

# Prediction of Viscosities of Fatty Compounds and Biodiesel by Group Contribution

Roberta Ceriani,<sup>\*,†</sup> Cintia B. Gonçalves,<sup>‡</sup> and João A. P. Coutinho<sup>§</sup>

<sup>†</sup>Departamento de Processos Químicos, Faculdade de Engenharia Química, Universidade Estadual de Campinas, 13083-852 Campinas, Brazil

<sup>‡</sup>Faculdade de Zootecnia e Engenharia de Alimentos, Universidade de São Paulo, 13635-900 Pirassununga, Brazil

<sup>§</sup>Departamento de Química, Centro de Investigação em Materiais Cerâmicos e Compósitos (CICECO), Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

**ABSTRACT:** In the present work, a group contribution method is proposed for the estimation of viscosity of fatty compounds and biodiesel esters as a function of the temperature. The databank used for regression of the group contribution parameters (1070 values for 65 types of substances) included fatty compounds, such as fatty acids, methyl and ethyl esters and alcohols, tri- and diacylglycerols, and glycerol. The inclusion of new experimental data for fatty esters, a partial acylglycerol, and glycerol allowed for a further refinement in the performance of this methodology in comparison to a prior group contribution equation (Ceriani, R.; Gonçalves, C. B.; Rabelo, J.; Caruso, M.; Cunha, A. C. C.; Cavaleri, F. W.; Batista, E. A. C.; Meirelles, A. J. A. Group contribution model for predicting viscosity of fatty compounds. *J. Chem. Eng. Data* **2007**, *52*, 965–972) for all classes of fatty compounds. Besides, the influence of small concentrations of partial acylglycerols, intermediate compounds in the transesterification reaction, in the viscosity of biodiesels was also investigated.

## 1. INTRODUCTION

The industries dealing with vegetable and animal fats and oils are of increasing importance nowadays mainly because of the growth in the biodiesel production in the past few years. However, the models for the prediction of physical properties of fatty compounds, required for the design and evaluation of transport and separation processes involved, are still wanting.<sup>1–3</sup> This situation results in part from the lack of accurate experimental data, which has encouraged researchers to measure new experimental data for these systems, trying to map the behavior of fatty compounds under a variety of processing conditions.<sup>4,5</sup> Among physical properties, viscosity has been under attention in this area of research, especially for biodiesel compounds (mainly fatty esters), because of the influence of this transport property during fuel injection and combustion. Recently, Su et al.<sup>6</sup> and Díaz-Tovar et al.<sup>6</sup> presented a systematic development of computer-aided methods and tools related to the prediction of physical properties of fatty compounds.

Because of the nature of fatty compounds, the concept of group contribution is suitable and has been used extensively for the prediction of thermodynamic and transport properties,<sup>1</sup> as vapor pressure,<sup>7</sup> viscosity,<sup>8</sup> heat capacity,<sup>9</sup> critical properties,<sup>6</sup> and surface tension.<sup>6</sup> Zong et al.<sup>10</sup> developed a chemical constituent fragment approach for some thermophysical properties of partial acylglycerols rather than a function group approach, but their methodology is not extendable for the other classes of fatty compounds.

The release of new experimental data for viscosities of pure fatty esters<sup>4</sup> and the incapability of the model by Ceriani et al.<sup>8</sup> of dealing with the prediction of viscosities of partial acylglycerols (mono- and diacylglycerols), as pointed out by Freitas et al.<sup>2</sup> and Díaz-Tovar et al.,<sup>6</sup> encouraged us to develop a refined methodology for the prediction of this relevant transport property in the oil and fat industry.

This paper aims to develop a flexible group contribution method for estimating the viscosity of fatty compounds using the same set of functional groups as proposed by Ceriani et al.<sup>8</sup> but with a different temperature dependence. In fact, Freitas et al.<sup>2</sup> pointed out that the temperature-dependency behavior of the model by Ceriani et al.<sup>8</sup> in the prediction of viscosities of biodiesels could be related to the poor description of the viscosity of pure unsaturated fatty acid esters. To overcome the limitations mentioned above, the experimental data used for regression considered the recent values published by Pratas et al.<sup>4</sup> for methyl and ethyl fatty esters and also values for diacylglycerol<sup>11</sup> and glycerol<sup>12</sup> in conjunction with the databank gathered by Ceriani et al.<sup>8</sup>

The predictive capability of the proposed model was tested against experimental data from Freitas et al.<sup>2</sup> for biodiesel from sunflower, soybean, palm, and rapeseed oils considering not only the presence of methyl esters but also partial acylglycerols, intermediate compounds in the transesterification reaction, following information given by the authors. Experimental data measured in this work for fairly good conversion transesterification reactions, i.e., biodiesel (from rapeseed, soybean, and palm oils) with the presence of considerable amounts of partial acylglycerols, was also used as a test databank.

## 2. EXPERIMENTAL SECTION

**2.1. Samples.** In this work, three biodiesel samples were synthesized in our laboratory (CICECO) by transesterification reactions of rapeseed, soybean, and palm oils, using the same procedure described by

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**Table 1. Properties and Composition of Biodiesels in the Mass Fraction**

	palm	rapeseed	soybean
density at 20 °C (g/cm <sup>3</sup> )	0.8815	0.8846	0.8909
ester content (%)	85.35	92.05	78.89
FAME			
C10:0	0.024	0.010	
C12:0	0.298	0.042	0.064
C14:0	0.828	0.064	0.061
C16:0	34.539	4.864	8.711
C16:1	0.124	0.190	0.058
C18:0	3.584	1.576	3.101
C18:1	37.067	57.210	18.065
C18:2	8.020	19.180	41.882
C18:3	0.120	6.393	5.462
C20:0	0.345	0.542	0.292
C20:1	0.139	1.236	0.176
C22:0	0.136	0.337	0.450
C22:1	0.000	0.178	0.221
C24:0	0.126	0.227	0.347
MAG <sup>d</sup>			
monopalmitin	7.066		
monolein	7.584	5.954	6.362
monolinolein		1.996	14.748
MAG + DAG <sup>d</sup>			
monopalmitin	3.533		
monolein	3.792		3.181
monolinolein			7.374
dipalmitin	3.533		
dirolein	3.792		3.181
dilinolein			7.374

<sup>d</sup> In the case of biodiesels from palm and soybean, it was considered that their acylglycerol fractions could be represented not only by monoacylglycerol (MAG) but also diacylglycerol (DAG). In this case, the incompleteness of the transesterification reaction could lead to the presence of these two classes of fatty compounds together with methyl esters in the final mixture.

Freitas et al.<sup>2</sup> However, the reaction times were selected conveniently to guarantee an incomplete reaction conversion, i.e., the presence of partial acylglycerols in the final product. Our goal was to study the influence of these compounds in the viscosity of biodiesel and test the predictive capability of our methodology. Density and composition in terms of methyl esters and monoacylglycerols of these biodiesels are presented in Table 1. Dependent upon the extension of the transesterification reaction, the acylglycerol fractions of biodiesels were represented by MAG or MAG + DAG. The specific compounds were selected on the basis of their fatty acid methyl ester (FAME) compositions.

**2.2. Experimental Measurements.** Viscosities were measured as a function of the temperature (283.15–373.15 K) in a 5 K interval at atmospheric pressure using an automated SVM 3000 Anton Paar rotational Stabinger viscometer. The temperature uncertainty is 0.02 K from 288.15 to 378.15 K. The uncertainty is inferior to 0.5% at each viscosity data point measured for the standard fluid SHL120 (SH Calibration Service GmbH). The fluid viscosities range from 2.554 mPa s at 20 °C to 0.727 mPa s at 100 °C. This viscometer has been used in previous experimental works with very good reproducibility.<sup>2–4</sup>

### 3. MODEL DEVELOPMENT

The first step has been to collect experimental data other than the ones included in the databank of Ceriani et al.<sup>8</sup> for four classes

of fatty compounds (acids, esters, alcohols and acylglycerols). A total of 306 new experimental values of viscosity has been found for 17 types of substances (7 methyl and 8 ethyl esters, 1 diacylglycerol and glycerol). The distribution over the classes of compounds for the complete databank considered in this work (1070 experimental points) is shown in Table 2. As one can see, the databank covers a representative range of temperatures and carbon chain lengths.

The following functional groups, as suggested by Ceriani et al.,<sup>8</sup> are able to represent all of the molecular structures of the compounds in the database: CH<sub>3</sub>, CH<sub>2</sub>, COOH, CH=, OH, COO, and CH<sub>2</sub>–CH–CH<sub>2</sub>. The last group is related to glycerol and acylglycerols and describes this special structure.<sup>8</sup> The group contribution equation chosen to correlate viscosity  $\eta$ , in mPa s, of component  $i$ , and temperature,  $T$ , in K, has a different temperature dependency in relation to the model proposed by Ceriani et al.<sup>8</sup>

$$\ln(\eta_i(\text{mPa s})) = \left( \sum_k N_k A_{1k} + \frac{\sum_k N_k B_{1k}}{T(\text{K}) + \sum_k N_k C_{1k}} \right) + \left[ M_i \left( \sum_k N_k A_{2k} + \frac{\sum_k N_k B_{2k}}{T(\text{K}) + \sum_k N_k C_{2k}} \right) \right] + Q \quad (1)$$

where  $N_k$  is the number of groups  $k$  in the molecule  $i$ ,  $M$  is the component molecular weight that multiplies the “perturbation term”,  $A_{1k}$ ,  $B_{1k}$ ,  $C_{1k}$ ,  $A_{2k}$ ,  $B_{2k}$  and  $C_{2k}$  are parameters obtained from the regression of the experimental databank,  $k$  represents the groups of component  $i$ , and  $Q$  is a correction term expressed as<sup>8</sup>

$$Q = \xi_1 q + \xi_2 \quad (2)$$

where  $\xi_1$  and  $\xi_2$  are related to each class of compounds.

In eq 2,  $q$  is a function of the absolute temperature<sup>4</sup>

$$q = \alpha + \frac{\beta}{T(\text{K}) + \gamma} \quad (3)$$

where  $\alpha$ ,  $\beta$ , and  $\gamma$  are optimized parameters obtained by regression of the databank as a whole.

The effect of functional groups on the dynamic viscosity is corrected by the term  $Q$  according to the total number of carbon atoms  $N_c$  in the molecules, as in eq 4.  $\xi_1$  is a function of  $N_c$  applicable to all compounds and stated as follows:<sup>8</sup>

$$\xi_1 = f_0 + N_c f_1 \quad (4)$$

where  $f_0$  and  $f_1$  are optimized constants.

The term  $\xi_2$  describes the differences between the viscosity of isomer esters at the same temperature and is related to the number of carbons of the substitute fraction ( $N_{cs}$ ) as follows:<sup>8</sup>

$$\xi_2 = s_0 + N_{cs} s_1 \quad (5)$$

where  $s_0$  and  $s_1$  are optimized constants. Equation 5 is mainly used to account for the effect of the alcoholic portion of fatty esters. Considering that fatty esters are obtained from the reaction of fatty acids and short-chain alcohols (C<sub>1</sub>–C<sub>3</sub>), their molecules can be split into two parts;  $N_{cs}$  represents the number of carbons of the short-chain alcohol that reacted with the fatty acid to produce the fatty ester.<sup>8</sup> In this way,  $N_{cs}$  equals 1, 2, or 3, respectively, for methyl, ethyl, and propyl esters.

**Table 2. Experimental Databank for Viscosities of Fatty Compounds and Glycerol<sup>a</sup>**

class of compounds	FA	FE	FOH	TAG	DAG	glycerol
number of data points	284	543	97	115	2	11
references	7	4 and 7	7	7	10	11
carbon chain length	6–22	7–25	6–14	27–57	39	3
temperature range (°C)	20–121.1	5–100	15–100	20–170	38.8–98.8	20–100

<sup>a</sup>FA, fatty acid; FE, fatty ester; FOH, fatty alcohol; TAG, triacylglycerol; DAG, diacylglycerol.

**Table 3. Adjusted Parameters for eqs 1–5**

group	$A_{1k}$	$B_{1k}$	$C_{1k}$	$A_{2k}$	$B_{2k}$	$C_{2k}$
CH <sub>3</sub>	-1.1369	83.6969	-72.3043	-0.00003	0.0109	-3.439
CH <sub>2</sub>	-0.0691	54.7992	2.7245	0.00003	-0.0101	4.2745
COOH	-0.6459	108.8	-102.2	-0.0104	13.1121	828.0
CH=	0.0472	12.9121	3.272	-0.00021	0.0518	8.2213
OH	-2.9095	704.5	-58.3105	0.00162	-0.1905	0.0
COO	-0.2149	16.8636	16.4977	-0.00089	0.6796	-115.4
CH <sub>2</sub> -CH-CH <sub>2</sub>	2.2105	-128.9	21.8036	0.00149	-1.807	85.1661

compound	$f_o$	$f_i$	$s_o$	$s_i$
fatty acids	-3.5733	0.2758		
alcohols	-23.4011	3.4594		
esters	-0.6442	0.0479	0.0747	-0.0478
acylglycerols	13.9884	-0.0681		

$q$	$\alpha$	$\beta$	$\gamma$
	0.00127	0.6458	-273.5

Table 3 shows the adjusted values of the parameters in eqs 1–5, fitted using the Statistical Analysis System package (SAS, Cary, NC) with the regression method suggested by Marquardt.<sup>13</sup> The following objective function was used:

$$f = \sum_{j=1}^n \left[ \frac{|\eta_{\text{exp}} - \eta_{\text{calc}}|}{\eta_{\text{exp}}} \right] \quad (6)$$

where  $n$  is the number of experimental data considered and  $\eta_{\text{exp}}$  and  $\eta_{\text{calc}}$  are the experimental and calculated dynamic viscosities, respectively. We started adjusting  $A_{1k}$ ,  $B_{1k}$ , and  $C_{1k}$  for the functional groups of fatty esters and acids, followed by the addition of the other classes and their representative groups. The  $Q$  term was adjusted as a final trial.

#### 4. VISCOSITY OF BIODIESELS

The viscosities of biodiesels were calculated using the simplified Grunberg–Nissan equation.<sup>2</sup>

$$\ln \eta_{\text{mix}} = \sum_{i=1}^n x_i \ln \eta_i \quad (7)$$

The group contribution thermodynamics viscosity model (GC-UNIMOD) by Cao et al.<sup>14</sup> was also used in the prediction of viscosities of biodiesel (results not shown), but no substantial improvements were achieved, evidencing that biodiesel is a non-associated liquid, and therefore, its viscosity is well-described by eq 7.

Although values for viscosities of biodiesel from different sources are quite common in the literature, information regarding the biodiesel ester content, which is indicative of the progression of

**Table 4. ARD for Dynamic Viscosity of Fatty Compounds**

class of compounds	ARD <sup>a</sup> (RD maximum value – RD minimum value)	
	this work	Ceriani et al. <sup>4</sup>
fatty acids	3.21 (15.17–0.02)	5.51 (23.59–0.03)
fatty esters	2.69 (16.43–0.0004)	7.73 (50.89–0.003)
fatty alcohols	3.98 (16.86–0.02)	3.98 (10.42–0.02)
triacylglycerols	4.81 (32.79–0.03)	4.85 (47.37–0.003)
diacylglycerol	4.15 (10.73–0.21)	NA <sup>b</sup>
total	3.18 (32.79–0.0004)	6.46 (50.89–0.003)

<sup>a</sup>(ARD = 100 ×  $\sum_n (|\eta_{\text{exp}} - \eta_{\text{calc}}|/\eta_{\text{exp}})/N$ ). <sup>b</sup>NA = not applicable.

the transesterification reaction, is quite unusual. This information, as will be shown later, is essential in the prediction of viscosities of biodiesel, because of the influence of small amounts of partial acylglycerols (DAG and MAG) in this transport property. Recently, Freitas et al.<sup>2</sup> measured the viscosity of biodiesels (sunflower, soybean, palm, and rapeseed oils) as a function of the temperature, given their compositions in terms of FAME and ester contents (%). These data are used together with the experimental values measured in this work for fairly good reaction conversions for biodiesel of palm, rapeseed, and soybean oils.

#### 5. RESULTS AND DISCUSSION

Table 4 shows the average relative deviations (ARD =  $\sum_{i=1}^n 1/n [100|\eta_{\text{exp}} - \eta_{\text{calc}}|/\eta_{\text{exp}}]_i$ ) between experimental and estimated values of viscosities for the classes of compounds studied in this work. It can be seen that a good representation of

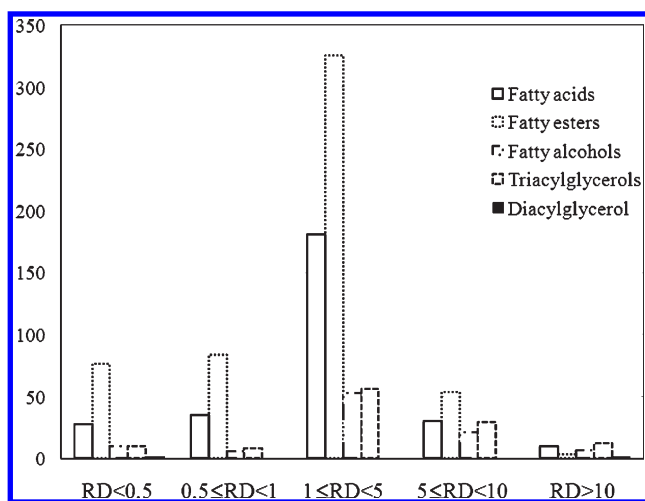


Figure 1. Distribution of the RD for each class of fatty compounds.

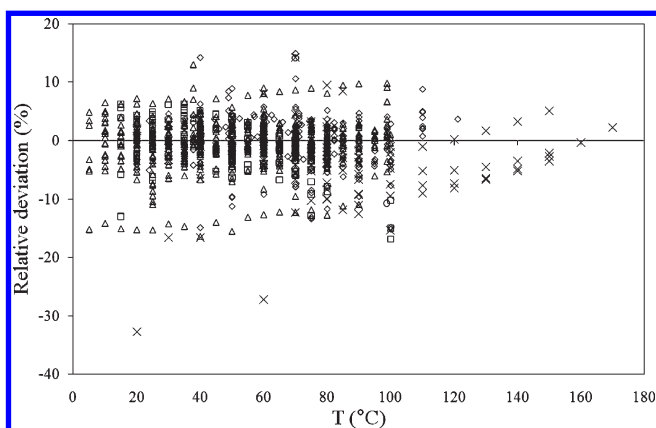


Figure 2. RDs between experimental and predicted dynamic viscosities using the model suggested in this work: ( $\diamond$ ) fatty acids, ( $\square$ ) fatty alcohols, ( $\triangle$ ) fatty esters, ( $\times$ ) triacylglycerols, and ( $\circ$ ) diacylglycerol.

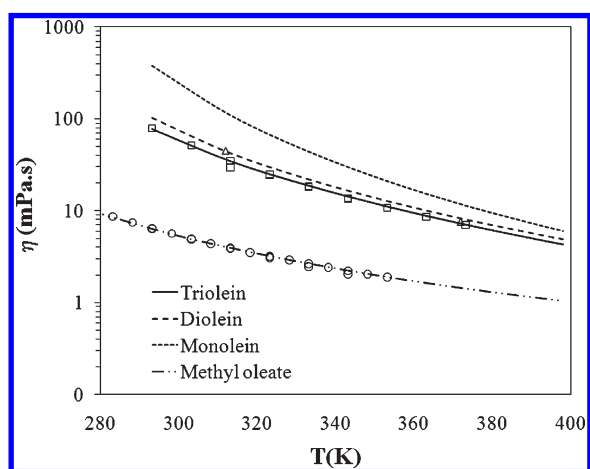


Figure 3. Predicted and experimental values for triolein, diolein, monolein, and methyl oleate. Legend for experimental data: ( $\circ$ ) methyl oleate, ( $\square$ ) triolein, and ( $\triangle$ ) diolein.

viscosity of fatty compounds has been achieved. In comparison to the model suggested previously by Ceriani et al.,<sup>8</sup> the new expression gives lower deviations for all classes of compounds

Table 5. Experimental Viscosities, in mPa s, for Biodiesels Measured in This Work

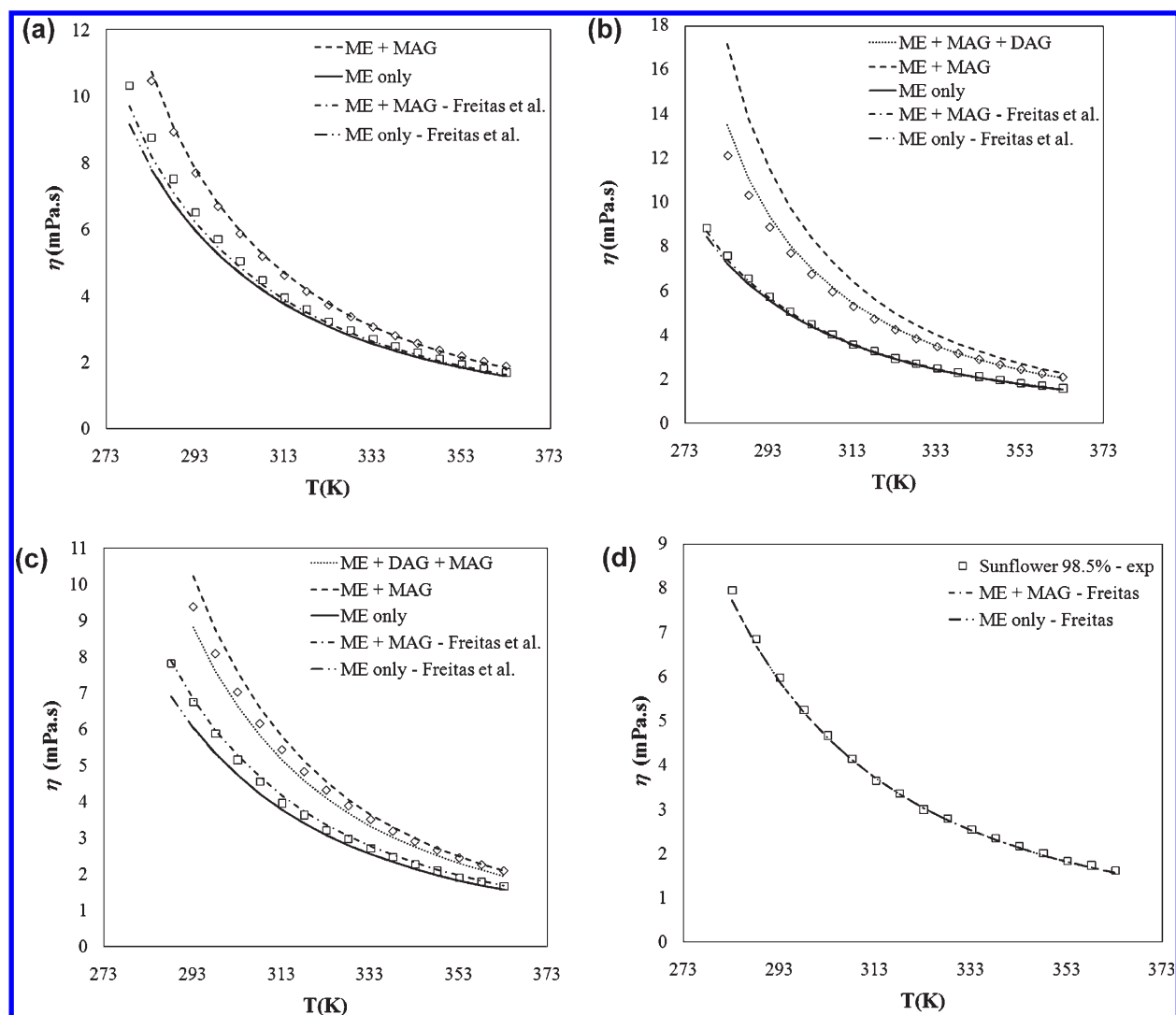
T (K)	viscosity (mPa s)		
	palm	rapeseed	soybean
273.15		10.471	12.070
273.15		8.933	10.282
293.15	9.376	7.699	8.845
298.15	8.082	6.695	7.679
303.15	7.022	5.873	6.725
308.15	6.152	5.193	5.934
313.15	5.431	4.622	5.273
318.15	4.827	4.140	4.706
323.15	4.315	3.728	4.228
328.15	3.880	3.375	3.819
333.15	3.504	3.070	3.461
338.15	3.182	2.806	3.158
343.15	2.902	2.574	2.892
348.15	2.657	2.369	2.654
353.15	2.443	2.190	2.441
358.15	2.255	2.030	2.252
363.15	2.088	1.887	2.087

with the exception of fatty alcohols, for which the same value was found. In fact, the inclusion of the experimental data by Pratas et al.<sup>4</sup> for esters and a few values found for diolein and glycerol improved its performance, lowering the maximum values of relative deviation (RD) of the model proposed here in comparison to the previous model by Ceriani et al. Figure 1 illustrates the distribution of the RD for each class of fatty compounds. As can be seen, most of the RDs are between  $\pm 1$  and  $\pm 5\%$  for all classes of compounds, and in the case of fatty esters, only 57 of the 543 experimental points were estimated with more than 5% deviation. Figure 2 shows a general distribution of the RDs ( $RD = 100|\eta_{exp} - \eta_{calc}|/\eta_{exp}$ ) for each fatty compound considered in the databank reported in Table 2. The results indicate that under- and overpredictions are well-distributed and that temperature dependency is not evident, except for some triacylglycerols over 120 °C. It is of note that the model was tested over a wide range of temperatures for 138 different fatty compounds in terms of the number of carbons and functional groups. No atypical profile was found, respecting the lower temperature limits shown in Table 2 and the melting temperature of each fatty compound. It should be highlighted that some compounds have dissimilar experimental viscosity values for the same temperature in our databank, which could explain a part of the RDs > 10% in Figure 1.

One interesting feature of the model developed in this work is that it allows for the estimation of viscosity values for fatty compounds for which experimental data is not available. Figure 3 illustrates the predicted and experimental values for triolein, diolein, monolein, and methyl oleate, which are important compounds in palm, soybean, and rapeseed oils and related products, such as biodiesel.

The viscosities of the three biodiesel samples measured in this work as a function of the temperature are reported in Table 5. Figure 4 shows the comparison between the viscosities of biodiesels of palm, sunflower, soybean, and rapeseed oils from Freitas et al.<sup>2</sup> with higher ester contents (96.5, 98.5, 99.4, and 98.8%, respectively) than ours (85.3, 78.9, and 92.1% for palm, soybean,





**Figure 4.** Predicted and experimental values for viscosities of biodiesels of palm, sunflower, soybean, and rapeseed oils from Freitas et al.<sup>2</sup> and biodiesels presented in Table 5: (A) rapeseed, (B) soybean, (C) palm, and (D) sunflower oils. Legend for experimental data: ( $\square$ ) Freitas et al.<sup>2</sup> and ( $\diamond$ ) this work. ME, methyl ester; MAG, monoacylglycerol; DAG, diacylglycerol, as in Table 1.

and rapeseed oils, respectively). The predicted curves, considering or not the presence of partial acylglycerols, are also shown. As one can see, the influence of small concentrations of monoacylglycerols and diacylglycerols (included just in the case of palm, 85.3%, and soybean, 78.9%) in the predictive capacity of our model is evident, even for the biodiesels by Freitas et al.,<sup>2</sup> which were produced from high conversion transesterification reactions. Taking into account the presence of partial acylglycerols allowed us to reduce the maximum ARDs observed to values lower than 4.7%.

## 6. CONCLUSION

We have presented a simple group contribution method for estimating the liquid viscosities of fatty compounds commonly found in biodiesel or edible oil industry processes as a function of the temperature. The new model has been compared to a previous model in the literature, and it has been found to be more accurate for all classes of compounds considered, besides being predictive for partial acylglycerols. Also, the capabilities of the proposed model were tested against biodiesel viscosities, considering the presence of partial acylglycerols with great accuracy.

## AUTHOR INFORMATION

### Corresponding Author

\*Telephone: +55-19-35213961. Fax: +55-19-35213965. E-mail: rceriani@feq.unicamp.br.

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## NOMENCLATURE

$A_{1k}, B_{1k}, C_{1k}, A_{2k}, B_{2k}, C_{2k}, f_o, f_1, s_o,$  and  $s_1$  = constants of eqs 1–5  
 $M_i$  = molecular weight of component  $i$   
 $N_c$  = total number of carbon atoms in the molecules

$N_{cs}$  = number of carbons of the alcoholic part in fatty esters

$N_k$  = number of groups  $k$  in the molecule

$T$  = temperature in K

### Greek Symbols

$\alpha$ ,  $\beta$ , and  $\gamma$  = constants of eq 3

$\eta$  = dynamic viscosity (mPa s)

### Subscripts

calc = calculated

exp = experimental

$i$  = component

$k$  = group of component  $i$

### Abbreviations

ARD = average relative deviation

exp = exponential

TAG = triacylglycerol

DAG = diacylglycerol

MAG = monoacylglycerol

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