# **Viscosity Prediction for Fatty Systems**

Juliana Rabelo, Eduardo Batista, Fl vio W. Cavaleri, and Antonio J.A. Meirelles\*

LASEFI (Physical Separation Laboratory), Food Engineering Department, State University of Campinas

(UNICAMP), Campinas, São Paulo, Brazil, 13083-970

ABSTRACT: Viscosity data have been measured as a function of temperature for two pure polyunsaturated fatty compounds (linoleic acid and trilinolein), for two multicomponent fatty systems, for a commercial-grade oleic acid (approximately 80% pure), and for canola oil. The measurements were performed in Cannon Fenske glass capillary kinematic viscometers. The contents of a large data bank, containing viscosity data for saturated, monounsaturated, and polyunsaturated pure fatty substances, were correlated by an equation based on the number of carbon atoms and double bonds. By using this equation for pure compounds and the UNIMOD group contribution method for mixtures, the viscosity data for model fatty systems, commercial oleic acid, and canola oil were predicted. The good results obtained in the present work indicate that this approach can be a valuable tool for designing or evaluating chemical process equipment for the oil industry.

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**KEY WORDS:** Canola oil, fatty acids, fatty mixtures, linoleic acid, oils, triglycerides, trilinolein, UNIMOD, viscosity, viscosity prediction.

Viscosity information on fatty mixtures and edible oils is essential for the design of heat transfer equipment, process piping, reactors, stripping columns, deodorizers, liquid extractors, distillation columns, crystallization equipment, and other units used in the oil and fat industry (1–5). Viscosity data on vegetable oils are also important for evaluating their use as alternative fuels and as base stocks for biodegradable lubricants (6,7). Despite this importance, viscosity estimation for fatty systems relies mainly on experimental measures and correlation of the experimental data.

Predictive methods are not often applied for estimating viscosities of fatty mixtures, although there are some successful examples of predictive methods used for calculating other physicochemical properties, such as densities of edible oils (8) and phase equilibria of fatty mixtures (9–12).

In the present work we have developed a generalized equation for calculating the viscosities of pure fatty compounds based on the number of carbon atoms and double bonds. To obtain a more significant set of parameters, we determined the

E-mail: tomze@ceres.fea.unicamp.br

viscosities of some polyunsaturated fatty substances (linoleic acid and trilinolein) not previously available in the literature. In the second part of this work, we used the UNIMOD equation (13) for estimating the viscosities of fatty mixtures. The prediction capacity of these equations was checked against the viscosities of some model fatty systems, commercial-grade oleic acid and canola oil; and the viscosities of these systems were also experimentally determined in the present work.

# **EXPERIMENTAL PROCEDURES**

Apparatus and measuring procedures. Viscosity data were obtained for linoleic acid ( $C_{18\cdot 2}$ ), trilinolein, a ternary mixture that contained capric acid ( $C_{10:0}$ ), oleic acid ( $C_{18:1}$ ) and tricaprylin, and a quaternary mixture composed of pelargonic  $(C_{9,0})$ , capric, lauric  $(C_{12,0})$ , and oleic acids. The solutions were prepared by mass, accurate to  $\pm 0.1$  mg, by using an analytical balance (Sartorius, Göttingen, Germany). Viscosities were also determined for a commercial-grade oleic acid (Riedel de-Häen, Germany) and for refined canola oil (Purilev, Brazil). The data were measured at temperatures above 20°C up to 90°C in glass capillary kinematic viscometers (sizes 75, 100, 150 and 200) from Cannon Fenske (Cannon Instrument Co., Pittsburgh, PA), immersed in a constant-temperature bath (Cole-Parmer Instrument Co., Niles, IL). This assembly maintains a temperature of ±0.05°C. Thermometers (Cole-Parmer Instrument Co.) with subdivisions of 0.1°C were used for monitoring bath temperature. The viscosities v, expressed in centistokes, were calculated from the efflux time  $\theta$  and the instrument constant c by using the following equation:

$$\upsilon = c\theta$$
[1]

Values for c were provided by the viscometer manufacturer, and the correction for temperature effects was considered. An electronic timer accurate to 0.01 s was used for measuring the efflux time. At each temperature, the viscosity was measured at least four times to give the average values presented in this work. All data correlations and predictions of experimental results were performed with version 6.12 of the Statistical Analysis System (SAS, Cary, NC) package.

*Materials and analytical procedures.* All pure chemicals were obtained from Sigma (St. Louis, MO), except for  $C_{18:2}$  and trilinolein, which were purchased from Nu-Chek-Prep (Elysian, MN). The acids had high purity (>99%), except for

<sup>\*</sup>To whom correspondence should be addressed at Food Engineering Department, Mail Box: 6121; UNICAMP, Cidade Universitária Zeferino Vaz, Campinas, SP, Brazil, Zip Code: Jao83-970.

 TABLE 1

 Composition of Commercial-Grade Oleic Acid and of Canola Oil

Fatty acid	Trivial name (abbreviation)	Commercial-grade oleic acid (mass %)	Canola oil (mass %)
14:0	Myristic (M)	1.88	0.10
16:0	Palmitic (P)	4.81	6.79
16:1	Palmitoleic (Po)	6.85	0.33
18:0	Stearic (S)	1.55	1.83
18:1	Oleic (O)	80.10	60.99
18:2	Linoleic (Li)	4.37	21.01
18:3	Linolenic (Le)	0.44	8.48
20:0	Arachidic (A)		0.32
22:1	Erucic (E)		0.15

 $C_{9:0}$  and  $C_{18:1}$ , which were 90 and 95% pure, respectively. The triglycerides had the following purities: 97–98% for tricaprylin and higher than 99% for trilinolein.

Linoleic acid, commercial-grade oleic acid, trilinolein, and canola oil were analyzed by gas chromatography of the fatty acid methyl esters according to Official Method 1-62 of AOCS (14). A Sigma 3b (PerkinElmer, Norwalk, CT) gas chromatograph with flame-ionization detector and integrator was used under the following conditions: stainless steel column with 0.125 in. external diameter and 4 m length, packed with 10% Silar 10C (10% cyanopropylsiloxane in Chromosorb W), nitrogen as the carrier gas at a rate of 25 mL/min, an injection temperature of 225°C, a column temperature of 175°C, and a detection temperature of 225°C. Samples were prepared in the form of fatty acid methyl esters according to the methodology developed by Hartman and Lago (15).

The chromatographic analysis confirmed the purity of linoleic acid as 99.3% and that of trilinolein as 99.2%. The purity of tricaprylin had also been confirmed in a prior study as 97.6% (16). The fatty acid composition of the commercial-grade oleic acid and of canola oil are shown in Table 1. From the data in Table 1, the triglyceride composition of the canola oil was estimated by using the procedure of Antoniosi Filho

TABLE 2	
Estimated Composition of Canola Oil <sup>a</sup>	

Group <sup>b</sup>	Principal triglyceride	M <sub>i</sub> (g/mol)	Mass (%)	Mole (%)
50:1	POP	833.37	0.86	0.90
50:2	PLiP	831.35	0.54	0.57
52:2	POO	859.40	8.91	9.09
52:3	POLi	857.39	6.53	6.68
52:4	POLe	855.37	3.80	3.90
52:5	PLiLe	853.36	1.02	1.05
54:2	SOO	887.46	2.17	2.14
54:3	000	885.44	23.99	23.76
54:4	OOLi	883.43	24.27	24.09
54:5	OOLe	881.41	17.85	17.76
54:6	OLiLe	879.40	7.58	7.56
54:7	OLeLe	877.38	2.49	2.49

 ${}^{a}M_{i}$ , molecular weight. For other abbreviations see Table 1.

<sup>b</sup>Isomer set including different triglycerides, but all with the same number of fatty acid carbons and double bonds. For example, Group 50:1 means the isomer set of triglycerides with 50 fatty acid carbons and one double bond.

*et al.* (17). This estimated composition is shown in Table 2. In this table, the principal triglyceride represents the component of major concentration in the isomer set with x fatty acid carbons and y double bonds. Groups with a total concentration of triglycerides less than 0.5% were ignored. For both reasons, some fatty acids (myristic, palmitoleic, arachidic, erucic) that appear in Table 1 do not appear explicitly in Table 2. A similar procedure has been employed by Batista *et al.* (12,18) for estimating the compositions of corn and canola oils. Such compositions were used by the authors in the correlation and prediction of liquid-liquid equilibrium data for systems that contained edible oils, fatty acids, and short-chain alcohols.

## **RESULTS AND DISCUSSION**

The kinematic viscosities for linoleic acid, commercial-grade oleic acid, trilinolein, and canola oil are tabulated in Table 3. The viscosity data for the mixtures are summarized in Table 4. The highest standard deviation observed in the experimental measures was 0.012 cSt and the lowest was 0.005 cSt, resulting in a mean standard deviation of 0.006 cSt for the whole set of experimental data. The highest coefficient of variation was 0.25%, suggesting an excellent reproducibility for the measured efflux times.

Viscosity correlation for pure fatty compounds. For corre-

#### TABLE 3

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Kinematic Viscosities of Linoleic Acid, Commercial-Grade Oleic Acid, Trilinolein, and Canola Oil

		Viscosity (c	St)	
Temperature (°C)	Linoleic acid (C <sub>18:2</sub> )	Commercial oleic acid	Trilinolein	Canola oil
20	_	39.206	_	79.251
30	17.452	27.252	34.896	52.104
40	13.193	18.854	25.269	36.084
50	10.313	14.285	18.881	26.167
60	7.962	11.105	13.213	19.663
70	5.808	8.782	10.247	14.956
80	4.574	7.067	7.493	11.951
90	3.864	5.775	6.011	9.749

IABLE 4	
Kinematic Viscosities of the Multicomponent Mixe	tures

	Visco	sity (cSt)
Temperature (°C)	Ternary mixture <sup>a</sup>	Quaternary mixture <sup>b</sup>
30	15.735	
40	11.566	
45		7.834
50	8.794	6.895
60	6.897	5.520
70	5.600	4.498
80	4.469	3.712
90	3.855	3.013

<sup>a</sup>Composition:  $C_{10:0} = 33.44$ ,  $C_{18:1} = 33.40$ , tricaprylin = 33.16 mass %. <sup>b</sup>Composition:  $C_{9:0} = 24.95$ ,  $C_{10:0} = 25.49$ ,  $C_{12:0} = 24.75$ ,  $C_{18:1} = 24.81$  mass %.

TABLE 5
Databank Used for Adjustment of the Parameters of Equations 2-5

		Temperature	
		range	
	Compound	(°C)	References
Fatty acids Triglycerides	C <sub>6:0</sub> , C <sub>7:0</sub> , C <sub>8:0</sub> , C <sub>9:0</sub> , C <sub>10:0</sub> , C <sub>12:0</sub> , C <sub>14:0</sub> , C <sub>16:0</sub> , C <sub>18:0</sub> , C <sub>18:1</sub> , C <sub>18:2</sub> , C <sub>22:1</sub> Tricaprylin, tricaprin, trilaurin, trimyristin, tripalmitin, tristearin, triolein, trilinolein	0–198 5–90	1, 22, 23, this work. 1, 24, this work.
Triglycerides	Tricaprylin, tricaprin, trilaurin, trimyristin, tripalmitin, tristearin, triolein, trilinolein	5-90	1, 24, this w

lating the pure fatty compound viscosities, we developed a generalized correlation following the procedure suggested by Cruz *et al.* (19) for a homologous series of poly(ethylene glycols). The dynamic viscosities ( $\eta$ ) for each fatty compound, expressed in 10<sup>-3</sup> Pa·s (= cP), were correlated by the following expression:

$$\ln \eta = A + B/(T - C)$$
<sup>[2]</sup>

where T represents absolute temperature, and A, B, and C are parameters determined by regression of the experimental data. The set of parameters A, B, and C obtained for each fatty compound class, acid or triglyceride was then correlated as a function of the number of carbon atoms and double bonds. The best results were obtained when a sigmoidal (Boltzmanntype) dependence on the number of carbon atoms and a quadratic dependence on the number of double bonds were assumed for the parameter A and a linear dependence on both were used for parameter C. The parameters were generalized as follows:

$$A = (A_1 - A_2) / \{1 + \exp[(n_C - A_3) / A_4]\} + A_2 + A_5 \times n_D^2$$
 [3]

$$B = B_1$$
 [4]

$$C = C_1 + C_2 \times n_C + C_3 \times n_D$$
<sup>[5]</sup>

where  $n_C$  and  $n_D$  are the number of carbon atoms, including the glycerol atoms in case of triglycerides, and double bonds, respectively.

Because part of the experimental measures available in the literature are kinematic viscosity data, we also used the prediction method described by Halvorsen *et al.* (8) for calculating the densities of fatty acids and triglycerides. For testing the predictive capacity of this method, we compared the experimental and calculated densities of the following compounds: fatty acids (pelargonic, capric, lauric, myristic, palmitic, stearic, oleic, and erucic) and triglycerides (tricaprin, trilaurin, trimyristin, tripalmitin, tristearin, triolein, trielaidin, trilinolein and trilinolenin). The average absolute deviation (AAD) was calculated according to Equation 6:

$$AAD = \left\{ \left[ \sum_{i=1}^{p} \left( \left| \rho_{i, \exp} - \rho_{i, \operatorname{cal}} \right| / \rho_{i, \exp} \right) \right] / p \right\} \times 100$$
[6]

where  $\rho_{i,exp}$  and  $\rho_{i,cal}$  are the experimental and calculated densities, respectively, and *p* is the number of experimental measures.

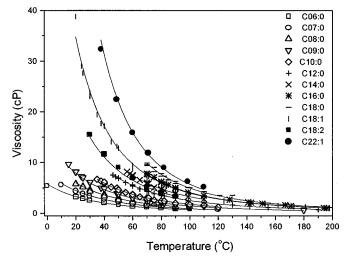
The experimental densities for the fatty acids were taken from Nourredini *et al.* (20) and those for triglycerides from Brockmann *et al.* (21) and Formo (22). The method works well for fatty acids, considering that the AAD was only 0.24%. For triglycerides, the AAD is higher (0.80%), but density data for such compounds are scarce in the literature. According to Halvorsen *et al.* (8), their method also works well for vegetable oils.

By using such estimated densities, we transformed the kinematic viscosity data into dynamic viscosities and built a comprehensive data bank, including viscosity data taken from the literature and the pure-compound viscosities determined in the present work (Table 5). This data bank was used for adjusting the parameters of Equations 2-5. The sets of parameters for each fatty compound class are given in Table 6, the first set being specific for fatty acids and the second one for triglycerides. AAD were 3.42 and 3.62% for fatty acids and triglycerides, respectively. The deviations were calculated according to Equation 6, substituting  $\rho_{i,exp}$  and  $\rho_{i,cal}$  by the experimental ( $\eta_{i exp}$ ) and calculated dynamic viscosities ( $\eta_{i calc}$ ), respectively. Figures 1 and 2 show the estimated and experimental results for each fatty compound class. As can be seen, the generalized equation allows a good estimation of the viscosities of the fatty compounds.

Viscosity prediction for fatty mixtures. Based on the group contribution concept, Cao *et al.* (13) developed the UNIMOD model for predicting the viscosities of multicomponent mixtures. In a way similar to the UNIFAC method (27), proposed for phase equilibrium, the UNIMOD equation takes into account two contributions for the mixture viscosity. The first one, named the combinatorial part, is related to the differences in size of the molecules present in the mixture, so that only properties for pure substances are considered in this contribution. The second one, the residual part, takes into consideration the energy of interaction between the different groups present in the mixture. The UNIMOD model is com-

TABLE 6Parameter Sets for Equations 2—5

Fatty	acids	Triglycerides			
$A_{1} = -6.09$ $A_{2} = -3.536$ $A_{3} = 5.40$ $A_{4} = 3.10$ $A_{5} = -0.066$	$B_1 = 1331.5$ $C_1 = 41.6$ $C_2 = 4.135$ $C_3 = -8.0$	$A_{1} = -4.01$ $A_{2} = -2.954$ $A_{3} = 28.9$ $A_{4} = 6.5$ $A_{5} = -0.0033$	$B_1 = 1156.$ $C_1 = 99.1$ $C_2 = 0.851$ $C_3 = -3.65$		



**FIG. 1.** Dynamic viscosities of fatty acids. The lines are correlation derivatives, and the points are experimental data.

municated in Equation 7:

$$\ln(\upsilon) = \sum_{i=1}^{n} \left[\xi_i^C + \xi_i^R\right],$$
[7]

1, 2, ..., *n* (number of components in the mixture)

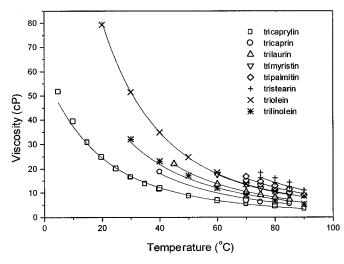
The combinatorial part is as follows:

$$\xi_i^C = \phi_i \ln\left(\upsilon_i \frac{M_i}{M}\right) + 2\phi_i \ln\left(\frac{x_i}{\phi_i}\right)$$
[8]

$$\phi_i = \frac{x_i r_i}{\sum_{j=1}^n x_j r_j}$$
[9]

$$r_i = \sum_{\substack{\text{all} \\ \text{groups } k}} v_k^{(i)} R_k$$
[10]

where  $M_i$ , M,  $r_i$ ,  $x_i$ ,  $R_k$ ,  $v_k^{(i)}$ ,  $v_i$ , v, and  $\phi_i$  are the molecular



**FIG. 2.** Dynamic viscosities of triglycerides. The lines are correlation derivatives, and the points are experimental data.

weight of component *i*, the mixture's molecular weight, the volume parameter for molecule *i*, the mole fraction of component *i*, the volume parameter for group *k*, the number of groups of type *k* in molecule *i*, the kinematic viscosity of pure compound *i* in cSt, the mixture viscosity in cSt, and the segment fraction, which is similar to the volume fraction of component *i*. Values for the group volume parameter  $R_k$  are obtained from the van der Waals group volume, given by Bondi (28). The values for  $R_k$  are taken from Fredenslund and Sorensen (29).

The residual part is represented by:

$$\xi_i^R = \sum_{\substack{\text{all} \\ \text{groups } k}} v_k^{(i)} \left[ \Xi_{ki} - \Xi_{ki}^{(i)} \right]$$
[11]

$$\Xi_{mi} = -\frac{Q_m}{R_m} N_{mi}^{\text{vis}} \phi_i \sum_{\substack{\text{all} \\ \text{groups } k}} \theta_{km} \ln(\Psi_{km})$$
[12]

where  $\Xi_{mi}$  is the group residual viscosity and  $\Xi_{ki}^{(i)}$  is the residual viscosity of group k in a reference solution that contains only molecules of type i. This last term is necessary to attain the normalization that the viscosity for the mixture v becomes the viscosity of pure compound i as  $x_i \rightarrow 1$ . Both terms,  $\Xi_{mi}$ and  $\Xi_{ki}^{(i)}$ , are calculated from Equation 12. Following are the expressions that define the other terms in the above set of equations:

$$\Psi_{mn} = \exp(-a_{mn}/T)$$
 [13]

$$\theta_{mn} = \frac{\theta_m \Psi_{mn}}{\sum_{\substack{\text{all} \\ \text{groups } k}} \theta_k \Psi_{kn}}$$
[14]

$$\theta_m = \frac{X_m \mathcal{Q}_m}{\sum_{\substack{\text{all} \\ \text{groups } k}} X_k \mathcal{Q}_k}$$
[15]

$$X_m = \frac{\sum_{i} x_i v_m^{(i)}}{\sum_{i} x_i \sum_{\substack{\text{all} \\ \text{groups } k}} v_k^{(i)}}$$
[16]

$$N_{ki}^{\text{vis}} = Q_k \left( \frac{q_i - r_i}{2} - \frac{1 - r_i}{z} \right)$$
[17]

and z = coordination number = 10

$$q_i = \sum_{\substack{\text{all}\\\text{groups }k}} v_k^{(i)} \mathcal{Q}_k$$
[18]

where  $X_k$ ,  $Q_k$ ,  $\theta_k$ ,  $q_i$ , and  $a_{mn}$  are the mole fraction of group k, the surface area parameter for group k (27,29), the area fraction of group k, the measure of the molecular surface area of component i, and the interaction parameter between groups mand n, respectively. There are two parameters ( $a_{mn} \neq a_{nm}$ ) for each pair of groups. For fatty acids and triglycerides, the following groups should be considered: CH<sub>2</sub> (with subgroups CH, CH<sub>2</sub>, and CH<sub>3</sub>), CH=CH (double bond), COOH (acid), and CH<sub>2</sub>COO (ester). Cao *et al.* (13) suggest taking the same

 TABLE 7

 Average Absolute Deviation (AAD) for Viscosities of Fatty Mixtures

	AAD (%)				
Mixtures	Without residual term	With residual term			
Binary <sup>a</sup>	3.40	3.20			
Ternary <sup>b</sup>	5.97	9.83			
Quaternary <sup>b</sup>	0.87	0.83			
Commercial oleic acid <sup>b</sup>	3.15	3.10			
Canola oil <sup>b</sup>	9.31	9.60			
Corn oil <sup>c</sup>					
"A"	9.90	10.15			
"B"	12.98	14.04			
Coconut oil <sup>c</sup>					
"A"	4.87	4.99			
"B"	1.52	1.60			

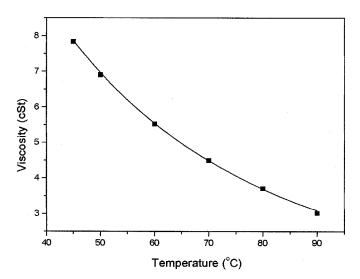
<sup>a</sup>Experimental data from Reference 1.

<sup>b</sup>Experimental data determined in this work.

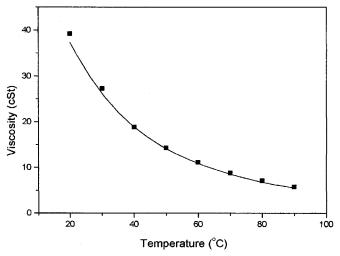
<sup>c</sup>Experimental data from Reference 2.

parameter values used for the UNIFAC-VLE (vapor-liquid equilibrium). Following this suggestion, we have used in the present work the group interaction parameters given by Fredenslund and Sorensen (29).

Using the generalized equation developed in this work for the pure compounds and the UNIMOD model for the mixtures, we have predicted the kinematic viscosities for many different fatty systems, including the data presented in this paper and some other data taken from the literature (1,2). Table 7 summarizes the obtained values for AAD. They were calculated according to Equation 6, substituting  $\rho_{i,exp}$  and  $\rho_{i,cal}$  by the experimental ( $v_{i,exp}$ ) and calculated ( $v_{i,cal}$ ) kinematic viscosities, respectively. Figures 3, 4, and 5 show the experimental and calculated kinematic viscosities for the quaternary mixture of fatty acids, the commercial-grade oleic acid and canola oil, respectively. The predictions are often good, especially considering the complexity and the large



**FIG. 3.** Kinematic viscosities for the quaternary mixture (composition:  $C_{9:0} = 24.95$ ,  $C_{10:0} = 25.49$ ,  $C_{12:0} = 24.75$ ,  $C_{18:1} = 24.81$  mass %). The line is a correlation derivative, and the points are experimental data.

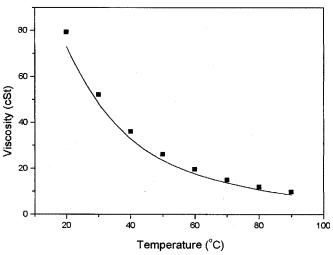


**FIG. 4.** Kinematic viscosities for commercial-grade oleic acid. The line is a correlation derivative, and the points are experimental data.

number in compounds of some systems, such as in canola oil.

For canola oil, we have also considered the possibility of estimating the viscosity by using only the generalized equation. The oil was treated as a pseudo-compound with approximately its average molecular weight (Table 2) and an average number of carbon atoms and double bonds rounded to the closest integer. This pseudo-compound was a triglyceride similar to OOLi, with 57 carbon atoms, 4 double bonds and a molecular weight of 883.43 g·mol<sup>-1</sup>. The triglyceride OOLi is exactly the principal triglyceride of the isomer set with the major concentration in canola oil. The value for the AAD was 9.79%, slightly higher than the AAD obtained with the UNI-MOD model (Table 7).

The methodology was further tested by predicting some of the viscosity data determined by Noureddini *et al.* (2). The authors give the composition of the vegetable oils used in their work according to the fatty acid class: saturated, mono-



**FIG. 5.** Kinematic viscosities for canola oil. The line is a correlation derivative (UNIMOD equation with residual term), and the points are experimental data.

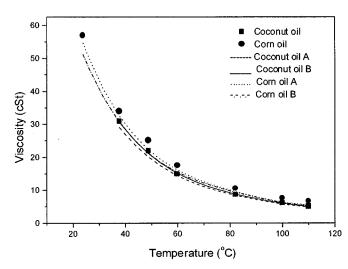
 TABLE 8

 Estimated Fatty Acid Composition for Corn and Coconut Oils<sup>a</sup>

			Corn oil		Coconut oil		
Fatty acid		Ref. 20	"A"	"B"	Ref. 20	"A"	"B″
Saturated	C <sub>6:0</sub>		0.00	0.00		0.80	0.41
	C <sub>8:0</sub>		0.00	0.00		9.02	7.22
	C <sub>10:0</sub>		0.00	0.00		10.02	8.25
	C <sub>12:0</sub>		0.00	0.00		52.11	49.54
	C <sub>14:0</sub>	14.30	0.00	0.00	94.00	13.03	16.51
	C <sub>16:0</sub>		8.80	11.00		8.02	9.80
	C <sub>18:0</sub>		5.50	3.30		1.00	2.06
	C <sub>20:0</sub>		0.00	0.00		0.00	0.21
Monounsat.	C <sub>16:1</sub>		0.09	0.44		0.00	0.36
	C <sub>18:1</sub>	21.40	21.31	20.96	5.00	5.00	4.64
Polyunsat.	C <sub>18:2</sub>		64.30	54.90		1.00	1.00
	C <sub>18:3</sub>	64.30	0.00	9.40	1.00	0.00	0.00

<sup>a</sup>"A" and "B" are two different concentrations that were estimated by information given by Nourredini *et al.* (20) and Sonntag (30). For further details see text.

unsaturated, and polyunsaturated fatty acids (20). Combining this information and the detailed fatty acid composition given by Sonntag (30), we have estimated two fatty acid compositions for each oil. They are presented in Table 8. The triglyceride compositions of these oils were then estimated, taking into account that coconut oil has a content of trisaturated triglycerides in the range of 84 to 89% (30,31), and corn oil has 0% of the same class of triglycerides. The deviations between predicted and experimental viscosities are given in Table 7. The results are shown in Figure 6. The simultaneous use of the generalized equation for pure compounds and the UNIMOD model predicts the coconut oil viscosities well for both estimated compositions. For corn oil, the deviations are higher, but by considering exclusively the temperature range of 0-90°C, the AAD for corn oil "A" reduces to 7.75%. This range coincides with the temperature range used in the experimental determination of the viscosities of the pure triglyc-



**FIG. 6.** Kinematic viscosities for corn and coconut oils. The lines are correlation derivatives (UNIMOD equation with residual term: —— coconut A, ----- corn B), and the points are experimental data ( $\blacksquare$  coconut,  $\bullet$  corn).

erides (see Table 6).

The AAD for canola and corn oils are comparatively higher than those obtained for coconut oil and most model systems. Probably the reason for that behavior is the high concentration of polyunsaturated triglycerides in those oils that cannot be well described by the set of parameters taken from the UNIFAC-VLE data bank. The inclusion of the residual term gives better predictions for most model systems and the commercial-grade oleic acid; however, especially for the ternary mixture and for canola and corn oils, the predictions become worse when this term is included (see Table 7). The ternary mixture, in contrast to the other systems studied in the present work, is the only one that includes simultaneously fatty acids and a triglyceride. A readjustment of some interaction parameters, especially those reflecting the interactions between groups such as CH=CH, COOH and CH<sub>2</sub>COO, should be considered in future work.

For comparison purposes some prediction results reported in the literature should be mentioned. Cao *et al.* (13) reported deviations in the range of 2.7 to 5.3% for predictions of the viscosities of mixtures with the UNIMOD model. They used a large data bank, including mostly binary mixtures of alkanes, alcohols, ketones, ethers, and esters, but also some ternary and quaternary systems.

Considering such reported deviations and the complexity of the systems used in the present work, we conclude that the simultaneous use of the generalized equation for pure compounds and the UNIMOD model often gives satisfactory viscosity predictions for fatty mixtures. The proposed approach to viscosity prediction can be a valuable tool for designing or evaluating chemical process equipment for the oil industry.

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