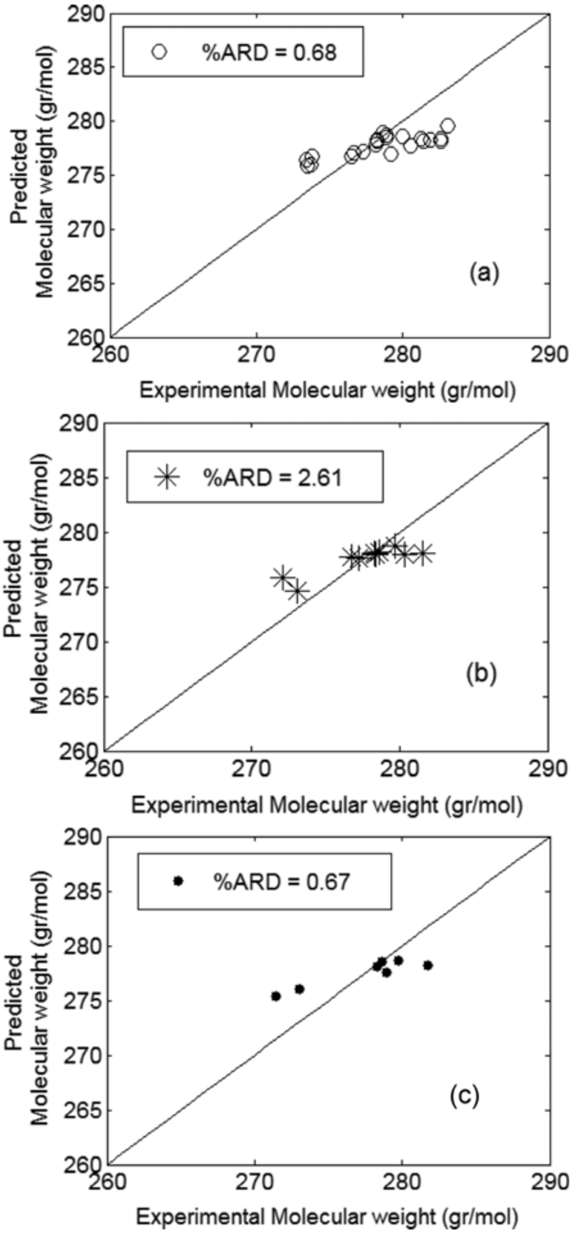

Fig. 2. Molecular weight of biodiesel obtained experimentally and calculated by Eq. (8) using experimental data of (a) reference [25] (b) reference [4] (c) this work.

two parameters which can describe the intermolecular interactions such as boiling point or molecular size like specific gravity. a, b, … and f are coefficients obtained by means of experimental data.

Various correlations based on the Daubert-Riazi equations were presented in which molecular weight is correlated with boiling point, specific gravity and viscosity of petroleum fractions [20].

Taking into account the structural similarity between the hydrogen-carbon chain of FAME and the unbranched alkanes in petroleum fractions [23], we set the Daubert-Riazi equations as a template for biodiesel fuels. In the present study, based on the regression of the Daubert-Riazi equations on the biodiesel data the coefficients were modified and the following correlations are developed:

$$MW=2.3347\ (BP^{0.747})(Vis^{-0.0137}) \tag{8}$$

$$MW=327.321\ (Sp\_Gr^{1.7815})(Vis^{0.0409}) \tag{9}$$

$$MW=0.6306\ (BP^{1.2023})(Sp\_Gr^{2.9154})\exp(-0.0023Sp\_Gr\times BP) \tag{10}$$

where MW, BP, Vis, Sp-Gr are molecular weight (gr/mol), BP (°K), viscosity (cSt) and specific gravity of biodiesel, respectively. The evaluation of Eq. (8), Eq. (9) and Eq. (10) is shown in Fig. 2, Fig. 3 and Fig. 4. Both references [4] and [25] have investigated average compositional profiles of different samples for a particular bio-

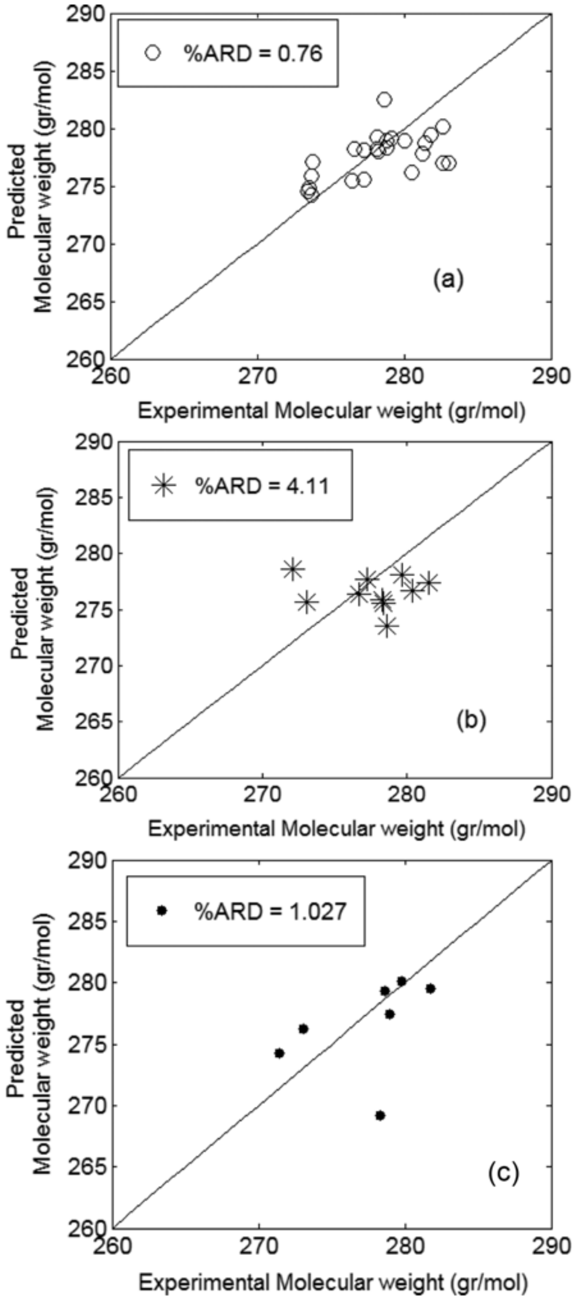

Fig. 3. Molecular weight of biodiesel obtained experimentally and calculated by Eq. (9) using experimental data of (a) reference [25] (b) reference [4] (c) this work.

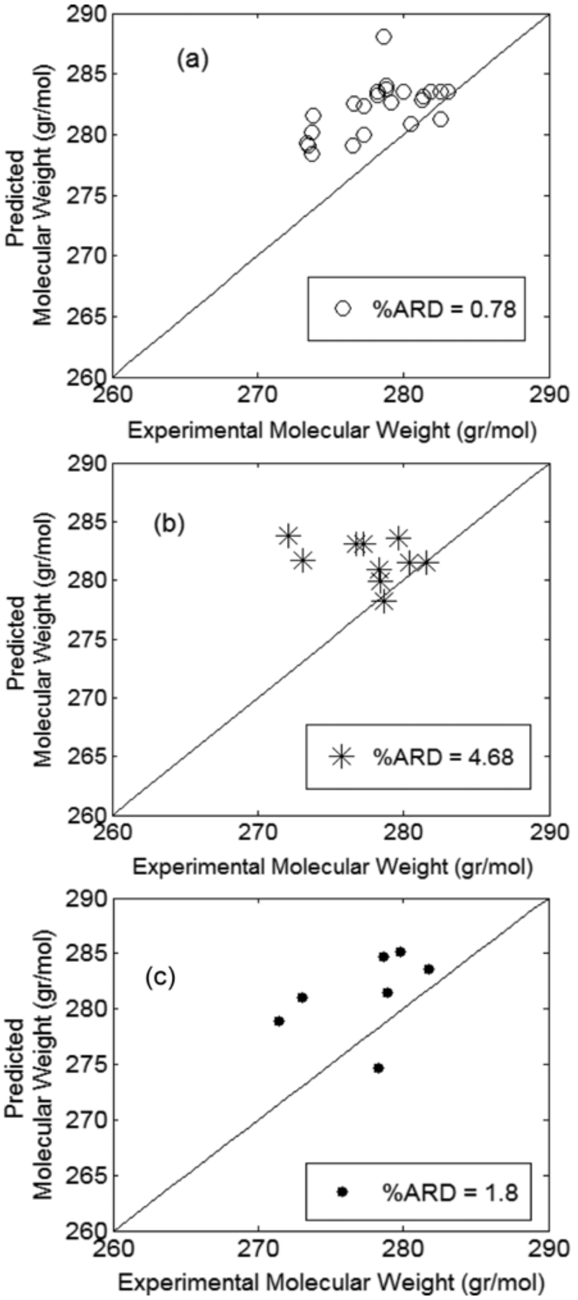

Fig. 4. Molecular weight of biodiesel obtained experimentally and calculated by Eq. (10) using experimental data of (a) reference [25] (b) reference [4] (c) this work.

Table 1. Fatty acid weight (mass) percentage of biodiesels produced in this work

Biodiesel	C14:0	C14:1	C16:0	C16:1	C18:0	C18:1	C18:2	C18:3	C20:0	C22:0	C24:0
Sunflower			6.68		3.44	29.92	58.39	0.68	0.24		
Soybean			9.73		3.68	20.4	56.12	9.09	0.29	0.28	
Rapeseed			3.92	0.12	2.01	65.13	18.67	6.81	0.64	0.3	
Olive			13.44	0.96	2.52	68.38	12.75	0.67	0.39		0.63
Chicken	0.35	0.1	25.42	6.29	6.47	47.17	12.78	0.52	0.26		
Tallow	2.17	0.91	21.98	3.29	13.72	40.76	2.9	0.52	0.49	0.49	
Waste oil	0.1		21		3.7	32.05	33.38	2.2	0.22	2.25	4.22

diesel reported in the literature. Biodiesel is dependent on FA composition, which consists primarily of C16:0, C18:0, C18:1 and C18:2 to meet ASTM D6751 standard criteria (Table 1). Biodiesel from sunflower, rapeseed, soybean, tallow and waste cooking oil is common in references [4,25] and this study. Biodiesel from olive oil and chicken fat is only studied in this study and reference [25]. The growing condition and locations cause variation in the compositions. Such variation in the compositional profiles is most likely due to the different analytical methods and skill levels in applying these methods. There are only few studies available in the literature that investigated the effect of growth condition (temperature, water and ...) on the FA profile of fats and oils [4]. One study with controlled experiment showed that the profile did not change noticeably with growth conditions [26]. Therefore, it is generally assumed that FA compositional profile remain unchanged through different conditions under which transesterification was carried out.

3. Viscosity

Viscosity at 40 °C is an important characteristic of biodiesel fuels [4]. A model that could make a good prediction of biodiesel viscosity based on its composition would be useful in the optimization of biodiesel production processes. Several methodologies have been used for prediction of biodiesel viscosity; Chang and Liu [8] developed Eq. (11) based on the fact that viscosity of a FAME is proportional to its number of carbon atoms and inversely proportional to its number of double bonds. Therefore, they proposed a linear correlation for viscosity of each FAME independently. They reported 3.51% ARD for 20 experimental data points.

$$\eta=0.235\,N_C-0.699N_{DB}-3.648 \tag{11}$$

The simplicity of the Chang and Liu method facilitates the modification of model parameters with new experimental data. Thus, Su et al. [9] refined the parameters of Eq. (11) with new experimental data for biodiesel viscosity instead of pure FAMEs and improved the accuracy of the prediction. The proposed equation, Eq. (12), is as follows:

$$\eta=0.235\,N_C-0.468\,N_{DB} \tag{12}$$

Here new terms are added to the Su model with the same parameters and the coefficients are modified. Correlation (13) is as follows:

$$V=39.9-5.77N_C+0.217N_C^2+22.7N_{DB}-1.334N_CN_{DB} \tag{13}$$

where V is viscosity in cSt. %ARD for biodiesels from 24 different raw materials is 4.24. Fig. 5 shows the verification of Eq. (13) by experimental data of present study (Table 2) as well as references

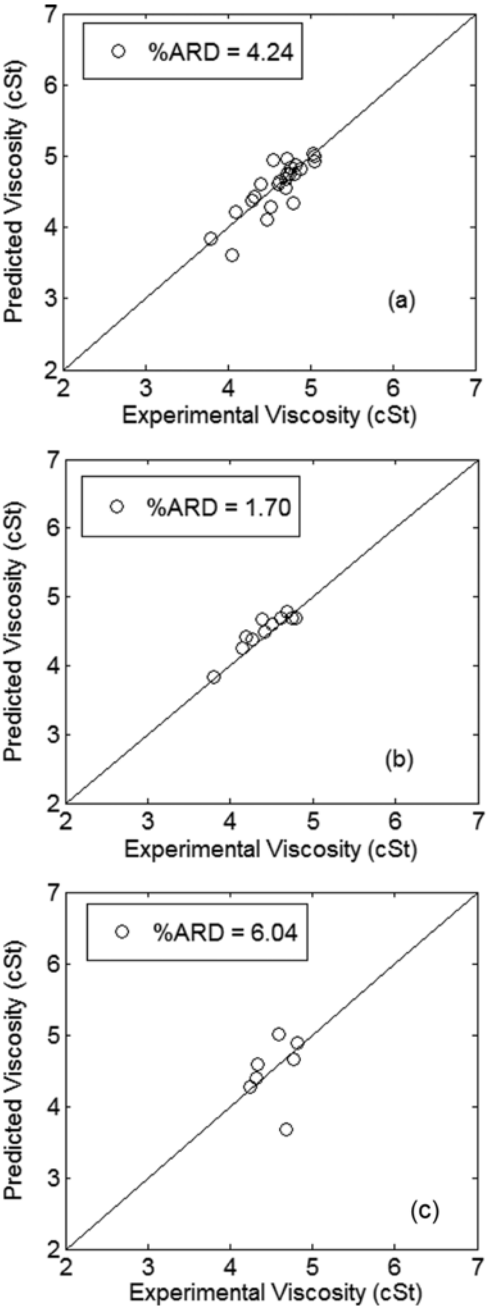

Fig. 5. Viscosity of biodiesel obtained experimentally and predicted by the method of this study (Eq. (13)) using experimental data of (a) reference [25] (b) reference [4] (c) this work.

Table 2. Experimental viscosity, density and flash point of biodiesels in this study

	Viscosity (cSt)	Density (kg/m^3) @ 40 °C	Flash point (°C)
Sunflower	4.31	886	171.3
Soybean	4.24	885	174.2
Rapeseed	4.77	883	179.1
Olive	4.81	879	173.3
Waste cooking oil	4.34	866	172.1
Chicken fat	4.58	878	169.9
Tallow	4.68	874	168.5

[4,25].

4. Flash Point

The flash point of a liquid is the lowest temperature at which the application of an ignition source causes vapor and air above the surface of the liquid to ignite. Flash point is measured to evaluate the explosion hazards of liquids. The development of reliable predictive methods for estimating flash points would significantly reduce the amount of experimental data required for a complete flammability characterization in biofuels [3]. Some techniques for estimation of flash point are discussed below.

4-1. Prediction of Flash Point Based on the Number of Carbon Atoms and Double Bonds

As pointed out previously, Su et al. [9] reported a correlation to predict the viscosity of biodiesel as a function of chain length (N_C) and unsaturation (N_{DB}). They investigated whether this basis also works for flash point. They correlated the biodiesel flash point with these two parameters and presented Eq. (14):

$$FP=23.362N_C+4.854N_{DB} \tag{14}$$

In this study, coefficients of the Su model are regressed with experimental data to present a more accurate correlation to predict the flash point of biodiesel. Also, new terms were added:

$$FP=284.1+3.861N_C-0.5154N_C^2-\frac{37.02}{N_{DB}}+\frac{2.372}{N_{DB}^2} \tag{15}$$

where FP is the flash point of biodiesel in °C. %ARD of Eq. (15) for 24 different kinds of biodiesels is 3.72. The evaluation of the proposed model is shown in Fig. 6.

Predictive models for viscosity and flash point of biodiesel presented in this study are compared with the Su models which were developed based on the soybean methyl ester [16]. However, in the current study biodiesels from 24 different kinds of feedstock are considered to present the correlations. The obtained results (% ARD values) indicate a higher degree of correlation in comparison with the Su study (Table 3).

5. Relationship between Viscosity and Density

Fuel density is a key property that affects engine performance. Since fuel injection pumps meter fuel by volume, not by mass, a greater or lesser mass of fuel is injected, depending on its density. Generally, densities of biodiesel fuels are higher than petroleum diesel. In many cases, it is preferable to use a dimensionless term, specific gravity [4].

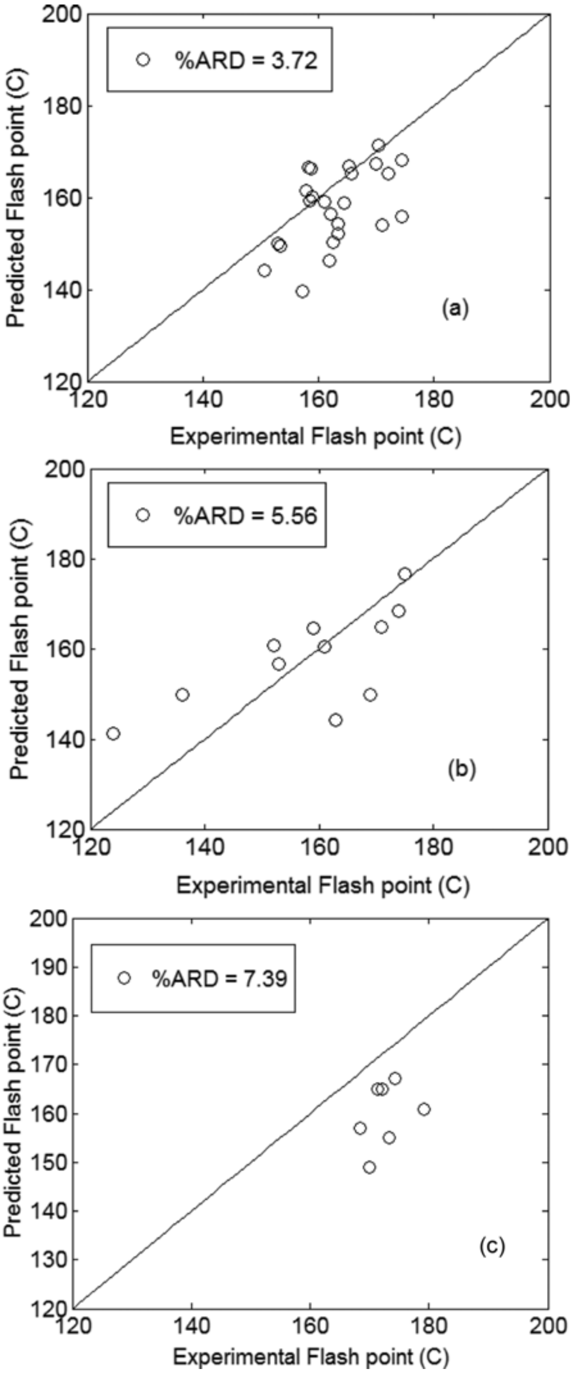

Fig. 6. Flash point of biodiesel obtained experimentally and predicted by the method of this study (Eq. (15)) using experimental data of (a) reference [25] (b) reference [4] (c) this work.

One of the parameters defined for petroleum characterization is the viscosity-gravity constant (VGC). This parameter is defined based on an empirical relationship developed between Saybolt viscosity (SUS) and specific gravity through a constant VGC and can be calculated as follows [20]:

$$VGC=\frac{10S-1.0752\log(V-38)}{10-\log(V-38)} \tag{16}$$

Table 3. Comparison of correlations to predict the viscosity and flash point of biodiesel

Model	Viscosity		Flash point	
	Equation	%ARD	Equation	%ARD
Su	η=0.235N_C−0.468 N_{DB}	21.8[a] 18.2[b] 21.1[c]	FP=23.362N_C+4.854N_{DB}	159.2[a] 132.2[b] 171.6[c]
This study	$V=39.9-5.77N_C+0.217N_C^2+22.7N_{DB}-1.334N_CN_{DB}$	4.2[a] 1.7[b] 6.0[c]	$FP=284.1+3.861N_C-0.5154N_C^2-\frac{37.02}{N_{DB}}+\frac{2.372}{N_{DB}^2}$	3.7[a] 5.5[b] 9.7[c]

[a] Experimental data of reference [25]
[b] Experimental data of reference [4]
[c] Experimental data of this study

where S stands for specific gravity (60 °F/60 °F) and V is Saybolt viscosity.

Based on the similarity between structure of some petroleum fractions and biodiesel (mixture of FAMEs), Eq. (16) was used to establish a new relationship specifically for biodiesel in which the specific gravity of biodiesels was logarithmically correlated to its viscosity. The coefficients are regressed with 24 different kinds of biodiesel.

$$\text{Sp-Gr}=0.8989-0.178\ln(\text{Vis}-1.765) \qquad (17)$$

where Sp-Gr and Vis are specific gravity (15 °C/15 °C) and viscosity in cSt (mm^2/s), respectively. A comparison of predicted and experimental data using Eq. (17) is shown in Fig. 7.

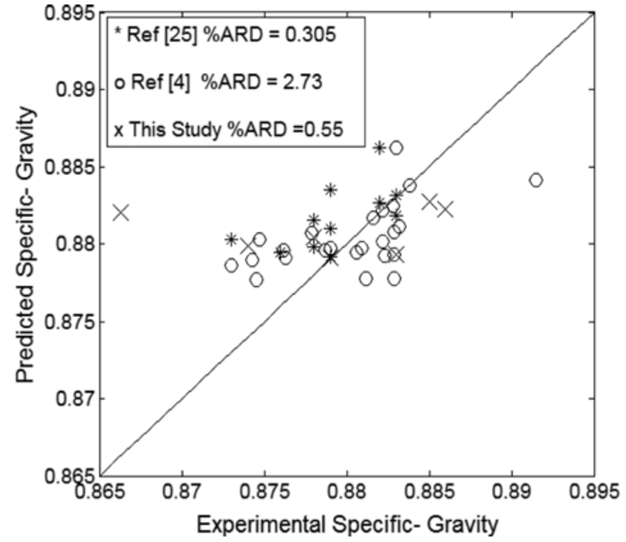

Fig. 7. Specific gravity of biodiesel obtained experimentally and predicted by the method of this study experimental data of reference [25], reference [4] and this work.

CONCLUSION

1. The compositional structure of biodiesel is similar to petroleum fractions. Considering the reported correlations of some petroleum fractions as a template, three correlations were presented to calculate biodiesel molecular weight. The first one is a function of boiling point and viscosity; the second one is a function of specific-gravity and viscosity; and the third one is a function of boiling point and specific-gravity. For 24 different kinds of biodiesel ARD of these correlations were calculated to be 0.68, 0.76 and 0.78%, respectively.

2. Based on the weighted-average number of carbon atoms (N_C) and weighted-average number of double bonds (N_{DB}), two correlations were developed to predict biodiesel flash point with ARD 3.72% and biodiesel viscosity with ARD 4.24%.

Specific gravity of biodiesel, a dimensionless form of density, was correlated with viscosity of biodiesel by a logarithmic function. ARD 0.30% was obtained for biodiesels of 24 different raw materials.

NOMENCLATURE

ARD	: average relative deviation
ASTM	: american standard test method
C & G	: constantinou and gani
FA	: fatty acid
FAME	: fatty acid methyl esters
FP	: flash point [°C]
MW	: molecular weight [gr/mol]
N_C	: weighted-average number of carbon atoms
NIST	: national institute of science and technology
N_{DB}	: weighted-average number of double bonds
P_c	: critical pressure
Sp-Gr	: specific gravity
T_b	: boiling point [°K]
T_c	: critical temperature
VGC	: viscosity gravity constant
Vis	: viscosity [cSt]
V_c	: critical volume

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