PREDICTION OF THERMAL CONDUCTIVITY OF VEGETABLE OILS AND BIODIESELS AT SEVERAL TEMPERATURES

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Abstract. *Biodiesel is an alternative fuel produced from renewable sources (vegetable oils and animal fats) that can substitute oil diesel in engines and is considered, chemically, as a mixture of saturated and unsaturated methyl or ethyl esters of fatty acids. The behavior of thermal properties of the lubrification fluids and the fuel must be well understood when designing engines and other mechanical equipments. The experimental measurement of thermal conductivity of fluids is susceptible to deviations because convective currents are formed during the experiment and thermal losses are often common. Group-contribution methods are a very useful tool to estimate physical properties of organic compounds and they take in account, basically, the molecular structure of the substance. From the type of the group and the quantity of these, compound's property is estimated; however, some methodologies need another property of the substance. The objective of this work is the estimation of thermal conductivity of vegetable oil and its biodiesels at different temperatures by applying a estimation method based on group-contribution. The estimations were carried out into a temperature range between 20 and 100°C, in 10°C steps. The comparison between the estimated data and the experimental ones was satisfactory although some higher deviations were observed.*

Keywords*: Thermal conductivity, biodiesel, prediction, group-contribution.*

1. INTRODUCTION

It does not matter the way to obtain or employ the vegetable oils, knowing the thermophysical properties, such as density, viscosity, thermal conductivity and diffusivity, has a fundamental importance to accomplish the steps of the design of equipments, processes or even product specification (Brock *et al.*, 2008). In the biofuels' scenario, product specification concerning to its properties has importance on its utilization and processing too. Knowing physical and transport properties is essential for the design of pipes, reactors, heat exchangers, liquid-liquid extractors and these values are used as input parameters on simulation software and optimization processes.

Although, it is very difficult to measure experimentally some properties of organic substances. As example, the determination of thermal conductivity is complex due to the formation of convective streams and thermal losses during the experiment. Critical properties are not easy to measure and require an accurate control of measure system.

Except for some liquids, like those containing multi-hydroxy and multi-amine groups, the thermal conductivity of organic liquids decreases with temperature. Below or near the boiling point over small temperature ranges, the variation in thermal conductivity with temperature can be represented by

$$k = A - BT \tag{1}$$

where k is the liquid thermal conductivity ($W.m^{-1}.K^{-1}$) at temperature T (K) and A and B are constants that depend on the liquid (Sastri e Rao, 1999).

2. METHODOLOGY

The thermal conductivity of the fatty acids/methyl esters was estimated by the methodology proposed by Sastri and Rao (1999). From these estimations, the thermal conductivity of vegetable oils and biodiesels was carried out by applying the Eq. (2).

$$k_{o/b} = \sum x_i k_i \tag{2}$$

where $k_{o/b}$ is the themal conductivity of oil/biodiesel and x_i and k_i are, respectively, the molar fraction and the thermal conductivity of the i fatty acid/methyl ester.

The composition of vegetable oils was obtained from literature – Tab. 1. Here, it was considered a full-conversion of fatty acid to methyl ester. So, the fatty acid composition in the oil is the same of its respective methyl ester in biodiesel.

Table 1. Percentage of fatty acid in vegetable oils and methyl esters in biodiesel.

Fatty acid	Castor	Sunflower	Soy	Moringa	Corn	Coconut	Jartropha	Cotton	Canola	Palm
C10:0						6.0				0.1
C12:0						46.7				0.9
C14:0		0.1	0.1			18.3		0.8	0.1	1.3
C16:0	2.3	6.0	10.3	6.5	9.9	9.2	16.4	22.9	3.9	43.9
C18:0	3.0	5.9	4.7	6.0	3.1	2.9	5.4	3.1	3.1	4.9
C18:1	9.0	16.1	22.5	72.2	29.1	6.9	40.3	18.5	60.2	39.0
$C18:1_{1OH}$	80.3									
C18:2	4.5	71.4	54.1	1.0	56.8	1.7	37.0	54.2	21.1	9.5
C18:3		0.6	8.3		1.1			0.5	11.1	0.3
Ref.	[2]	[1]	[1]	[3]	[1]	[1]	[2]	[1]	[1]	[1]

[1] – Allen et al. (1999)
[2] – Peres and Lucena (2007)
[3] – Rashid et al. (2008)

The methodology proposed by Sastri and Rao (1999) can be resumed as a first-order group contribution method, in which:

$$k = k_B a^{\left\{1-\left[\frac{1-T_r}{1-T_{br}}\right]^n\right\}} \tag{3}$$

$$k_B = \sum \Delta k_B + \sum \Delta k_{cor} \tag{4}$$

where: k is the thermal conductivity of the compound, Tr is the reduced temperature, $T_{br} = T_b/T_c$, T_b is the boiling point (K), T_c is the critical temperature (K), $\Sigma\Delta k_B$ is the sum of incremental values of constituent groups and Δk_{cor} is the correction factor required for some specific cases. These two last parameters are given in Sastri and Rao (1999). Table 2 shows the incremental parameters (Δk_B) used in this work.

Table 2. Incremental parameters applied in this work.

Group	Δk_B (W.m^{-1}.K^{-1})
-CH3	0.0545
-CH2	-0.0008
=CH-	0.0020
-OH	0.0830
-COOH	0.0650
-COO-	0.0070

The critical temperature and the boiling point were estimated by the method proposed by Constantinou and Gani (1994). Detailing this methodology is out of the objective of this work.

3. RESULTS AND DISCUSSION

3.1. Vegetable oils

Figure 1 shows the estimation of thermal conductivity of vegetable oils with temperature. Figure 2 shows the comparison between some estimations and experimental measurements available on literature (Brock *et al.*, 2008); the deviations are between 2 and 15%. The data from the estimations, for each vegetable oil, were fitted according Eq (1) and its coefficients are presented on Table 3.

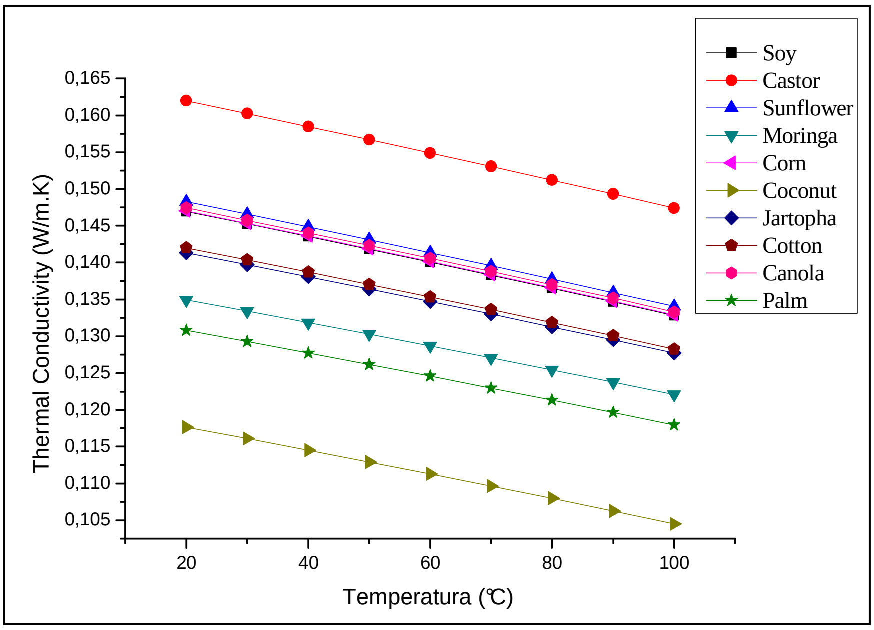
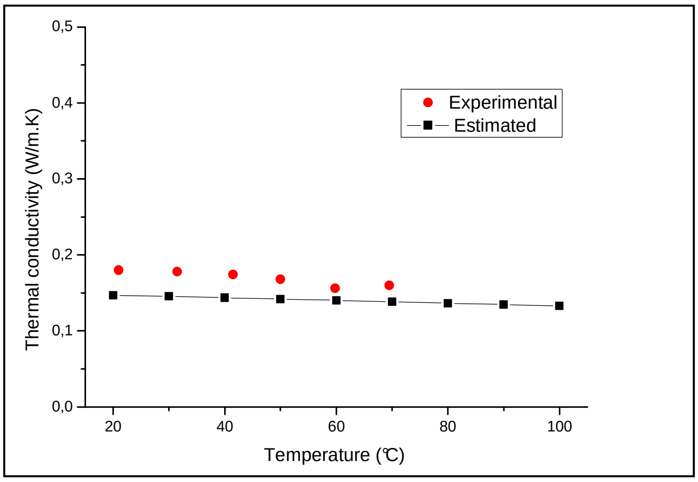
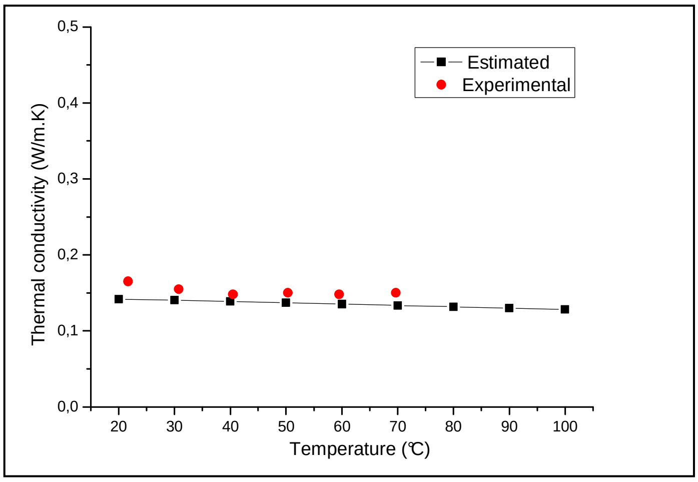


Figure 1. Estimation of thermal conductivity of vegetable oils with temperature.



(a)



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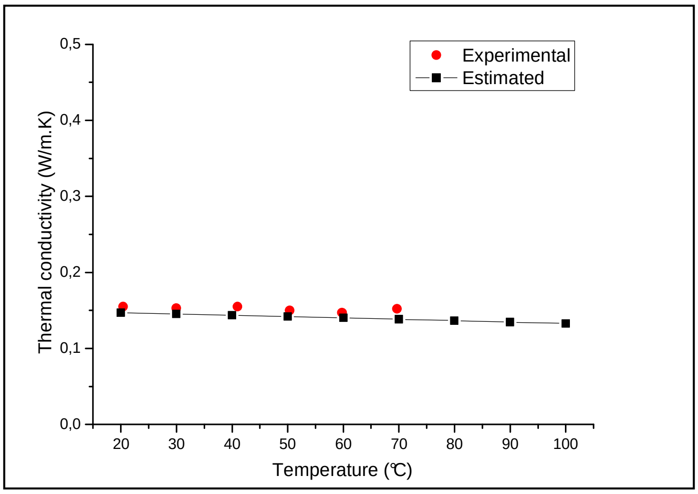

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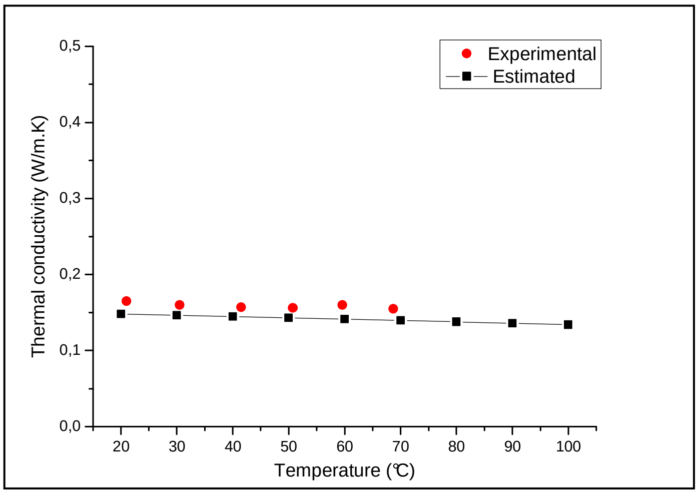

(d)

Figure 2. Comparison between experimental and estimated values for (a) soy, (b) cotton, (c) corn and (d) sunflower oil.

Table 3. Constants to correlate thermal conductivity and temperature – Eq (1)* - for vegetable oils.

Oil	A	B
Soy	0.1506	0.00020
Castor	0.1657	0.00019
Sunflower	0.1519	0.00017
Moringa	0.1382	0.00020
Corn	0.1507	0.00021
Coconut	0.1210	0.00021
Jartropha	0.1448	0.00019
Cotton	0.1455	0.00020
Canola	0.1511	0.00018
Palm	0.1341	0.00019

* Eq (1) with T in °C.

From the figures above, it is possible to notice that the thermal conductivity of vegetable oils decreases with temperature. This dependence is well described by Eq. (1) and the coefficients presented on Table 3. The values of thermal conductivities, for the ten oil plants, are very close; excepting to castor and coconut: the higher and the smaller one, respectively.

3.2. Biodiesels

Figure 3 shows the estimation of thermal conductivity of biodiesels with temperature. These data, for each biodiesel, were fitted according Eq (1) and its coefficients are presented on Table 4. Once experimental measurements of biodiesel thermal conductivity were not found on literature, it is not possible affirm anything about the accuracy of the estimations.

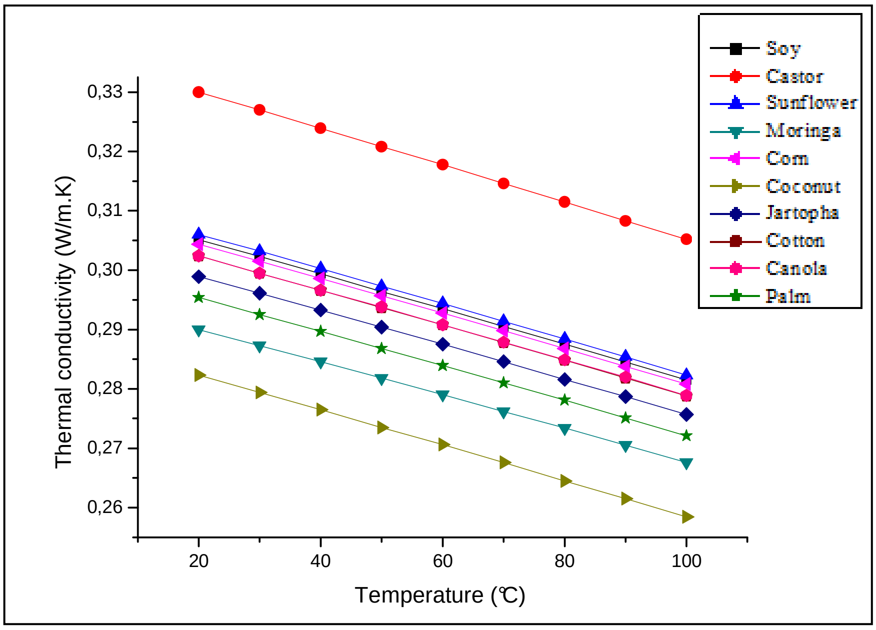

Figure 3. Estimation of thermal conductivity of biodiesel with temperature.

Table 4. Constants to correlate thermal conductivity and temperature – Eq (1)* - for biodiesels.

Biodiesel	A	B
Soy	0.3112	0.00030
Castor	0.3363	0.00032
Sunflower	0.3121	0.00033
Moringa	0.2957	0.00029
Corn	0.3104	0.00031
Coconut	0.2887	0.00030
Jartropha	0.3049	0.00029
Cotton	0.3084	0.00028
Canola	0.3083	0.00030
Palm	0.3013	0.00029

* Eq (1) with T in °C.

The values of the estimations - from Fig. (3) - shows an increase in the fluid's thermal conductivity when the oil is transformed into biodiesel. This increase helps in the heat transfer to burn the fuel.

4. CONCLUSION

The application of group-contribution methods to estimate the thermal conductivities of vegetable oils and biodiesels were investigated. These methods were efficient when applied to oils, with deviations between 2 and 15%. Concerning to the accuracy in biodiesel estimations, it is not possible to affirm anything once experimental values were not found on literature. The estimations show an increase in the thermal conductivity of biodiesel compared to the oil's. This increase makes more efficient the utilization of biodiesel as fuel once the heat transfer in burning is improved.

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