J Am Oil Chem Soc (2009) 86:375–382
DOI 10.1007/s11746-009-1354-y

ORIGINAL PAPER

Predicting Properties of Biodiesel Fuels using Mixture Topological Index

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Received: 21 September 2008 / Revised: 14 January 2009 / Accepted: 15 January 2009 / Published online: 12 February 2009

Abstract A new topological index for individual components based on the information of molar mass, bond length and bond energy was established to reflect the molecular structure of fatty acid methyl esters (FAME). Combined with the modified Grunberg–Nissan or Hind equation, the two series mixture topological index values of the biodiesels (mixture of FAME) were calculated, respectively. Some basic properties such as the density, viscosity, flash point (FP), high heating value (HHV) for biodiesel were correlated with these mixture topological indexes to find the relationship of structure and properties. The results show that the topological index can reflect the information of the molecular structure for FAME, such as the size of molecule, unsaturated bond, intensity of bond and branch degree. The modified Grunberg–Nissan equation has a higher precision of predicting for the properties of biodiesel studied than the Hind equation.

Keywords Biodiesel · Mixture topological index · Structure · Properties

Introduction

Biodiesel is an alternative fuel for petroleum fuel that can be commercially produced through transesterification of vegetable oils or animal fats and methanol or ethanol with an alkaline or acidic catalyst [1, 2]. Biodiesel is a mixture of fatty esters with each ester component contributing to the properties of the fuel. The properties of biodiesel are decided by the structure of the fatty acid methyl esters (FAME) that constitute biodiesel [3–5].

The main properties of biodiesel fuels include density, viscosity, flash point (FP) and high heating value (HHV). Generally, the properties of biodiesel are measured by standard method such as ASTM [6–8]. The values from standard test are accurate and acceptable. However some methods of testing always incur time and material resources.

For these reasons, a Quantitative Structure–Property Relationship (QSPR) model can be considered as a useful means of relating the properties of biodiesels with their molecular structure. This method has been successfully used for some organic substances [9, 10]. However, reported QSPR methods by different researchers can only be used for an individual component but not for the mixture. It cannot reflect the difference in physical properties among several mixtures which have same components but different mass fractions.

To use the QSPR method in predicting the properties of biodiesel fuels successfully, a topological index based on the distance matrix and adjacent matrix of the molecular structure was developed in our laboratory [11]. However, the molecular structure parameters were not introduced fully, so the calculated results were not sufficiently accurate and only the viscosity of biodiesel fuels was calculated and predicted.

Based on these considerations, the purpose of this work is to attempt to establish a novel topological index which will include more information on the molecular structure such as molar mass, bond length and bond energy of FAME. Then by introducing the modified Grunberg–Nissan or Hind equation to get the topological index for

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FAME mixture [12, 13], we may obtain the mathematical relationships between the topological index of FAME mixture with the properties of biodiesel, such as density, viscosity, flash point (FP) and high heating value (HHV).

Using this method, there is a lower requirement for expensive measurement of the properties of the FAME mixture and the feedstock can be appropriately selected to meet the specifications necessary for biodiesel production.

Model for Mixture Topological Index

Foundation of the Individual Component Topological Index

The Quantitative Structure–Property Relationship (QSPR) models are widely used nowadays to perform property estimation. A QSPR model consists of a correlation between a property of substance and a topological index derived from molecular structure of the substance.

The relationship between topological index and molecular structure may be developed as follows: firstly, the molecular structure graph is described according to the molecular structural formula by using a connected graph, then, the topological structure is obtained by translating the molecular structure graph into matrix. Finally, the molecular matrix diagram is numerically represented. In the mean time, to connect the molecular structural graph with physical properties, it is necessary to translate the matrix into a dimensionless factor to ultimately develop the relationship.

Traditionally, the molecular structure graph was hydrogen-depleted graphs which the hydrogen atom was ignored, based on this consideration, the topological index is expressed in Eq. (1):

$$Xu = \sqrt{n}\lg\left(\sum_{i}^{n} v_i s_i^2 \Big/ \sum_{i}^{n} v_i s_i\right) \tag{1}$$

where n is the vertex number of the molecular structure graph, s_i is distance matrix, v_i is the vertex value which is not consider the number of hydrogen [11].

The topological index Xu consists of a number of carbon and oxygen atoms in a molecule, the vertex value and the bond length. Nevertheless there are some disadvantages in this topological index Xu.

(1) The parameter of Xu is not sufficiently comprehensive.
(2) It is difficult to distinguish when the molecular structure is similar but the atoms are different.
(3) The topological index Xu is not available during the chemical reaction since it can not reflect the bond's cleavage.

To overcome these disadvantages for the topological index Xu, the bond length (C–C, C=C, C–O and C=O), bond energy and molar mass will be taken as the basis to develop a novel topological index in this work.

Firstly, the molar mass M is directly proportional with to the physical properties of FAME. It is an indispensable parameter of the molecule. So the molar mass M is introduced into the topological index expression.

Secondly, the vertex degree v_i is corrected:

The number of hydrogen atoms connected to each carbon atom or heteroatom is different, this fact was taken into account in the corrected vertex degree v_i in our work [14].

(1) The point valence adjustment of the hetero-atom is $\delta^{\mathrm{v}} = (z^{\mathrm{v}} - h)/(z - z^{\mathrm{v}} - 1)$. Here z is the total number of extranuclear electrons, z^{v} is the number of valence electrons and h is the number of hydrogen atoms linking with the hetero-atom [15].
(2) With relation to the unsaturated bonds, a double bond is treated as two single bonds and a triple bond as three single bonds. The point valence after adjustment is $\delta^{\mathrm{v}} = z^{\mathrm{v}} - h$.

Thirdly, the relative intensity of the bond is modified. By substituting the topological distance with relative bond distance defined as the ratio of topological distance with corresponding C–C distance when the latter is set to be 1.0. The ratio is defined as f_{ij}. For example, the real length of the C–C bond is 0.154 nm and the C–O bond is 0.134 nm in esters, so the relative bond distance of the C–O bond in esters is $0.134/0.154 = 0.8701$. By substituting the topological bond energy with relative bond energy defined as the ratio of topological energy with the corresponding C–C bond energy when the latter is set to be 1.0. The ratio is defined as e_{ij}. For example, the real bond energy of C–C bond is 345.6 KJ/mol and that of the C–O bond is 357.9 KJ/mol in esters, so the relative bond energy of the C–O bond in esters is $357.9/345.6 = 1.035$. If we consider that the bond energy is smaller when the bond length is longer, then the relative bond intensity r_{ij} is defined as the ratio of relative bond energy e_{ij} and relative bond length f_{ij}.

$$\begin{cases} r_{ij} = e_{ij}/f_{ij} \ (i \neq j) \\ r_{ij} = 0 (i = j) \end{cases} \tag{2}$$

The r_{ij} is the sum of the relative bond intensity for all the bonds from the vertex i to j. Using this modification, the molecular relative bond intensity matrix R is found, then, the column sum of matrix R is calculated and a new matrix R_i is obtained.

The bond parameters of some ordinary bonds are tabulated in Table 1.

Combined, the M, V, R and a novel topological index A is expressed in Eq. (3):

Table 1 Bond parameter of some ordinary bonds

Name of bond	Real bond length (nm)	Relative bond length	Real bond energy (KJ/mol)	Relative bond energy	Relative bond intensity
C–C	0.154	1	345.6	1	1
C–O (ester)	0.134	0.8701	357.9	1.035	1.1895
C=O	0.123	0.7987	749	2.1672	2.7134

$$A = M \ln\left(\sum_{i}^{n} v_i R_i^2 \Big/ \sum_{i}^{n} v_i R_i\right) \tag{3}$$

The M, V, R contain an abundance of molecular structure information, so a new topological index A can be assumed to reflect the molecular structure more accurately and obtain a better correlation results with the properties of FAME.

Foundation of the Mixture Topological Index to Correlate Properties

The Grunberg–Nissan equation is expressed in Eq. (4), and the Hind equation is expressed in Eq. (5):

$$\ln \eta_{\mathrm{m}} = \sum_{i}^{n} x_i \ln \eta_i + \sum_{i}^{n}\sum_{j>i}^{n} x_i x_j S_{ij} + \sum_{i}^{n}\sum_{j>i}^{n}\sum_{k>j}^{n} x_i x_j x_k S_{ijk} \tag{4}$$

$$\eta_{\mathrm{m}} = \sum_{i}^{n} x_i^2 \eta_i + 2\left(\sum_{i}^{n}\sum_{j>i}^{n} x_i x_j S_{ij} + \sum_{i}^{n}\sum_{j>i}^{n}\sum_{k>j}^{n} x_i x_j x_k S_{ijk}\right) \tag{5}$$

where, η_{m} is the mean value of the mixture's properties, η_i the value of the individual component's properties, x_i, x_j and x_k the mole fraction of i, j and k component, and S_{ij} the binary interaction parameter, S_{ijk} the ternary interaction parameter, n the number of components.

Biodiesel is the mixture of FAME in which the chemical structures are similar (aliphatic chains) and it may be regarded as a non-ideal solution due to their similarity. Therefore, the Grunberg–Nissan equation or Hind equation can be modified to simplify computation. Because the individual component topological index can reflect the structural information of the fatty acid methyl esters component, Eqs. (4) or (5) are applied to obtain the relationship of topological index between individual components and mixtures. Some simplification and assumptions may be made here.

(1) Since the biodiesel can be regarded as a near-ideal solution, the binary and ternary interaction parameters in Eqs. (4) and (5) would be small and thus can be neglected, as in other works [16].
(2) Since the mass fraction is commonly used in current literatures, the mole fraction is replaced by the mass fraction in calculating properties of biodiesel.
(3) The properties η_i of i component was replaced by its topological index value A_i.

With these modifications, Eqs. (4) or (5) were modified as Eqs. (6) or (7) respectively and used to calculate the topological index of the FAME mixture.

$$\ln A_{\mathrm{m}}^{\mathrm{G}} = \sum_{i=1}^{n} x_i \ln A_i \tag{6}$$

$$A_{\mathrm{m}}^{\mathrm{H}} = \sum_{i=1}^{n} x_i^2 A_i \tag{7}$$

where, A_{m} is the mixture topological index value, A_i the topological index value of the individual i component, and x_i the mass fraction of the individual i component. Superscripts G and H represent the method of Grunberg–Nissan and the Hind, respectively.

The correlation process of the mixture topological index values with the properties of biodiesels can be realized as follows. Firstly, the individual topological index value (A_i) of FAME was calculated according to Eq. (3). Secondly, combining the individual topological index value with the mass fraction (Z_i) for each kind of FAME in biodiesel, the mixture topological index values (A_{m}) of biodiesels were calculated according to Eqs. (6) or (7), respectively. Thirdly, two quantitative regression equations were obtained from the mixture topological index values and properties of biodiesels. Lastly, the coefficients of regression (R_{c}) of these two regression equations were compared and the better solution was chosen to illustrate the correlation of the mixture topological index values and properties of biodiesels.

Results and Discussion

The Calculation Process of Topological Index Value

It is known from Eq. (6), that the mixture topological index values of biodiesels are decided by the topological index

Table 2 Fatty acid methyl esters and their mass percentage of 11 types of biodiesels provided by Allen et al

Biodiesel type	C8:0	C10:0	C12:0	C14:0	C16:0	C18:0	C18:1	C18:2	C18:3	C22:1
Soybean	0	0	0	0.1	10.3	4.7	22.5	54.1	8.3	0
Rapeseed	0	0	0	0	2.7	2.8	21.9	13.1	8.6	50.9
Beef tallow	0	0.1	0.1	3.3	25.2	19.2	48.9	2.7	0.5	0
Peanut	0	0	0	0	10.4	8.9	47.1	32.9	0.5	0.2
Olive	0	0	0	0	11	3.6	75.3	9.5	0.6	0
Palm	0.1	0.1	0.9	1.3	43.9	4.9	39	9.5	0.3	0
Safflower	0	0	0	0.1	6.6	3.3	14.4	75.5	0.1	0
Sunflower	0	0	0	0.1	6	5.9	16	71.4	0.6	0
Cottonseed	0	0	0	0.8	22.9	3.1	18.5	54.2	0.5	0
Crambe	0	0	0	0	2.07	0.7	18.86	9	6.85	58.51
Linseed	0	0	0	0	4.92	2.41	19.7	18.03	54.94	0

value of individual components (FAME) and their mass percentage in the biodiesels. The fatty acid methyl esters components and their mass percentage for eleven biodiesels are tabulated in Table 2 [16].

$CH_3(CH_2)_6COOCH_3$ (Caprylic methyl ester, CME) is a common component of different biodiesel fuels, and its structure diagram is shown in Fig. 1.

The molar mass of CME is 0.158 kg/mol. Matrix R, R_i and the vertex degree matrix v_i of CME are obtained as follows.

Firstly, taking r_{15} as an example to illustrate the calculation process for matrix element r_{ij} of relative bond intensity matrix R:

$$\begin{aligned} r_{15} &= 2\ \text{Relative bond intensity(C--O)} \\ &\quad + 2\ \text{Relative bond intensity(C--C)} \\ &= 4.379 \end{aligned}$$

These relative bond intensities can be seen in Table 1.

Similarly, other matrix elements r_{ij} can be obtained, and the relative bond intensity matrix R of CME is shown as follows.

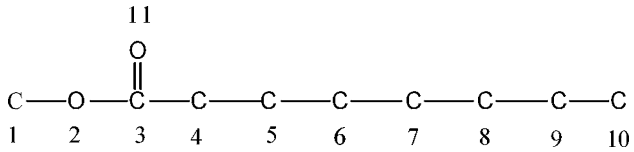

Fig. 1 The structure diagram of CME

Next, the matrix R_i is obtained by the summation of each column of matrix R.

$$R_i = [53.3139\ 42.6084\ 34.2819\ 31.2819\ 30.2819\ 31.2819\ 34.2819\ 39.2819\ 46.2819\ 55.2819\ 58.2819]$$

Finally, taking v_3 (double bond), v_{11} (hetero-atom) as examples, the vertex degree matrix v_i of CME is calculated as follows:

$$v_3 = (z^{\mathrm{v}} - h) = 4 \quad (z^{\mathrm{v}} = 4,\ h = 0)$$

$$v_{11} = (z^{\mathrm{v}} - h)/(z - z^{\mathrm{v}} - 1) = 6 \quad (z^{\mathrm{v}} = 6,\ h = 0,\ z = 8)$$

The vertex degree matrix v_i is obtained as follows:

$$v_i = [1\ \ 6\ \ 4\ \ 2\ \ 2\ \ 2\ \ 2\ \ 2\ \ 2\ \ 1\ \ 6]$$

$$R = \begin{bmatrix} 0 & 1.1895 & 2.379 & 3.379 & 4.379 & 5.379 & 6.379 & 7.379 & 8.379 & 9.379 & 5.0924 \\ 1.1895 & 0 & 1.1895 & 2.1895 & 3.1895 & 4.1895 & 5.1895 & 6.1895 & 7.1895 & 8.1895 & 3.9029 \\ 2.379 & 1.1895 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 2.7134 \\ 3.379 & 2.1895 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 3.7134 \\ 4.379 & 3.1895 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 4.7134 \\ 5.379 & 4.1895 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5.7134 \\ 6.379 & 5.1895 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 6.7134 \\ 7.379 & 6.1895 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 7.7134 \\ 8.379 & 7.1895 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 8.7134 \\ 9.379 & 8.1895 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 9.7134 \\ 5.0924 & 3.9029 & 2.7134 & 3.7134 & 4.7134 & 5.7134 & 6.7134 & 7.7134 & 8.7134 & 9.7134 & 0 \end{bmatrix}$$

The topological index value of CME is calculated according to Eq. (3), and the topological index value of CME is 0.2203.

The individual topological index value A_i of FAME is calculated and the process is similar. According to Eqs. (6) or (7), combined the A_i with mass percentage of FAME in biodiesel, the mixture topological index value A_m of biodiesel is calculated. For example, the mixture topological index value of Soybean oil is 0.3562 using Eq. (6) and 0.1300 using Eq. (7).

The mixture topological index values of biodiesels were calculated based on Eqs. (6) and (7), respectively, correlated with each property such as density, viscosity, flash point, cloud point, and higher heating value of biodiesel, respectively, so that the correlated precision can be compared by two regression coefficients (R_c).

Density

Density (D) is an important property of biodiesel, where it is the weight of a unit volume of fluid. The density of biodiesels was discussed in more recent literature [17].

The densities and topological index values of six types of biodiesels are tabulated in Table 3.

The correlation between the density (D) and the mixture topological index value (A_m) of biodiesel is expressed in regression Eqs. (8) and (9) respectively:

$$D^G = 981.3291 - 327.7233A_m^G \quad Rc = 0.9834 \tag{8}$$

$$D^H = 858.0202 - 18.7781A_m^H \quad Rc = 0.0972 \tag{9}$$

It can be seen that these two equations have a large difference in the coefficient of regression. The Hind equation shows a lower correlated precision.

Figure 2 shows the correlation results between the topological index values and densities of biodiesels. The densities of biodiesels decrease with increasing mixture topological index values.

Table 3 Density and topological index of six types of biodiesels

Biodiesel type	Density (g/L)		A_m^G	A_m^H
	D (experimental)	D^G (calculated)		
Crambe	848	849.0	0.4037	0.1578
Rapeseed	857	855.7	0.3834	0.1328
Sunflower	863	864.2	0.3573	0.1947
Soybean	865	864.6	0.3562	0.1300
Safflower	866	864.3	0.3571	0.2139
Palm	867	868.2	0.3453	0.1229

A_m^G, topological index calculated by the Grunberg–Nissan equation

A_m^H, topological index calculated by the Hind equation

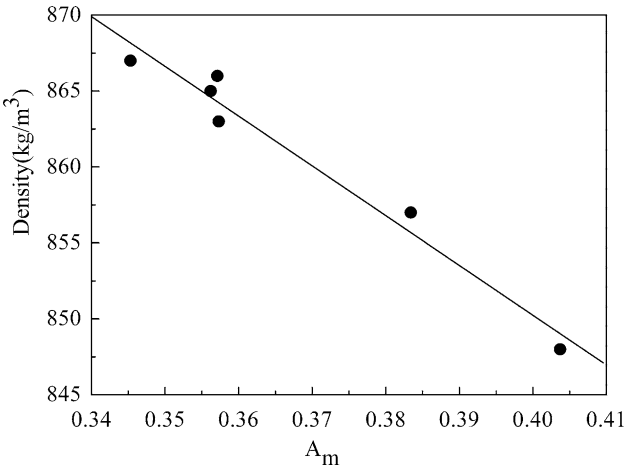

Fig. 2 Correlation between A_m^G and density for biodiesels

The properties of FAME are decided by their molecular structures. The topological index A is established based on the molecular structure of FAME so it can indicate the properties of FAME and biodiesels. The topological index values of individual components increase with increasing chain length (M) and saturation (R_i) from Eq. (3). The same rule is also applicable to the mixture topological index. Although the densities of individual components decrease with increasing chain length and increase with decreasing saturation. However, the decreasing effect of saturation is much less than the decreasing effect of chain length. Thus, the densities have smaller values when the biodiesels contain longer chain components. Accordingly, the densities of biodiesels decrease with an increase in mixture topological index values.

Viscosity

Viscosity is another important property of biodiesel since it affects the fluidity of the fuel and the operation of fuel injection equipment. High viscosity leads to poorer atomization of the fuel spray and less accurate operation of fuel injectors. The viscosity values of vegetable oil methyl esters are between 2.8 and 5.2 Cts and greatly decrease after transesterification process [8].

The viscosities [17] and topological index values of seven types of biodiesels are tabulated in Table 4.

The correlation between the viscosity (V) and the mixture topological index values (A_m) of biodiesel is expressed in regression Eqs. (10) and (11) respectively:

$$V^G = -3.0781 + 20.1877A_m^G \quad Rc = 0.9875 \tag{10}$$

$$V^H = 4.5752 - 1.6478A_m^H \quad Rc = 0.1567 \tag{11}$$

It can be seen that these two equations have a large difference in the coefficient of regression. The Hind equation shows a lower correlated precision.

Table 4 Viscosity and topological index of seven types of biodiesels

Biodiesel type	Viscosity (cts)		A_m^G	A_m^H
	V (experimental)	V^G (calculated)		
Crambe	5.12	5.07	0.4037	0.1578
Rapeseed	4.60	4.66	0.3834	0.1328
Olive	4.18	4.10	0.3558	0.2111
Sunflower	4.16	4.14	0.3573	0.1947
Soybean	4.08	4.11	0.3562	0.1300
Safflower	4.03	4.13	0.3571	0.2139
Palm	3.94	3.89	0.3453	0.1229

A_m^G, topological index calculated by the Grunberg–Nissan equation
A_m^H, topological index calculated by the Hind equation

Table 5 Flash point and topological index values of five types of biodiesels

Biodiesel type	Flash point (K)		A_m^G	A_m^H
	FP (experimental)	FP^G (calculated)		
Rapeseed oil	453	453.0	0.3834	0.1328
Soybean	441	439.6	0.3562	0.1300
Safflower oil	440	440.0	0.3571	0.2139
Sunflower	439	440.1	0.3573	0.1947
Palm	434	434.2	0.3453	0.1229

A_m^G, topological index calculated by the Grunberg–Nissan equation
A_m^H, topological index calculated by the Hind equation

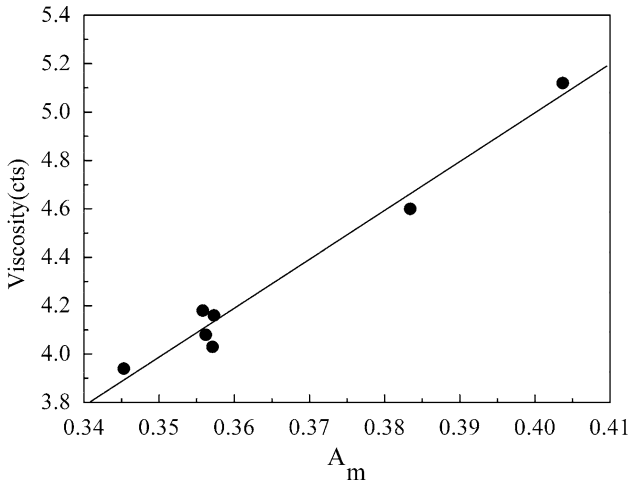

Fig. 3 Correlation between A_m^G and viscosity for biodiesels

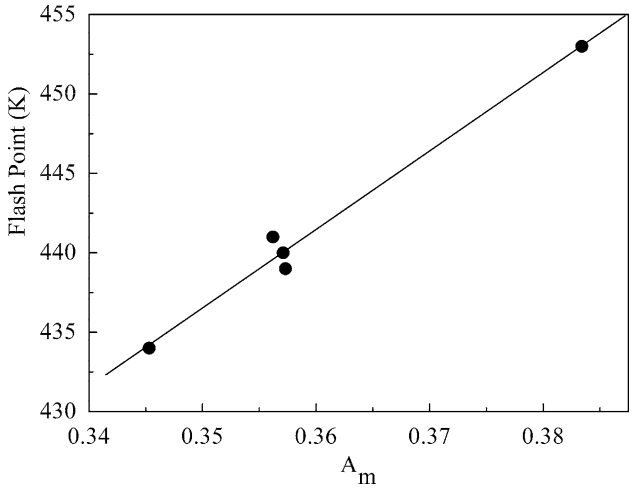

Fig. 4 Correlation between A_m^G and flash point for biodiesels

Figure 3 shows the correlation between the topological index values and viscosities.

The viscosities of individual components increase with increasing chain length and decrease with decreasing saturation. However, the decreasing effect of saturation is much less than the increasing effect of chain length. Thus the viscosities have larger values when the biodiesels contain more long chain components. Accordingly, the viscosities of biodiesels increase with an increase in the value of the mixture topological index values.

Flash Point

The flash point (FP) is the lowest temperature at which a liquid produces flammable vapor near its surface that will ignite when brought in contact with air and a spark or a flame.

Flash point is one of the most important and widely used flammability characteristics of liquids and low melting substances. It provides a simple, convenient index of the flammability and combustibility of substances since it provides the knowledge needed for the handling and transporting of the liquid in bulk quantities [18].

The flash points [17] and topological index values of five types of biodiesels are tabulated in Table 5.

The correlation between the flash point and the mixture topological index values (A_m) of biodiesel is expressed in regression Eqs. (12) and (13) respectively:

$$FP^G = 263.5402 + 494.2471A_m^G \quad Rc = 0.9916 \tag{12}$$

$$FP^H = 445.5889 - 26.3687A_m^H \quad Rc = 0.1584 \tag{13}$$

It can be seen that these two equations have a large difference in the coefficient of regression. The Hind equation shows the lower correlated precision.

Figure 4 shows the correlation between the topological index values and flash points.

The values of flash points of individual components increase with increasing chain length and decrease with decreasing saturation. However, the decreasing effect of

Table 6 Higher heating value (HHV) and topological index of six types of biodiesels

Biodiesel type	HHV (MJ/kg)		A_m^G	A_m^H
	HHV (experimental)	HHV^G (calculated)		
Rapeseed	41.55	41.54	0.3834	0.1328
Olive	41.35	41.30	0.3558	0.2111
Sunflower	41.33	41.32	0.3573	0.1947
Soybean	41.28	41.31	0.3562	0.1300
Safflower	41.26	41.32	0.3571	0.2139
Palm	41.24	41.22	0.3453	0.1229

A_m^G, topological index calculated by the Grunberg–Nissan equation
A_m^H, topological index calculated by the Hind equation

saturation is much less than the increasing effect of chain length. Thus the flash points have larger values when the biodiesels contain longer chain components. Accordingly, the values of flash points of biodiesels increase with increasing topological index values of the mixture.

Higher Heating Value

The higher heating value (HHV) is an important property defining the energy content and thereby efficiency of fuels. The HHV is obtained by an oxygen-bomb calorimeter method as the latent heat of moisture in the combustion products is recovered. The HHVs of biomass-derived fuels have been estimated using their proximate and ultimate analysis data [19].

The higher heating values [17] and topological index values of six types of biodiesels are tabulated in Table 6.

The correlation between the higher heating value and the mixture topological index values (A_m) of biodiesel is expressed in regression Eqs. (14) and (15) respectively:

$$HHV^G = 38.3080 + 8.4274A_m^G \quad Rc = 0.9455 \tag{14}$$

$$HHV^H = 41.4086 + 0.4389A_m^H \quad Rc = 0.1680 \tag{15}$$

It can be seen that these two equations have a large difference in the coefficient of regression. The Hind equation shows a lower correlated precision.

Figure 5 shows the correlation between the topological index and higher heating values.

The higher heating values of individual components increase with increasing chain length and decrease with decreasing saturation. However, the decreasing effect saturation is much less-than the increasing effect of chain length. Thus the higher heating values have larger values when the biodiesels contain longer chain components. Accordingly, the higher heating values of biodiesels increase with increasing mixture topological index values.

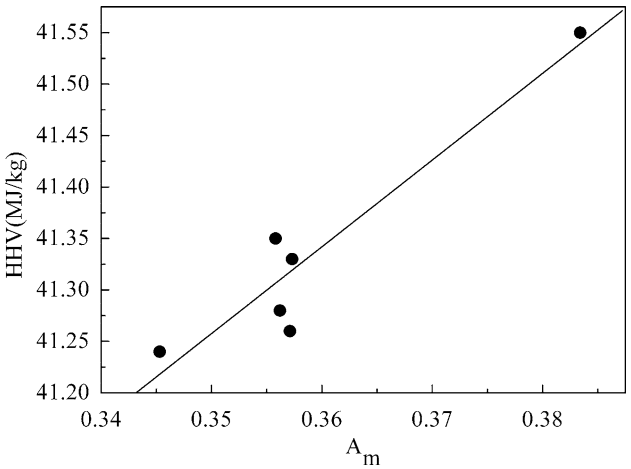

Fig. 5 Correlation between A_m^G and HHV for biodiesels

Table 7 The average relative errors (ARE)

	Density (g/L)	Viscosity (Cts)	Flash point (K)	HHV (MJ/kg)
ARE (%)	0.13	1.16	0.12	0.07

Average Relative Errors

The average relative errors (ARE) were calculated according to Eq. (16):

$$ARE\,(\%) = \frac{\sum |(y_E - y_C)/y_E|}{n} \tag{16}$$

here, y_E and y_C are experimental values reported in the literature and calculated values in this work, respectively.

The ARE of density, viscosity, flash point (FP) and high heating value (HHV) are presented in Table 7. It can be seen from this table, that values for all ARE is less than 2%. From the reported literature, the maximum allowable error for a prediction equation to estimate the viscosities of the ester mixtures was set at 5% [16]. So, the average relative error of less than 2% is acceptable.

Conclusion

Combining the novel topological index which contains more molecular structure information such as the molar mass, bond length and bond energy with the modified Grunberg–Nissan or Hind equations, the topological index values of biodiesel (mixture of FAME) were calculated then related with the density, viscosity, flash point and higher heating value of biodiesel, by using the QSPR model. The correlated results show that the Grunberg–Nissan equation more closely agrees with the properties of biodiesel than the Hind equation.

Due to the different effects of chain length and saturation toward the properties of FAME, the topological index values and the properties present different regression relations. It can be seen that the density of the biodiesel decrease with increase in topological index value. The viscosity, flash point and higher heating value of the biodiesel increase with increase in the topological index value.

Acknowledgments Financial support for this work from the National Basic Research Program of China (973 Program, 2009CB219906), National Natural Science Foundation of China (20776117) and Specialized Research Fund for the Doctoral Program of Higher Education of China (20070698037) are gratefully acknowledged.

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