Estimation of Biodiesel Cetane Number, Density, Kinematic Viscosity and Heating Values from its Fatty Acid Weight Composition

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ABSTRACT

A detailed statistical investigation is conducted in order to correlate some important biodiesel properties with the respective methyl ester weight composition in fatty acids. The examined properties are cetane number, density, kinematic viscosity and heating values (lower and higher). The chosen method for the correlation is the multiple linear regression analysis. A comprehensive data set was chosen for each interesting property as the basis for the formulation of the linear relations with respect to the eight, most important, fatty acids (lauric, myristic, palmitic, stearic, palmitoleic, oleic, linoleic, linolenic). The derived correlations were then verified against other experimental data, selected from various sources, with the aim to assess their predictive capability. It was found that for both the cetane number and density, the derived correlations were, on the one hand highly statistical, and, on the other, proved successful in predicting the corresponding properties from randomly selected samples reported in the literature. On the contrary, for both

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heating values and kinematic viscosity, the statistical correlations were weaker, although for the HHV the relative error between experimental and predicted values was adequately small.

Keywords: Biodiesel; Fatty acid composition; Cetane number; Density; Heating value; Kinematic viscosity; Multiple linear regression

1. Introduction

An extensive research has been carried out in the last decades regarding the use of biodiesel in engines. This is not surprising since methyl esters produced from agricultural or animal products succeed in reducing the dependence on oil imports, while at the same time they enhance the local economy and energy security, and manifest a positive CO_2 balance [1–6]. Furthermore, when burned in compression ignition engines, the combustion of biodiesel usually produces lower carbonaceous pollutant emissions [3,5].

One peculiar aspect of biodiesels (and their originating vegetable oils) is the fact that they are produced from a variety of feedstocks possessing different chemical composition. Since the structure of each oil/fat in fatty acids varies (sometimes by a lot) depending on its origin, the physical and chemical properties of biodiesel differ too; prominent examples here are the cetane number and the cold-flow properties [1–5]. Thus, the combustion characteristics and emissions from engines vary, sometimes by a lot, depending on the exact biodiesel used [3,5].

A logical question arises here, as to which feedstock possesses the ‘best’ composition, or, better still, what would be a superior fatty acid (FA) composition, with the ultimate goal to achieve ‘better’ engine performance and lower emissions. Many researchers have investigated such issues in the past [7–11], and it seems that a

reasonable step is to try and correlate biodiesel properties with specific oil attributes such as fatty acid composition, chain length, molecular weight, degree of unsaturation or number of double bonds [e.g. 12–22]. For example, Bamgboye and Hansen [12] reported one such correlation with respect to the FA composition for cetane number (CN) applying linear regression analysis. Piloto-Rodriguez et al. [13] focused on cetane number too applying both multiple linear regression (MLR) and artificial neural networks (ANN). The latter approach was the one followed by Ramadhas et al. [14], while the former (MLR) was chosen by Gopinath et al. [15]. Apart from CN, existing reports on other properties have correlated, for example, density with temperature [18]; density, viscosity, CN and higher heating value were inter-related with molecular weight and number of double bonds by Ramirez-Verduzco et al. [19]. Ramos et al. [20] correlated oxidation stability, cetane number, iodine value and cold filter plugging point with the methyl ester degree of unsaturation and long chain saturated factor. Lastly, a quadratic correlation with the number of carbon atoms in the original fatty acid and the number of double bonds was statistically selected as the most suitable by Lapuerta et al. [22], again for cetane number.

The research group involving the first author has studied broadly the use of biodiesels in engines, under both steady-state [23] and transient conditions [5,24]. Moreover, two extensive statistical analyses have been conducted, aiming to identify and analyze the effects of the biodiesel originating feedstocks on engine emissions [25], and on the properties of the fuel [26]. For the current work, which is, in a sense, continuation of [26], the focus is again on the biodiesel properties, but now aiming to formulate *predictive correlations with respect to the fatty acid weight composition applying multiple linear regression techniques.*

The target is to expand on previous analyses on the subject [12,13,15] as regards: a) the sample of oils/biodiesel feedstocks taken under consideration, b) the predictive

capability of the obtained correlations and c) the number of investigated properties. With respect to the latter, the usually investigated property is cetane number. In this work, we also focus on density, kinematic viscosity and heating values (lower and higher).

2. Methodology

In order to proceed to the formulation of a reliable correlation between biodiesel properties and the respective fatty acid weight composition, the first step was the selection of an appropriately large and representative sample of reported (experimental) values from the literature. It was our intention to use a broad sample so as to include a great variety of published data from many sources and feedstocks, including also neat fatty acids. Particularly in regard to the fatty acids chosen for the correlation, these were the major four saturated, i.e. lauric, myristic, palmitic and stearic, and the major four unsaturated, namely, palmitoleic, oleic, linoleic and linolenic. The regression equation chosen for the multiple linear regression analysis is of the form:

$$\text{Property} = A + a_1x_1 + a_2x_2 + a_3x_3 + a_4x_4 + a_5x_5 + a_6x_6 + a_7x_7 + a_8x_8 \quad (1)$$

with A, $a_{1\div8}$, constants to be computed by the least squares method, and $x_{1\div8}$ the percentage weight of each fatty acid in the sample for every examined property (1: lauric; 2: myristic; 3: palmitic; 4: stearic; 5: palmitoleic; 6: oleic; 7: linoleic; 8: linolenic).

The obtained correlations from Eq. (1), for each examined property, will then be compared against (different) experimental data in order to assess their predictive capability; where applicable, they will also be compared with other similar relations developed from past research.

3. Results and discussion

3.1. Cetane Number

The dimensionless cetane number is one of the most critical fuel properties. It is highly responsible for ignition delay (a relation between CN and ignition delay is, for example, reported in [21]), hence percentage of premixed vs. diffusion combustion in a diesel engine [27]. In this way, it influences not only the exact heat release rate but is also responsible for the emission of pollutants and the radiation of combustion noise [3,5,26,28]. It is not surprising then that CN has been widely reported in the literature, with the published values differing by a lot. European specifications EN 14214:2008 dictate a minimum biodiesel CN of 51, whereas in the U.S. (ASTM D6751) the minimum acceptable value is 47. On the other hand, since the experimental determination of CN is both time consuming and quite difficult [7], it is quite reasonable that several predictive models have been developed in the past.

Figure 1 is indicative of the large variability in the reported CN values (density, viscosity and heating values too that will be discussed later in the text). These range from lower than that of the respective automotive diesel fuel up to much higher. The variability can be mostly attributed to the different FAME structure and fatty acid composition as Fig. 2 eloquently demonstrates for the feedstock sample of Fig. 1 (experimental and computational uncertainties and errors are not to be excluded too). It seems that a quite strong correlation between CN and number of double bonds exists [26,28], as Fig. 3 illustrates

$$CN = 62.32 - 6.13\bar{n}_{DB} \quad (2)$$

with $\bar{n}_{DB}$ the average number of double bonds in the biodiesel molecule. From Fig. 3, it is made clear that increasing the number of double bonds, i.e. increasing the FA unsaturation level, results in lower CN values. Highly saturated feedstocks, on the other hand, such as palm, coconut and tallow exhibit the highest CN values, in the order of 60 (but worse cold-flow properties [26,28]). Klopfenstein [29] determined a second-order polynomial correlation between CN and chain length, whereas Ramirez-Verduzco et al. [19] between CN, molecular weight and number of double bonds. Mishra et al., [30] correlated biodiesel CN with the straight-chain saturated factor and a modified degree of unsaturation. Various correlations between CN and other properties such as boiling point, heat of vaporization, heat of combustion etc. are summarized in [15].

Table 1 provides the sample used for the MLR analysis, containing 45 different sets of CN and FA weight composition values. The first 20 lines in Table 1 correspond to values reached during past research by the first author [26], and refer to average values (CN and FA composition) from a huge sample of data, from published reports up to 2011. The rest of the data in Table 1 derive from Refs. [12,13] and refer to individual experimental measurements, including also neat fatty acids (last eight lines, taken from [31]). Thus, it is believed that the data sample used for the regression analysis is satisfactorily broad. Notice in the neat FAs data in Table 1 that methyl stearate exhibits the highest CN, possessing also the highest molecular weight. The dependence between CN and molecular weight (chain length too) is well established in the literature as, for example, detailed in [15,19,21,31].

Applying the multiple linear regression analysis, Eq. (1) is transformed into

$$CN = 55.87 + \overbrace{0.0747x_1 + 0.098x_2 + 0.164x_3 + 0.176x_4}^{\text{saturated}} - \overbrace{0.050x_5 + 0.001x_6 - 0.140x_7 - 0.273x_8}^{\text{unsaturated}} \quad (3)$$

The first (constant) term in Eq. (3) is quite high (of the same order of magnitude to past similar research — see Eqs. (4a)–(4c) later in this section). Further, saturated acids contribute towards an increase in the CN, with the magnitude of the respective coefficients increasing with increasing carbon number. Unsaturated acids, on the other hand, contribute towards a decrease of the predicted CN, as previous research [12,13,15,28] confirms. Therefore, it is believed that the derived equation has a sound theoretical basis.

The statistical coefficients of the model are summarized in Table 2, with the R^2 found approx. 90%, i.e. a quite high value, despite the wide variability of the selected data set. In any case, the most important aspect is the model's predictive capability. This was performed on a separate sample, randomly selected from various sources [32–35]; the details of the experimental data as well as the predicted ones from Eq. (3) are provided in Table 3. In all cases, the error is satisfactorily small, and the prediction of the CN quite successful, a fact that proves the reliability of the derived correlation.

The next step of the analysis was to compare the correlation reached in the current work with those from past research, namely the models of (notice the difference in the obtained coefficients from each study)

a) Bamgboye and Hansen [12],

$$CN = 61.1 + 0.088x_2 + 0.133x_3 + 0.152x_4 - 0.101x_5 - 0.039x_6 - 0.243x_7 - 0.395x_8 \quad (4a)$$

b) Piloto-Rodriguez et al. [13] (notice that this model also includes the percentage of gondoic 20:1 and erucic 22:1 mono-unsaturated fatty acids in the derived correlation, with 'res' indicating the sum of other FAs found in the molecule)

166 $$CN = 56.16 + 0.07x_1 + 0.1x_2 + 0.15x_3 + 0.23x_4 - 0.05x_5 - 0.03x_6 - 0.19x_7 - 0.31x_8 + 0.08x_{20:1} + 0.18x_{22:1} - 0.1x_{res} \quad (4b)$$

167 c) Gopinath et al. [15].

168 $$CN = 62.2 + 0.017x_1 + 0.074x_2 + 0.115x_3 + 0.177x_4 - 0.103x_6 - 0.279x_7 - 0.366x_8 \quad (4c)$$

169

170 Figure 4 compares graphically the experimental vs. predicted CN values for all four
171 models. The model of Bamgboye and Hansen [12] and Gopinath et al. [15] exhibit R^2
172 values 0.82 and 0.81 respectively, that of Piloto-Rodriguez [13] lies slightly lower at 0.80,
173 whereas the new model slightly higher at R^2=0.83, confirming its predictive capability
174 against well-established previous research. Closer look at the graphs in Fig. 4 reveals
175 another interesting feature, namely, there are two discrete groups of CN values. One is
176 located between CN 40 and 52, and the other between 60 and 65. The former
177 corresponds to vegetable oil-derived biodiesels, and the latter mostly to animal-derived
178 ones (palm is included here too).

179 *3.2. Density*

180 The density of a material or liquid is defined as its mass per unit volume. Vegetable
181 oils (methyl esters too) possess higher density than conventional diesel fuel. This means
182 that diesel engine fuel pumps, which operate on a volumetric basis, will inject larger mass
183 of biodiesel (or vegetable oil) than neat diesel fuel, a fact that will influence the air–fuel
184 ratio in the engine (performance and emissions too [2–5]). In the EU (EN 14214:2008), the
185 acceptable range of biodiesel density is rather wide (860–900 kg/m^3), whereas in the US
186 (ASTM D6751) there is no density specification.

187 Figure 1 demonstrates the quite high variability in density values from various
188 feedstocks (average values); again, it is the different fatty acid composition of the

originating oil that is mostly responsible for the observed differences. A quite strong correlation between density and the degree of unsaturation is also established from Fig. 5 (R^2=0.87); the respective correlation found in [26] is

$$\rho = 869.25 + 9.17\,\bar{n}_{DB} \quad (5)$$

with ρ the density in kg/m^3. In general, density increases with the increase in the number of double bonds; alternatively, the more saturated the originating oil, the lower the density of the derived methyl ester. Ramirez-Verduzco et al. [19] correlated density not only with the number of double bonds but also with molecular weight. Similarly, Lapuerta et al. [36] correlated density with the degree of unsaturation and the chain length. No correlation between density and fatty acid composition has been found in the literature, and one such correlation is provided below.

Table 4 contains the data set used for the multi regression analysis between density and fatty acid composition. Overall 23 values from a variety of different feedstocks were used. The derived MLR equation is

$$\rho = 923 - \overbrace{1.01x_1 - 0.99x_2 - 0.54x_3 - 0.62x_4}^{\text{saturated}} - \overbrace{0.70x_5 - 0.44x_6 - 0.37x_7 - 0.24x_8}^{\text{unsaturated}} \quad (6)$$

where $x_{1\div8}$ are the percentage weights of the eight fatty acids. An interesting feature in Eq. (6) is that the saturated FAs assume higher values compared to the unsaturated ones; this is related to the rather high constant term (923).

The statistical coefficients of the derived MLR analysis are summarized in Table 5. A quite high R^2 value of 94.5% was established, along with a very small standard error of 1.22, indicating a very good correlation between the derived equation and the data sample it was based on.

In order to check the reliability of the derived density model, a set of 10 (different from those of Table 5) experimental values from [18] was used, detailed in Table 6. This table provides both the experimental and predicted from Eq. (6) values. For all examined cases, a practically negligible error of less than 0.45% was established, proving the predictive capability of the model. Figure 6 expands on the results of Table 6 illustrating the correlation of the predicted results with the experimental data. An R^2 value of 0.84 was determined which is believed to be quite satisfactory. It is of the same order as the one from Fig. 4 for cetane. Due to lack of other relevant (MLR) analyses, no comparison with similar approaches was feasible in this case.

3.3. Kinematic Viscosity

Viscosity is a measure of the resistance of a fluid which is being deformed by either shear or tensile stress. For liquid fuels, the less viscous the fluid, the greater its ease of movement. As regards compression ignition engines, low values of viscosity are favorable facilitating faster atomization of the fuel spray; this in turn reduces the ignition delay period. On the other hand, and with regard to mechanical fuel pumps, higher kinematic viscosity results in reduced fuel leakage losses, and this ultimately leads to both higher injection pressures and injected fuel mass [27].

Figure 1 demonstrates average values of kinematic viscosity for methyl esters from various vegetable and animal feedstocks (it is reminded here that biodiesels are Newtonian fluids for temperatures above 5^{o}C [37]). The corresponding European and U.S. specification limits are also highlighted in Fig. 1. A rather moderate correlation between viscosity and unsaturation level (or number of double bonds) was established, as illustrated in Fig. 7 (R^2=0.57). Past research [19,37,38] had correlated kinematic viscosity

apart from the number of double bonds with molecular weight too. It was found that viscosity increased with increasing molecular weight, and decreased with increasing number of double bonds. Hong et al., [39], on the other hand, developed a biodiesel viscosity equation based on the individual pure FAMEs viscosities. Based on the statistical analysis in [26], a quite high (R^2=96.7%) statistical relation between viscosity (μ in mm^2/s) and CN can be established

$$\mu = 960.77 - 0.0059CN^3 + 0.9665CN^2 - 52.694CN \quad (7)$$

To the best of the authors' knowledge, no correlation between viscosity and fatty acid weight composition has been reported in the literature. In order to determine such a relation, the viscosity and FA values provided in Table 7 have been used (data from Ref. [26]). From the data set of this table, a MLR analysis was performed and the results are summarized in Table 8. Contrary to the preceding CN and density analysis, the derived viscosity results do not seem that encouraging. A rather moderate R^2 in the order of 66% was established. Equation (8) provides the corresponding MLR correlation

$$\mu = 5.3380^{\overbrace{-0.79593x_1 - 0.04417x_2 + 0.000731x_3 + 0.009571x_4}^{\text{saturated}}} \overbrace{-0.00102x_5 - 0.00578x_6 - 0.01179x_7 - 0.01726x_8}^{\text{unsaturated}} \quad (8)$$

The derived correlation is more on the mathematical rather than the 'physical' side. Table 9 and Fig. 8 demonstrate the predictive capability of the developed model. As was rather anticipated, the prediction error is quite large, in the order of 10% for all six experimental values used, a fact that indicates the relatively low predictive capability of the derived model. Experimental uncertainties and errors aside, it is rather obvious that correlating biodiesel viscosity only with its FA weight composition does not prove

adequate and reliable. Perhaps it is the oxygen content in the biodiesel molecule that is responsible here.

3.4. Heating Values

The lower (LHV or net) and the higher (HHV or gross) heating values are measures of the fuel's heat of combustion; the difference between HHV and LHV is the water's heat of vaporization. Since methyl esters contain on average 10−12% per weight oxygen, they exhibit proportionally lower heating values than conventional diesel fuel. This means that in order to achieve the same engine power, the injected fuel quantity should be larger. Figure 1 illustrates typical average values for biodiesel lower and higher heating values from many common feedstocks. Interestingly, there is no specification as regards the biodiesel heating value (for automotive applications), neither in the EU nor in the U.S.

As was the case with CN, density and viscosity, Ramirez-Verduzco et al. [19] correlated HHV with molecular weight and number of double bonds; Hong et al. [39], as well as Fassinou et al. [40,41], correlated the methyl ester HHV with the individual FAs heating values. Demirbas [42], on the other hand, developed relations between HHV and viscosity, density and flash point, while Mehta and Anand [43] between LHV and carbon-to-oxygen ratio and number of double bonds. Lastly, Tesfa et al. [44] proposed a LHV correlation with density and kinematic viscosity (notice that previous fuel-oriented research has mostly focused on HHV, whereas engine/emissions-oriented studies on LHV).

Table 10 contains a wide set of data (23 observations) for LHV and the respective fatty acid compositions from various feedstocks (data from [26]). From the data set of this table, a MLR analysis was performed for HHV (a similar one was performed for LHV). The only other citation in the literature directly relating HHV with the fatty acid composition is

[45], but that study only dealt with oils and, in particular, waste frying ones. A rather weak R^2 in the order of approx. 51% was established for HHV (approx. 59% for LHV). For what is worth, the statistical correlation between both heating values and the degree of unsaturation was equally weak, as previous research confirms [26,28] and Fig. 9 demonstrates. One possible reason for this might be the uncertainty in the experimental results, as, for example, not all researchers have been using the same calorimeters. Equations (9a) and (9b) provide the derived MLR correlations for HHV and LHV respectively

$$\mathrm{HHV} = 39{,}839.54\overbrace{-1159.62x_1 + 24.96x_2 + 14.03x_3 + 1.71x_4}^{\text{saturated}} \overbrace{-52.32x_5 + 1.51x_6 + 2.78x_7 + 8.27x_8}^{\text{unsaturated}} \quad (9a)$$

In general, the coefficients of saturated acids are higher than those of the unsaturated ones, but their influence is not monotonic. More specifically, the composition in lauric acid decreases the HHV, whereas myristic, palmitic and stearic increase it. On the other hand, the contribution of palmitoleic acid is quite large (e.g. in tallow or mahua FAMEs). A conclusive observation from Eq. (9a) is the strong dependence of lauric acid on HHV. Similar comments can be made for the respective LHV correlation Eq. (9b)

$$\mathrm{LHV} = 37{,}667.45\overbrace{-316.73x_1 + 96.79x_2 - 3.07x_3 - 37.64x_4}^{\text{saturated}} + \overbrace{25.82x_5 - 2.76x_6 + 9.46x_7 + 3.86x_8}^{\text{unsaturated}} \quad (9b)$$

The predictive capability of the HHV model against experimental data from the literature is investigated in Table 12. As can be observed, the resulting (relative) errors between model and experiment are quite small (always less than 4%; for many cases even less than 1%), as was also the case in [45]. This proves the quite good predictive

capability of the derived equations despite the weak R^2 value mentioned above between the model and the data it was based on.

4. Summary and conclusion

A comprehensive statistical analysis was performed with the aim to formulate predictive correlations between biodiesel properties and the respective fatty acid weight composition. The examined properties were cetane number, density, heating values and kinematic viscosity. The FAs used for the analysis were the four major saturated ones lauric, myristic, palmitic, stearic, and the four major unsaturated palmitoleic, oleic, linoleic and linolenic. Multi-linear regression analysis was chosen for the formulation of the predictive correlations. A large sample of data was used for each case, covering a wide range of feedstocks and property values.

For cetane number and density, the derived correlations were both highly statistical regarding the data set they were based on, and, more importantly, proved quite successful in predicting the properties from other sources (small relative error and high correlation between experimental and predicted values). Particularly for CN, for which previous correlations exist, the new model seemed to provide a slightly higher degree of predictive capability.

For both heating values, however, as well as for kinematic viscosity, the obtained correlations did not prove statistically strong (R^2 between 50.5 and 66%). As regards their predictive capability, the relative error for viscosity ranged between 7 and 13%; for HHV it was much better, on average 1%.

It is believed that the results from this study can prove useful to researchers and institutions with respect to simulation and planning. Furthermore, the results of such

analyses can provide insight into designing a ‘better’ biodiesel feedstock, with desired attributes, hence favorable diesel engine performance and emissions behavior.

Nomenclature

CN	Cetane number
EU	European Union
FA	Fatty acid
FAME	Fatty acid methyl ester
HHV	Higher heating value
LHV	Lower heating value
ME	Methyl ester
MLR	Multiple linear regression
PME	Palm methyl ester
RME	Rapeseed methyl ester
SME	Soybean methyl ester
TME	Tallow methyl ester

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461 **Table 1.** Cetane number and fatty acid weight composition of the examined data set

		12:0 $C_{12}H_{24}O_2$	14:0 $C_{14}H_{28}O_2$	16:0 $C_{16}H_{32}O_2$	18:0 $C_{18}H_{36}O_2$	16:1 $C_{16}H_{30}O_2$	18:1 $C_{18}H_{34}O_2$	18:2 $C_{18}H_{32}O_2$	18:3 $C_{18}H_{30}O_2$	**Cetane Number (CN)**
	Mol. weight (kg/kmol)	200.32	228.37	256.42	284.48	254.41	282.46	280.45	278.43	
	Formal (common) name / **Animal Fat or Vegetable Oil**	Dodecanoic (Lauric)	Tetradecanoic (Myristic)	Hexadecanoic (Palmitic)	Octadecanoic (Stearic)	*cis*-9 Hexadecenoic (Palmitoleic)	*cis*-9 Octadecenoic (Oleic)	*cis*-9, *cis*-12 Octadecadienoic (Linoleic)	*cis*-9,*cis*-12, *cis*-15 Octadecatrienoic (Linolenic)	
	Index	*1*	*2*	*3*	*4*	*5*	*6*	*7*	*8*	
1	Beef tallow	0.15	2.41	24.39	19.08	2.66	41.65	5.91	0.72	60.9
2	Canola	0	0	4.51	2	0.36	60.33	21.24	9.49	54.8
3	Chicken fat	0.1	0.73	24.06	6.42	5.65	41.43	18.83	1.06	57.0
4	Coconut	46.91	18.74	9.69	0	0.11	2.83	6.83	0	61.0
5	Corn	0	0	11.81	2.13	0.12	27.35	57.74	0.63	52.5
6	Cottonseed	0	0.72	25.93	1.74	0.36	15.98	55.12	0.16	53.3
7	Hazelnut	0	0	6.32	3.71	0.3	79.17	10.67	0.15	53.8
8	Jatropha	0	0.15	14.42	5.82	0.69	42.81	35.38	0.23	55.7
9	Karanja	0	0	10.89	7.89	0	53.56	21.34	2.09	55.4
10	Mahua	0	0.15	22.23	22.49	0	39.01	14.87	0.1	56.9
11	Olive	0	0.05	11.47	2.83	0.9	74.52	9.54	0.51	58.9
12	Palm	0.37	1.13	42.39	4.2	0.17	40.91	9.7	0.29	61.2
13	Peanut	0	0	10.33	2.79	0	47.63	31.52	0.64	54.9
14	Rapeseed	0	0.04	4.07	1.55	0.23	62.24	20.61	8.72	54.1
15	Rice bran	0.08	0.45	18.12	2.17	0.2	42.35	34.84	0.93	56.3
16	Rubber seed	0	0.51	9.39	9.41	0.13	24.22	38.12	17.54	50.4
17	Safflower	0	0.08	7.42	2.38	0.05	14.41	75.31	0.09	51.8
18	Soybean	0.08	0.12	11.44	4.14	0.16	23.47	53.46	6.64	51.8
19	Sunflower	0	0.04	6.26	3.93	0.06	20.77	67.75	0.15	51.9
20	Waste cooking	0.2	0.67	15.69	6.14	0.73	42.84	29.36	2.03	56.2
21	Actinodapne angust	87.9	1.9	0.5	5.4	0	0	0	0	63.2
22	Aleurites oluccana	0	0	5.5	6.7	0	10.5	48.5	28.5	37.2
23	Argemone Mexicana	0	0.8	14.5	3.8	0	18.5	61.4	0	44.5
24	Canola	0	0.1	5.2	2.5	0.2	58.1	28.1	0.4	57.0
25	Lard	0.1	1.9	24.5	14.4	2.8	38.3	13.4	0.3	63.6
26	Eurhorbia helioscopia L.	2.8	5.5	9.9	1.1	0	15.8	22.1	42.7	38.2
27	Garnica morella3	0	0	0.7	46.4	0	49.5	0.9	0	63.5
28	Holoptelia integrifolia	0	3.5	35.1	4.5	1.9	53.3	0	0	61.2
29	Inedible tallow	0.1	2.1	23.9	19.5	2.8	38.5	6.4	0.3	61.7
30	Litsea glutinosa Robins	96.3	0	0	0	0	2.3	0	0	64.8
31	Moringa oleifera Lam	0	0	9.1	2.7	2.1	79.4	0.7	0.2	56.7
32	Neolitsa cassia Linn	85.9	3.8	0	0	0	4	3.3	0	64.0
33	Peanut	0	0	4.9	1.6	0	33	20.4	7.8	53.0

34	Pongamia pinnata	0	0	10.6	6.8	0	49.4	19	0	55.8
35	Thevetia peruviana	0	0	15.6	10.5	0	60.9	5.2	7.4	57.5
36	Vallaris solanacea	0	0	7.2	14.4	0	35.3	40.4	0	50.3
37	Yellow grease	0	1.1	17.3	9.5	2.2	45.3	14.5	1.3	52.9
38	Lauric	100	0	0	0	0	0	0	0	61.2
39	Myristic	0	100	0	0	0	0	0	0	66.2
40	Palmitic	0	0	100	0	0	0	0	0	74.3
41	Stearic	0	0	0	100	0	0	0	0	75.6
42	Palmitoleic	0	0	0	0	100	0	0	0	51.0
43	Oleic	0	0	0	0	0	100	0	0	55.0
44	Linoleic	0	0	0	0	0	0	100	0	38.2
45	Linolenic	0	0	0	0	0	0	0	100	31.6

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466 **Table 2.** Statistical coefficients of the developed MLR model for cetane number

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Regression Statistics	**Multiple Regression Model**
Multiple R	0.947
R^2 (%)	89.6
St. error	3.044
Observations	45

468 **Table 3.** Comparison between experimental and computed CN values for model
469 verification
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FAME	Ref.	12:0	14:0	16:0	18:0	16:1	18:1	18:2	18:3	Exp. CN	Pred. CN	Abs. Error (%)
Soybean	32			11.7	3.97		21.27	53.7	8.12	**51.3**	48.8	5.2
Peanut	32			17.2	2.7		40.5	36.6	0.5	**54.0**	53.9	0.1
Corn	32			11.4	1.3		27.1	60.2	0	**55.4**	48.8	5.7
Sunflower	32			4.9	2.3		32.6	59.4	0	**51.6**	52.9	3.1
Rapeseed	32			5.2	1.4		66	18.9	5.6	**54.5**	63.9	2.9
Palm	32	0.5	1.6	49.8	2.9		38.6	6.6		**62.0**	62.8	1.1
Palm kernel	32	48	14.7	11.5	1.4	0	15.9	1.8		**62.1**	57.4	4.2
Waste frying	32	1.6	1.5	27.3	4.9		36.1	25.7	1.9	**55.0**	66.2	8.9
Beef tallow	33		2.72	25.33	34.7	2.02	31.69	0.75		**60.3**	54.6	4.6
Jatropha	33			14.2	6.9	1.4	43.1	34.4		**57.1**	47.4	3.4
Soybean	34		0	9	4		23	51	13	**49.0**	48.2	2.5
Sunflower	34		0	9	7		10	74		**47.0**	56.8	5.9
Koroch	35	0	0	7.9	8.9	0	57.9	14.5	0	**53.4**	54.6	4.5
Jatropha	35	0	0	16	6.5	0	43.5	34.4	0.8	**57.1**	48.8	5.2

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Table 4. Density and fatty acid weight composition of the examined data set

		12:0 $C_{12}H_{24}O_2$	14:0 $C_{14}H_{28}O_2$	16:0 $C_{16}H_{32}O_2$	18:0 $C_{18}H_{36}O_2$	16:1 $C_{16}H_{30}O_2$	18:1 $C_{18}H_{34}O_2$	18:2 $C_{18}H_{32}O_2$	18:3 $C_{18}H_{30}O_2$	**Density (kg/m^3)**
	Mol. weight (kg/kmol)	200.32	228.37	256.42	284.48	254.41	282.46	280.45	278.43	
	Formal (common) name	Dodecanoic (Lauric)	Tetradecanoic (Myristic)	Hexadecanoic (Palmitic)	Octadecanoic (Stearic)	*cis*-9 Hexadecenoic (Palmitoleic)	*cis*-9 Octadecenoic (Oleic)	*cis*-9, *cis*-12 Octadecadienoic (Linoleic)	*cis*-9,*cis*-12, *cis*-15 Octadecatrienoic (Linolenic)	
	Animal Fat or Vegetable Oil									
	Index	*1*	*2*	*3*	*4*	*5*	*6*	*7*	*8*	
1	Beef tallow	0.15	2.41	24.39	19.08	2.66	41.65	5.91	0.72	874.3
2	Canola	0.00	0.00	4.51	2.00	0.36	60.33	21.24	9.49	881.6
3	Chicken fat	0.10	0.73	24.06	6.42	5.65	41.43	18.83	1.06	876.3
4	Corn	0.00	0.00	11.81	2.13	0.12	27.35	57.74	0.63	882.2
5	Cottonseed	0.00	0.72	25.93	1.74	0.36	15.98	55.12	0.16	879
6	Croton	0.00	0.10	7.25	3.43	0.10	10.80	77.25	5.40	883.2
7	Hazelnut	0.00	0.00	6.32	3.71	0.30	79.17	10.67	0.15	877.9
8	Jatropha	0.00	0.15	14.42	5.82	0.69	42.81	35.38	0.23	878.7
9	Karanja	0.00	0.00	10.89	7.89	0.00	53.56	21.34	2.09	882.9
10	Linseed	0.00	0.00	5.18	3.26	0.10	19.04	16.12	54.54	891.5
11	Mahua	0.00	0.15	22.23	22.49	0.00	39.01	14.87	0.10	874.5
12	Neem	0.40	0.18	17.57	16.6	0.00	45.83	17.79	0.72	876.2
13	Olive	0.00	0.05	11.47	2.83	0.90	74.52	9.54	0.51	881.2
14	Palm	0.37	1.13	42.39	4.20	0.17	40.91	9.70	0.29	874.7
15	Peanut	0.00	0.00	10.33	2.79	0.00	47.63	31.52	0.64	882.9
16	Rapeseed	0.00	0.04	4.07	1.55	0.23	62.24	20.61	8.72	882.2
17	Rice bran	0.08	0.45	18.12	2.17	0.20	42.35	34.84	0.93	880.9
18	Rubber seed	0.00	0.51	9.39	9.41	0.13	24.22	38.12	17.54	882.3
19	Safflower	0.00	0.08	7.42	2.38	0.05	14.41	75.31	0.09	883.8
20	Soybean	0.08	0.12	11.44	4.14	0.16	23.47	53.46	6.64	882.8
21	Sunflower	0.00	0.04	6.26	3.93	0.06	20.77	67.75	0.15	882.9
22	Waste cooking	0.20	0.67	15.69	6.14	0.73	42.84	29.36	2.03	880.6
23	Lard	0.25	1.62	25.1	13.23	2.68	44.36	12.06	1.18	873.0

Table 5. Statistical coefficients of the developed MLR model for density

Regression Statistics	**Multiple Regression Model**
R	0.972
R^2 (%)	94.54
St. error	1.22
Observations	23

Table 6. Comparison between experimental (from [18]) and predicted density values for model verification

Biodiesel	Experimental Values (kg/m^3)	Predicted Values (kg/m^3)	Error (%)
Soybean (SME)	887.3	883.4	0.44
Rapeseed (RME)	886.0	882.8	0.36
Palm (PME)	877.9	875.2	0.31
SME+RME	885.7	882.3	0.32
RME+PME	882.1	878.7	0.38
SME+PME	882.0	879.8	0.25
SME+RME+PME	883.0	880.5	0.28
Sunflower	887.2	882.9	0.50
SME+RME	884.3	882.6	0.49
SME+RME	884.7	880.7	0.46

Table 7. Kinematic viscosity and fatty acid weight composition of the examined data set

		12:0 $C_{12}H_{24}O_2$	14:0 $C_{14}H_{28}O_2$	16:0 $C_{16}H_{32}O_2$	18:0 $C_{18}H_{36}O_2$	16:1 $C_{16}H_{30}O_2$	18:1 $C_{18}H_{34}O_2$	18:2 $C_{18}H_{32}O_2$	18:3 $C_{18}H_{30}O_2$	**Kinematic Viscosity (mm^2/s @40°C)**
	Mol. weight (kg/kmol)	200.32	228.37	256.42	284.48	254.41	282.46	280.45	278.43	
	Formal (common) name	Dodecanoic (Lauric)	Tetradecanoic (Myristic)	Hexadecanoic (Palmitic)	Octadecanoic (Stearic)	*cis*-9 Hexadecenoic (Palmitoleic)	*cis*-9 Octadecenoic (Oleic)	*cis*-9, *cis*-12 Octadecadienoic (Linoleic)	*cis*-9,*cis*-12, *cis*-15 Octadecatrienoic (Linolenic)	
	Animal Fat or Vegetable Oil									
	Index	*1*	*2*	*3*	*5*	*4*	*6*	*7*	*8*	
1	Beef tallow	0.15	2.41	24.39	19.08	2.66	41.65	5.91	0.72	4.83
2	Canola	0	0	4.51	2	0.36	60.33	21.24	9.49	4.40
3	Chicken fat	0.1	0.73	24.06	6.42	5.65	41.43	18.83	1.06	4.81
4	Corn	0	0	11.81	2.13	0.12	27.35	57.74	0.63	4.32
5	Cottonseed	0	0.72	25.93	1.74	0.36	15.98	55.12	0.16	4.70
6	Croton	0	0.1	7.25	3.43	0.1	10.8	77.25	5.4	4.48
7	Hazelnut	0	0	6.32	3.71	0.3	79.17	10.67	0.15	4.55
8	Jatropha	0	0.15	14.42	5.82	0.69	42.81	35.38	0.23	4.72
9	Karanja	0	0	10.89	7.89	0	53.56	21.34	2.09	5.04
10	Linseed	0	0	5.18	3.26	0.1	19.04	16.12	54.54	4.06
11	Mahua	0	0.15	22.23	22.49	0	39.01	14.87	0.1	5.06
12	Neem	0.4	0.18	17.57	16.6	0	45.83	17.79	0.72	4.72
13	Olive	0	0.05	11.47	2.83	0.9	74.52	9.54	0.51	5.05
14	Palm	0.37	1.13	42.39	4.2	0.17	40.91	9.7	0.29	4.61
15	Peanut	0	0	10.33	2.79	0	47.63	31.52	0.64	4.77
16	Rapeseed	0	0.04	4.07	1.55	0.23	62.24	20.61	8.72	4.63
17	Rice bran	0.08	0.45	18.12	2.17	0.2	42.35	34.84	0.93	4.70
18	Rubber seed	0	0.51	9.39	9.41	0.13	24.22	38.12	17.54	4.79
19	Safflower	0	0.08	7.42	2.38	0.05	14.41	75.31	0.09	4.10
20	Soybean	0.08	0.12	11.44	4.14	0.16	23.47	53.46	6.64	4.29
21	Sunflower	0	0.04	6.26	3.93	0.06	20.77	67.75	0.15	4.53
22	Waste cooking	0.2	0.67	15.69	6.14	0.73	42.84	29.36	2.03	4.75
23	Lard	0.25	1.62	25.1	13.23	2.68	44.36	12.06	1.18	4.89

Table 8. Statistical coefficients of the developed MLR model for kinematic viscosity

Regression Statistics	**Multiple Regression Model**
R	0.8148
R^2 (%)	66.39
St. error	0.199
Observations	23

Table 9. Comparison between experimental (from [19,39]) and predicted kinematic viscosity values for model verification

Biodiesel	Experimental Values (mm^2/s)	Predicted Values (mm^2/s)	Error (%)
Beef tallow	4.36	4.71	8.0
Soybean	4.01	4.5	12.2
Sunflower	4.03	4.45	10.4
Corn	4.18	4.52	8.1
Cottonseed	4.06	4.6	13.3
Canola+Lard	4.47	4.78	6.94

Table 10. Heating values and fatty acid weight composition of the examined data set

		12:0 $C_{12}H_{24}O_2$	14:0 $C_{14}H_{28}O_2$	16:0 $C_{16}H_{32}O_2$	18:0 $C_{18}H_{36}O_2$	16:1 $C_{16}H_{30}O_2$	18:1 $C_{18}H_{34}O_2$	18:2 $C_{18}H_{32}O_2$	18:3 $C_{18}H_{30}O_2$	**Higher Heating Value (kJ/kg)**	**Lower Heating Value (kJ/kg)**
	Mol. weight (kg/kmol)	200.32	228.37	256.42	284.48	254.41	282.46	280.45	278.43		
	Formal (common) name	Dodecanoic (Lauric)	Tetrade-canoic (Myristic)	Hexade-canoic (Palmitic)	Octa-decanoic (Stearic)	*cis*-9 Hexa-decenoic (Palmitoleic)	*cis*-9 Octa-decenoic (Oleic)	*cis*-9, *cis*-12 Octadeca-dienoic (Linoleic)	*cis*-9,*cis*-12, *cis*-15 Octa-decatrienoic (Linolenic)		
	Animal Fat or Vegetable Oil										
	Index	*1*	*2*	*3*	*5*	*4*	*6*	*7*	*8*		
1	Beef tallow	0.15	2.41	24.39	19.08	2.66	41.65	5.91	0.72	40,040	37,220
2	Canola	0	0	4.51	2	0.36	60.33	21.24	9.49	39,975	37,980
3	Chicken fat	0.1	0.73	24.06	6.42	5.65	41.43	18.83	1.06	39,890	37,630
4	Corn	0	0	11.81	2.13	0.12	27.35	57.74	0.63	40,190	37,610
5	Cottonseed	0	0.72	25.93	1.74	0.36	15.98	55.12	0.16	40,480	38,600
6	Croton	0	0.1	7.25	3.43	0.1	10.8	77.25	5.4	40,280	38,175
7	Hazelnut	0	0	6.32	3.71	0.3	79.17	10.67	0.15	39,800	37,825
8	Jatropha	0	0.15	14.42	5.82	0.69	42.81	35.38	0.23	40,380	37,230
9	Karanja	0	0	10.89	7.89	0	53.56	21.34	2.09	40,275	38,050
10	Linseed	0	0	5.18	3.26	0.1	19.04	16.12	54.54	40,410	36,490
11	Mahua	0	0.15	22.23	22.49	0	39.01	14.87	0.1	40,180	37,830
12	Neem	0.4	0.18	17.57	16.6	0	45.83	17.79	0.72	39,960	36,880
13	Olive	0	0.05	11.47	2.83	0.9	74.52	9.54	0.51	40,280	37,155
14	Palm	0.37	1.13	42.39	4.2	0.17	40.91	9.7	0.29	39,985	37,290
15	Peanut	0	0	10.33	2.79	0	47.63	31.52	0.64	39,930	37,080
16	Rapeseed	0	0.04	4.07	1.55	0.23	62.24	20.61	8.72	40,335	38,050
17	Rice bran	0.08	0.45	18.12	2.17	0.2	42.35	34.84	0.93	40,475	37,625
18	Rubber seed	0	0.51	9.39	9.41	0.13	24.22	38.12	17.54	40,350	38,045
19	Safflower	0	0.08	7.42	2.38	0.05	14.41	75.31	0.09	40,155	37,820
20	Soybean	0.08	0.12	11.44	4.14	0.16	23.47	53.46	6.64	40,020	38,145
21	Sunflower	0	0.04	6.26	3.93	0.06	20.77	67.75	0.15	40,000	37,750
22	Waste cooking	0.2	0.67	15.69	6.14	0.73	42.84	29.36	2.03	39,805	37,800
23	Lard	0.25	1.62	25.1	13.23	2.68	44.36	12.06	1.18	39,950	37,880

Table 11. Statistical coefficients of the developed MLR model for both heating values

Regression Statistics	**HHV**	**LHV**
R	0.711	0.7673
R^2 (%)	50.52	58.88
St. error	188	396
Observations	23	

Table 12. Comparison between experimental (from [19,39,40,45,46]) and predicted HHV for model verification

Biodiesel	Experimental HHV (kJ/kg)	Predicted HHV (kJ/kg)	Error (%)
Beef tallow	39,570	40,229	1.67
Soybean	40,230	40,232	0.01
Sunflower	40,665	40,163	1.23
Corn	41,140	40,194	2.30
Cottonseed	40,665	40,368	0.73
Corn	39,930	40,210	0.70
Waste cooking	39,741	40,549	2.03
Canola+Lard	40,050	40,206	0.39
Safflower	39,500	40,212	1.80
Sesame	39,300	40,223	2.35
Linseed	39,840	40,461	1.56
Jatropha	39,000	39,374	0.96
Palm	39,110	40,579	3.76
Rice bran	38,600	40,155	4.03

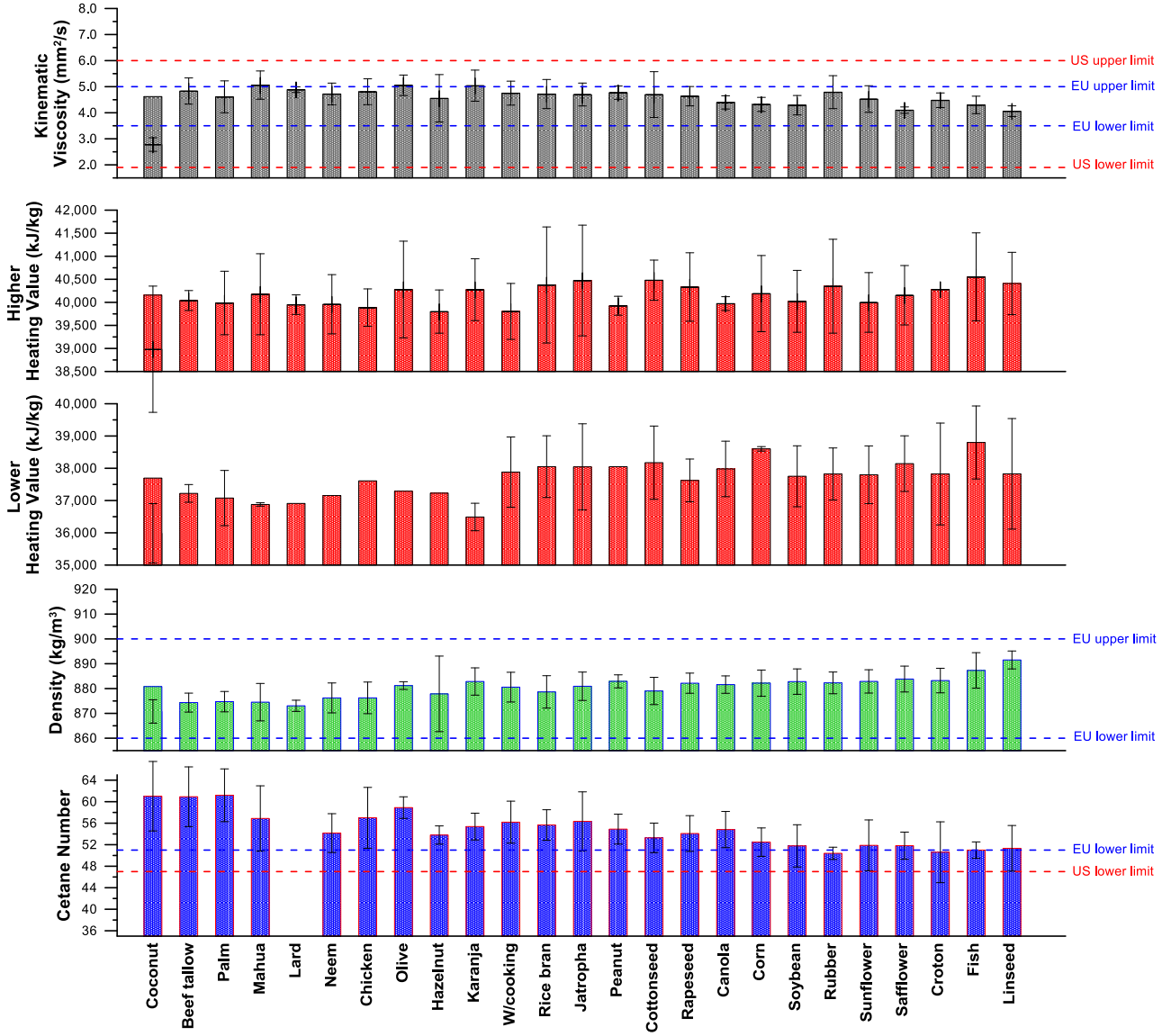

Fig. 1. Cetane number, density, heating values and kinematic viscosity for biodiesels from various feedstocks (data from [26])

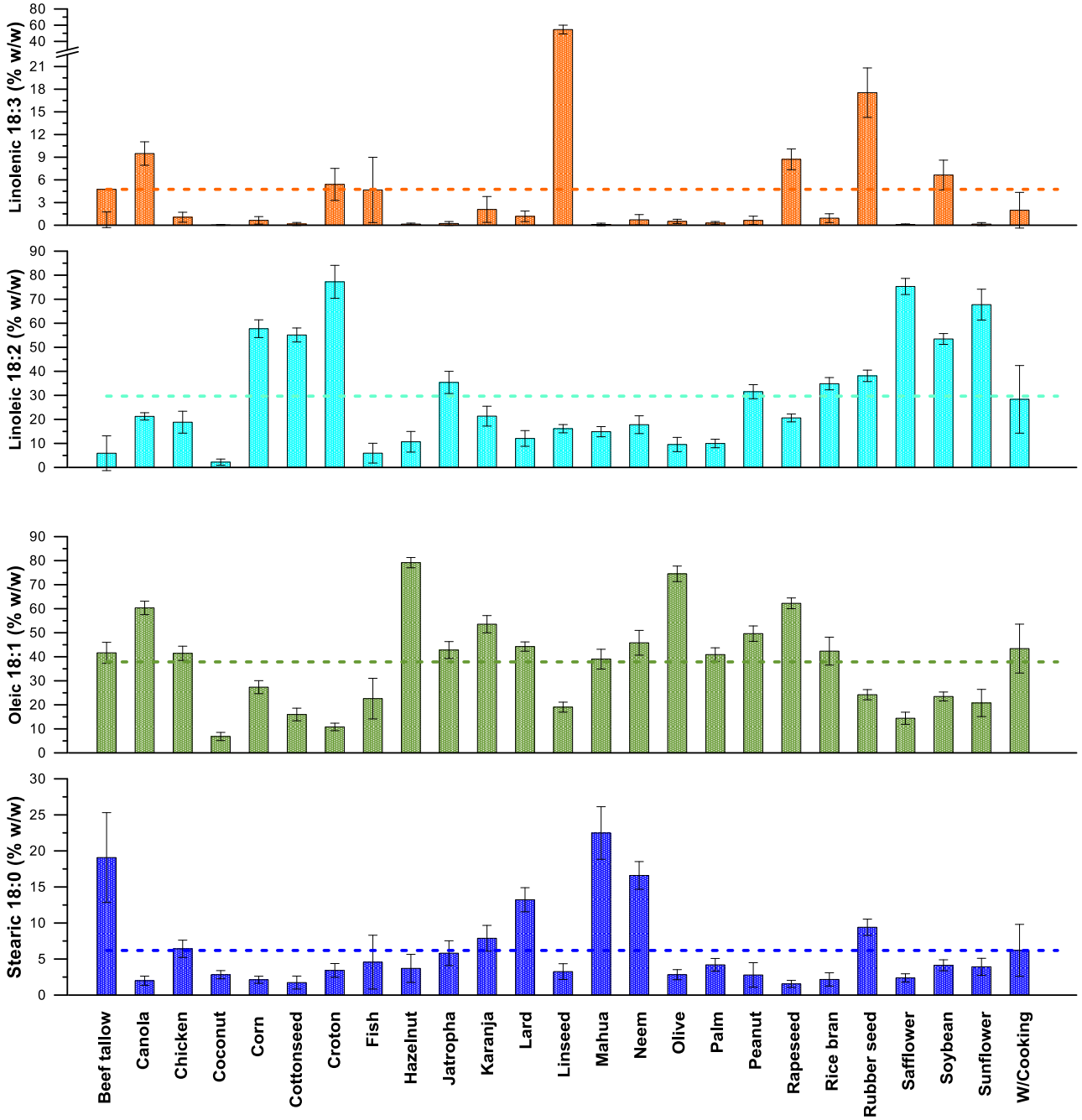

Fig. 2. Percentage weight of individual fatty acids in oil and animal feedstocks (solid line corresponds to average values) (data from [26])

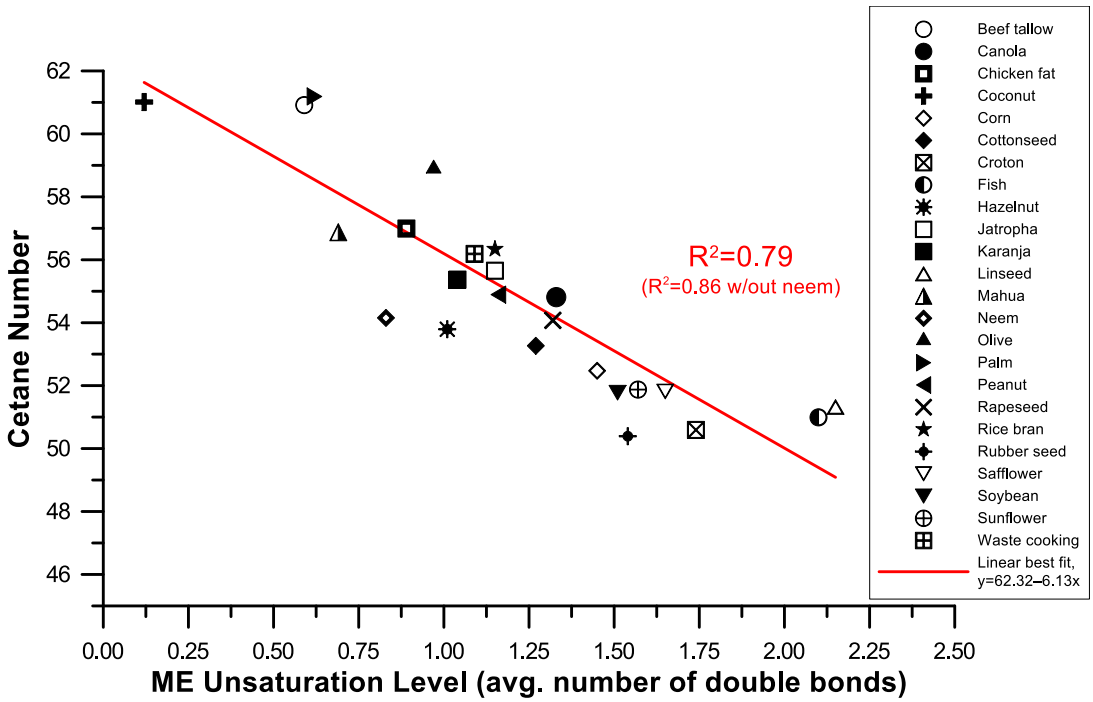

Fig. 3. Correlation between oil/fat unsaturation level and biodiesel average cetane number from 25 feedstocks (data from [26])

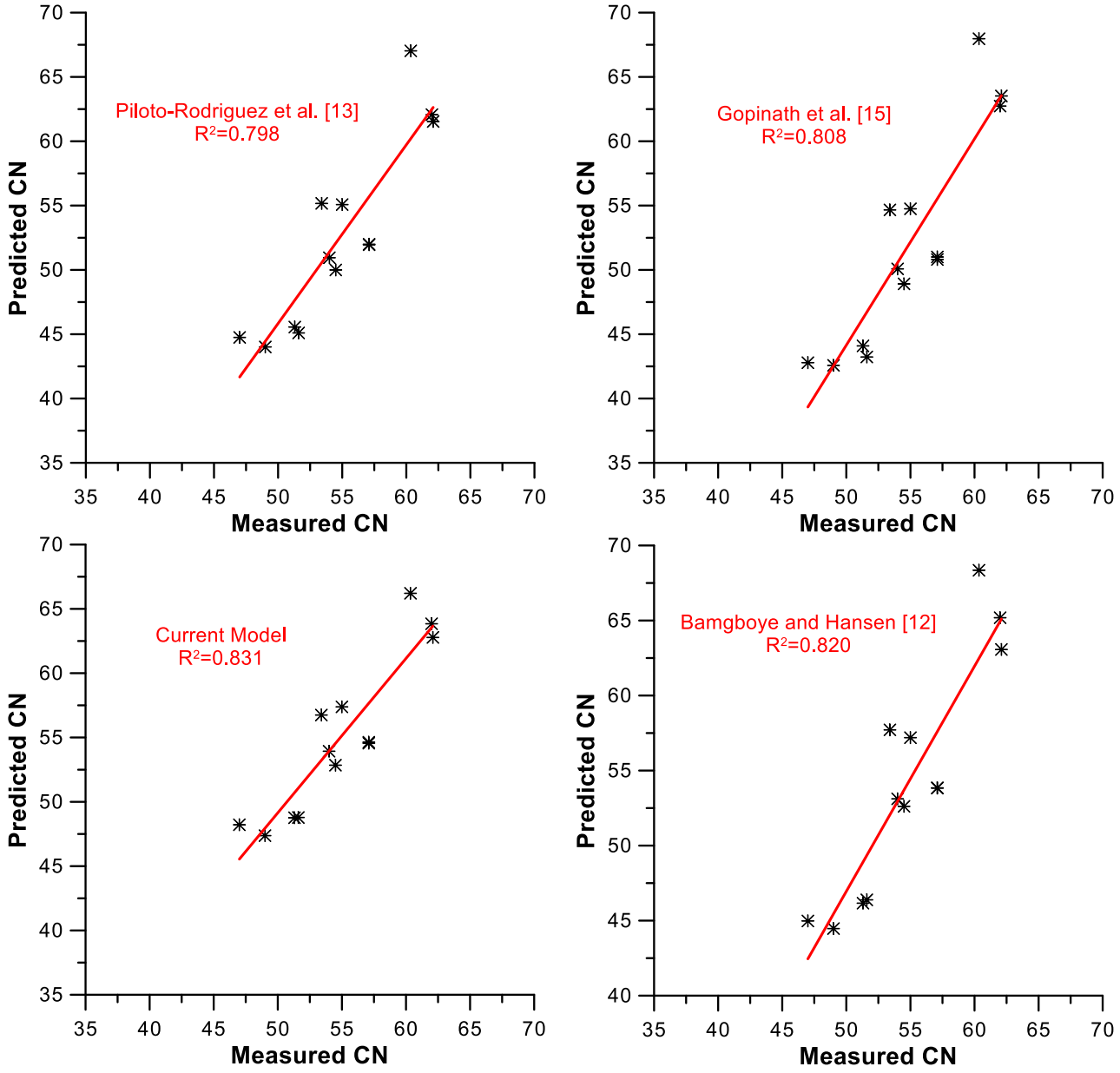

Fig. 4. Comparison of the predictive capability of the current model vs. three earlier ones (experimental data from Table 3)

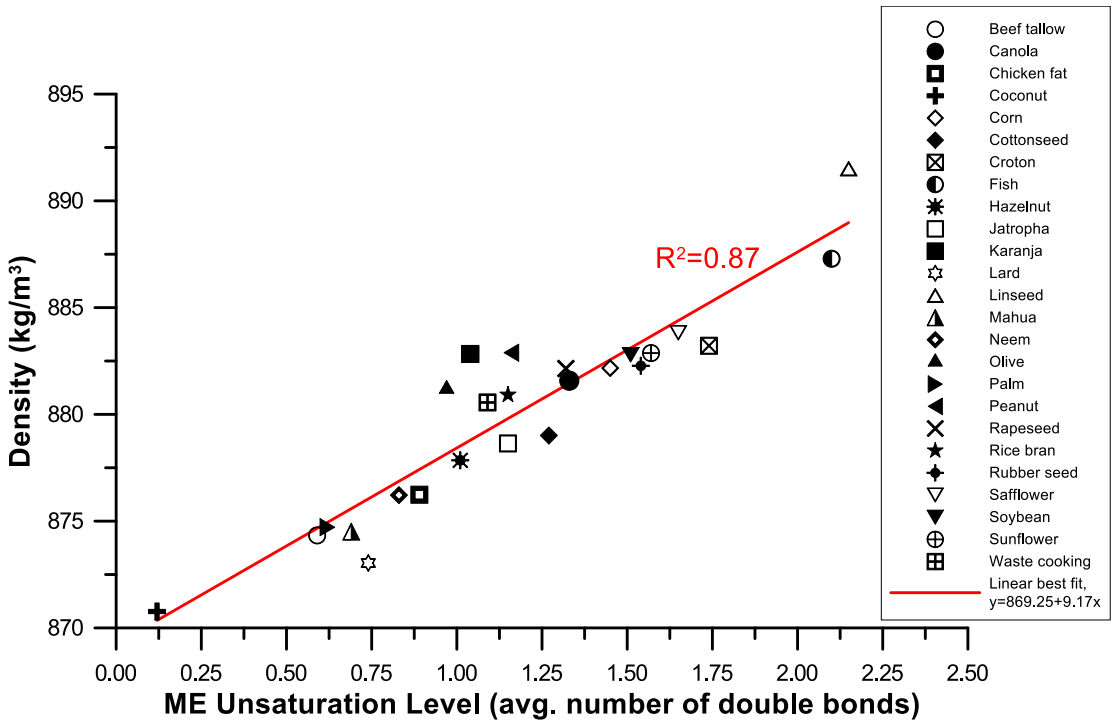

Fig. 5. Correlation between oil/fat unsaturation level and biodiesel average density from 25 feedstocks (data from [26]).

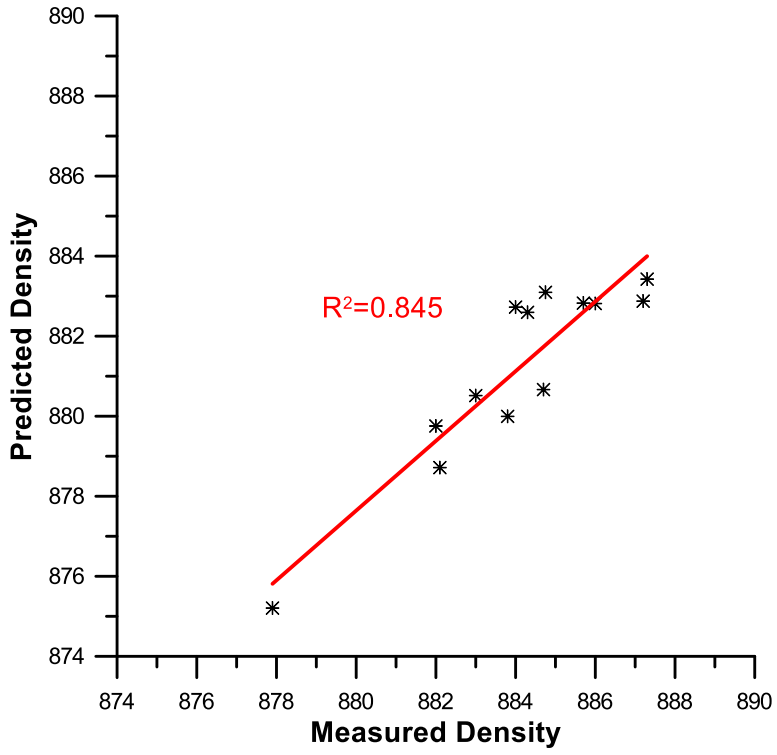

Fig. 6. Predictive capability of the developed model for density (kg/m^3) (experimental data from [18])

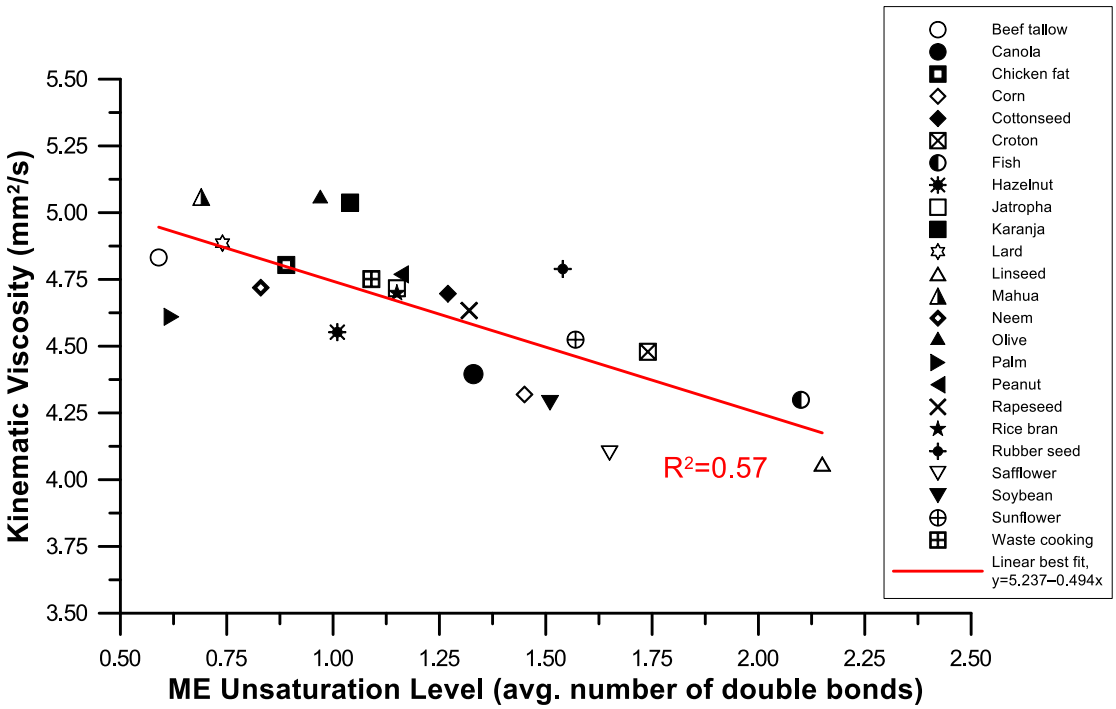

Fig. 7. Correlation between oil/fat unsaturation level and biodiesel average kinematic viscosity from 24 feedstocks (data from [26]).

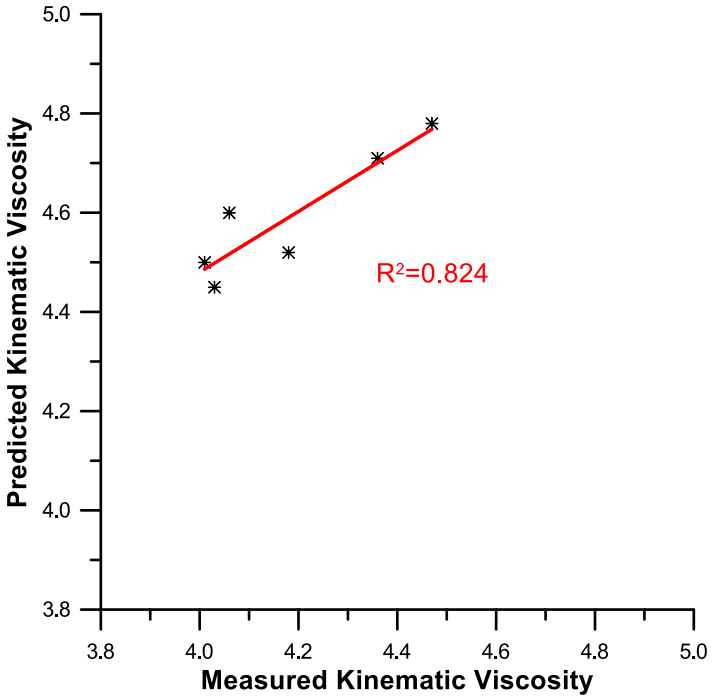

Fig. 8. Predictive capability of the developed model for kinematic viscosity (mm^2/s@40°C) (experimental data from [19,39])

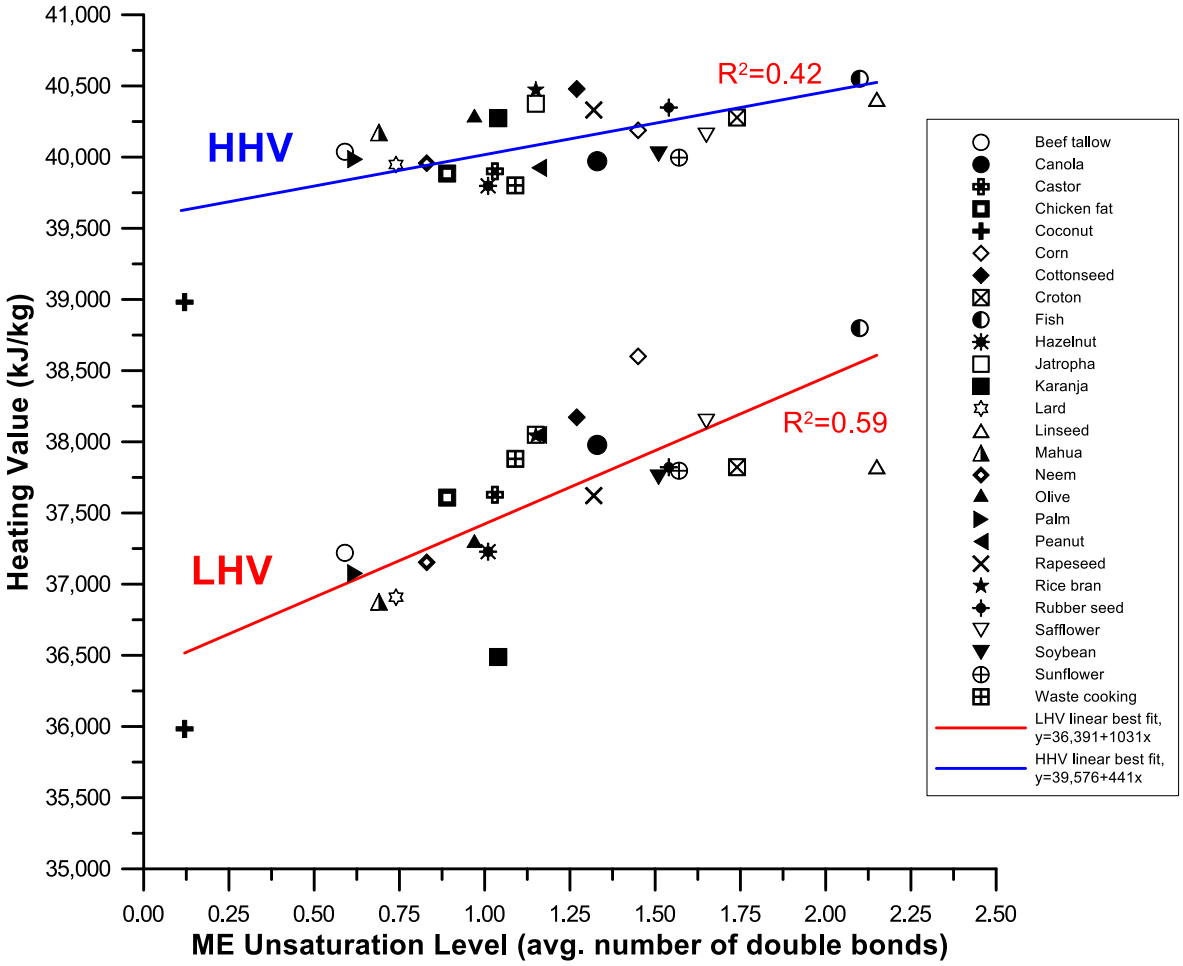

Fig. 9. Correlation between oil/fat unsaturation level and biodiesel average LHV and HHV from 25 feedstocks (data from [26]).