Density and Viscosity of Vegetable Oils

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ABSTRACT: A generalized method was developed to estimate the liquid density of vegetable oils and fatty acids. The correlation for vegetable oils was based on fatty acid critical properties and composition of the oil. The correlations predicted the density of vegetable oils and fatty acids with an average absolute deviation of 0.21 and 0.77%, respectively. The present method is slightly more accurate in predicting vegetable oil density and simpler than the method of Halvorsen *et al*. Also, a method is introduced that predicts viscosity from density data, thus relating two key properties of vegetable oils.

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The importance of vegetable oils in industries such as foods, soaps, cosmetics, and pharmaceuticals has been well documented (1,2). The estimation of the density and viscosity of vegetable oils is essential in the design of unit processes such as distillation, heat exchangers, piping, and reactors.

For vegetable oils, it has been shown that density decreases linearly with increases in temperature (1). This correlation takes the simple form:

$$\rho = b + m\,T \qquad [1]$$

where ρ is the density, T is the temperature, b is the intercept, and m is the negative slope. In Equation 1, the density decreases by about 0.00064 g/cm^3 per temperature increase of 1°C (1), and the constants are different for each of the oils.

A widely used method for the prediction of the density of vegetable oils was developed by Lund, which is discussed by Halvorsen *et al.* (3). The Lund relationship is:

$$\text{sg (15/15°C)} = 0.8475 + 0.00030\ \text{SV} + 0.00014\ \text{IV} \qquad [2]$$

where sg is the specific gravity of the vegetable oil at 15°C, SV is the saponification value, and IV is the iodine value of the oil. Equation 2 can be used for a wide variety of oils. Halvorsen *et al.* (3) examined the use of the modified Rackett equation to estimate the density of vegetable oils and compared the results to the Lund equation. This method makes use of the fatty acid composition and respective critical properties for each of the oils. Halvorsen *et al.* use the following equation to estimate the density of vegetable oils:

$$\rho_{\text{oil}} = \frac{(\Sigma x_i \text{MW}_i)}{R\left(\Sigma \dfrac{x_i T_{c_i}}{P_{c_i}}\right)\left(\Sigma x_i Z_{\text{RA}_i}\right)\left[1 + (1 - T_r)^{2/7}\right]} + F_c \qquad [3]$$

where ρ_{oil} is the density of the vegetable oil, R is the universal gas constant, T_r is the reduced temperature, and F_c is a correction factor characteristic of the oil (3). For each fatty acid component, x_i is the mole fraction, MW$_i$ is the molecular weight, P_{ci} is the critical pressure, Z_{RA_i} is the Rackett parameter, and T_{ci} is the critical temperature. The reduced temperature is defined as:

$$T_r = \frac{T}{T_{c,\text{mix}}} \qquad [4]$$

where

$$T_{c,\text{mix}} = \Sigma x_i T_{c_i} \qquad [5]$$

The correction factor is given by the relation:

$$F_c = 0.0236 + k\ |875 - \text{MW}_{\text{oil}}| \qquad [6]$$

The value of the constant k is equal to 0.000082 when the molecular weight of the oil is greater than 875, and equal to 0.000098 when the molecular weight is less than 875.

The molecular weight of the oil is defined as:

$$\text{MW}_{\text{oil}} = 3\ \Sigma x_i \text{MW}_i + 38.0488 \qquad [7]$$

Halvorsen *et al.* state that the results of Equation 3 predict density data within an average absolute deviation of 0.14%, as compared to 0.16% for the Lund equation.

Experimental liquid viscosity data have been shown to generally follow the well-known Andrade equation:

$$\ln \eta = A + \frac{B}{T} \qquad [8]$$

where η is the viscosity and T is the absolute temperature. Noureddini *et al.* (4) introduced a third constant to Equation 8 to predict the viscosities of oils with a mean deviation of less than 2%. To determine the constants in Equation 8 for each of the individual oils, experimental data are required.

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Dutt and Prasad (5) presented two generalized relations for the prediction of the viscosity of fatty oils based on the coefficients of an Antoine-type equation. The first equation developed related the viscosity of the oil to the ratio of iodine value over the saponification value (IV/SV):

$$\log \eta = (-1.4 + 1.25\frac{\text{IV}}{\text{SV}}) + (500 - 375\frac{\text{IV}}{\text{SV}})/[T + 140) - 85\frac{\text{IV}}{\text{SV}}] \quad [9]$$

where η is the viscosity in centipoise and T is the temperature in °C. The second equation developed related the viscosity of the oil to temperature:

$$\log \eta = -0.6298 + [273.66/(T + 88.81)] \quad [10]$$

Dutt and Prasad state that the results of Equations 9 and 10 predict viscosity of vegetable oils with an average absolute deviation of 13.0 and 14.5%, respectively.

A new generalized method to estimate the density of vegetable oils is presented in this paper. Vegetable oils primarily consist of fatty acids in the form of triglycerides. The exact composition of a vegetable oil varies depending on certain conditions such as climate. Physical property estimation results of vegetable oils thus depend on the composition used. As the composition of vegetable oils is restricted to a fairly homologous series, a relationship between reduced properties of the oils is examined. The new generalized method was developed using critical temperature and critical pressure fatty acid data found in Halvorsen *et al.* (3). The present method is somewhat simpler and is slightly more accurate than the modified Rackett estimation presented by Halvorsen *et al.* (3). The new method of estimating the density of vegetable oils is also extended to predict the viscosity of these oils thus relating two key physical properties of the oils. The relationship developed in this paper to estimate viscosity of vegetable oils is similar in accuracy to the generalized methods given by Dutt and Prasad (5).

Experimental density data were gathered for 14 different vegetable oils (1,6–13). An examination of the literature data shows trends of increasing density with increases in the level of unsaturation, and decreasing with increases in molecular weight.

The new method to predict the density of vegetable oils was developed with a plot of reduced density vs. reduced temperature. The reduced density was defined as:

$$\rho_r = \frac{\rho}{\rho_c} \quad [11]$$

where ρ is the experimental density (kg/m^3) and ρ_c is the critical density of the oil. The critical density is defined as:

$$\rho_c = \frac{\Sigma x_i \text{MW}_i}{R\left(\Sigma \frac{x_i T_{c_i}}{P_{c_i}}\right)} \quad [12]$$

The reduced temperature is defined in Equation 4. For each of the oils, the reduced density formed a linear relationship with reduced temperature. In general, at a given reduced temperature, the higher the molecular weight of the oil, the greater the reduced density. Oils with molecular weights within a range of approximately 2% of each other for a given reduced temperature had similar reduced densities. In an attempt to have all the data form one linear relationship, the equation for the reduced density was adjusted. The equation was corrected by defining a new reduced density as:

$$\rho' = \rho\left(\frac{A}{\rho_c} + B\right) \quad [13]$$

Figure 1 is a plot of the corrected density vs. reduced temperature. In Equation 13, the variable A equals 29.73 and B equals 2.00. The sum of the molecular weights of the fatty acids can also be used to correlate the density with reasonable accuracy:

$$\rho'' = \rho(A^*\Sigma x_i \text{MW}_i + B^*) \quad [14]$$

Figure 2 is a plot of the density adjustment based on the molecular weight of the fatty acids vs. reduced temperature. In Equation 14, the variable A^* equals 0.00022 and B^* equals 0.58. Table 1 shows a comparison of the results of Equations 13 and 14 along with the modified Rackett equation (Eq. 3) proposed by Halvorsen *et al.* (3). The method of using critical density to adjust the density of the oil is slightly more accurate than Equation 3 in predicting the density of vegetable oils within an absolute average deviation of 0.21%. A regression analysis of the results gave an R^2 value of 0.987 for Equation 13, as compared to 0.976 for Equation 3. Equation 13 is simpler than the modified Rackett equation in that it does not use a variable that needs to be determined experimentally. Equation 3 contains Z_{RA}, which is specific to each fatty acid and needs to be determined with known density data. Equation 13 also does not have a correction factor specific to each vegetable oil, such as F_c in Equation 3. Equation 14 uses molecular weight to adjust the density of the oil and it is as accurate as the modified Rackett equation in predicting the density of vegetable oils. The average absolute devia-

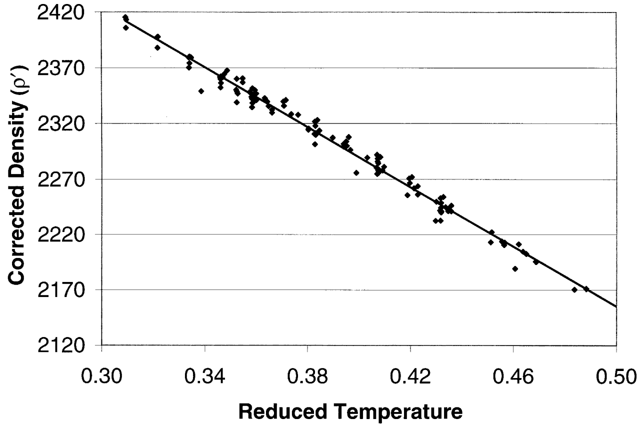

FIG. 1. Generalized correlation of the density of vegetable oils based on critical density.

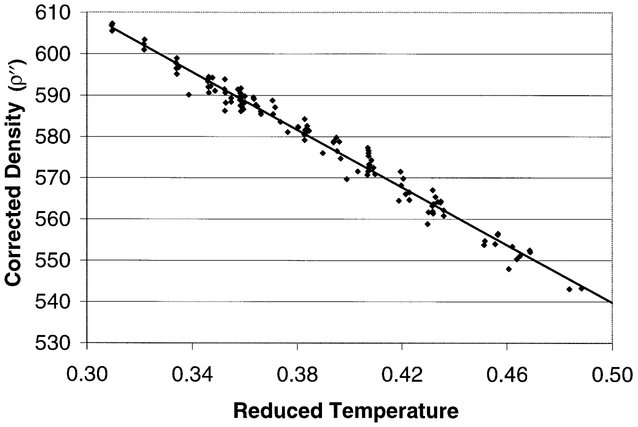

FIG. 2. Generalized correlation of the density of vegetable oils based on molecular weight.

tion is 0.28%. The R^2 value of Equation 14 is 0.981. This method is simpler than using the critical density adjustment (Eq. 13) in that it does not require critical pressure data, which can be difficult to estimate. An examination of the results of Table 1 shows that the new methods seem to predict vegetable oils with different molecular weights and levels of unsaturation with an equivalent degree of accuracy. Equations 13 and 14 can be used to predict the density of pure fatty acids that are part of the composition of vegetable oils. Experimental density data were gathered for 16 fatty acids (1,6,12–15, 17–21). For the prediction of the density of fatty acids, the constant A in Equation 13 is 39.10, and B is 1.93. The average absolute deviation predicted by Equation 13 for the density of fatty acids is 0.80%. For the prediction of the density of fatty acids, the constant A^* in Equation 14 is 0.000011, and B^* is 0.019. The average absolute deviation predicted by Equation 14 for the density of fatty acids is 0.77%. Figures 3 and 4 show the corrected density plotted against reduced temperature for pure fatty acids. The modified Rackett equation used by Halvorsen *et al.* (3) predicts the gathered fatty acid density data within an average absolute deviation of 0.20%. Table 2 shows the results of these predictive methods. Halvorsen *et al.* also reviewed other methods to predict the density of fatty acids. Though Equations 13 and 14 do not predict fatty acid densities as accurately as the modified Rackett equation (Eq. 3), both have the advantage of not having a variable that needs to be fitted to experimental data and fewer parameters.

Viscosity data were gathered for 12 vegetable oils from different literature sources (1,4,7,11,14–16). An examination of the literature data shows trends of viscosity decreasing with increase in level of unsaturation and increasing with increase in molecular weight.

An empirical relation between velocity of sound in a liquid and viscosity was given by Parthasarathy and Bakshi (22). The relation is:

$$\frac{U^{1/3}}{\rho} = A + \frac{B}{\eta^{1/2}} \qquad [15]$$

where U is the velocity of sound and η is the viscosity in centipoise. By starting with Equation 15, a useful relationship between density and viscosity can be developed. At ordinary pressures it can be shown using the relationship developed by Glasstone *et al.* (23) that

$$\eta^{1/2} = \frac{K^{1/2}M^{1/4}\Delta H^{1/2}}{2RV^{1/3}T^{1/4}} \qquad [16]$$

where M is molecular weight, ΔH is the enthalpy of vaporization, R is the gas constant, V is molal volume, and T is the absolute temperature. The velocity of sound through a liquid and enthalpy of vaporization are related in the following manner assuming constant specific heat:

TABLE 1
Comparison of Experimental and Calculated Densities of Oils

			Equation 13		Equation 14		Modified Rackett	
Oil	Points	*T* range (K)	AAD%[a]	MAD%[b]	AAD%	MAD%	AAD%	MAD%
Coconut	14	303.2–383.2	0.09	0.22	0.14	0.35	0.36	0.53
Corn	13	288.2–383.2	0.11	0.26	0.20	0.39	0.11	0.23
Cottonseed	8	283.2–353.2	0.12	0.27	0.17	0.26	0.16	0.31
Soybean	17	253.2–383.2	0.12	0.32	0.25	0.46	0.12	0.31
Sesame	10	253.2–353.2	0.21	1.03	0.15	0.99	0.36	0.63
Peanut	10	273.2–353.2	0.25	0.67	0.27	0.84	0.30	0.49
Palm	3	323.2–373.2	0.79	0.88	0.96	1.00	0.21	0.24
Safflower	2	292.6–333.2	0.26	0.50	0.62	0.90	0.24	0.45
Olive	3	288.2–305.2	0.17	0.31	0.26	0.48	0.31	0.52
Rapeseed	10	288.2–383.2	0.18	0.39	0.32	0.43	0.24	0.33
Sunflower	19	253.2–353.2	0.34	0.66	0.38	0.79	0.33	0.58
Palm kernel	3	323.2–373.2	0.36	0.40	0.52	0.63	0.18	0.23
Babassu	1	333.2	0.13	0.13	0.37	0.37	0.51	0.51
Rice bran	9	273.2–253.2	0.32	0.53	0.33	0.49	0.95	1.15
Overall	122	253.2–383.2	0.21		0.28		0.30	

[a]AAD%: average absolute deviation % = (sum of *d*)/*N*, where *d* = (|exp − calc|/exp)*100, *N* = number of data points.

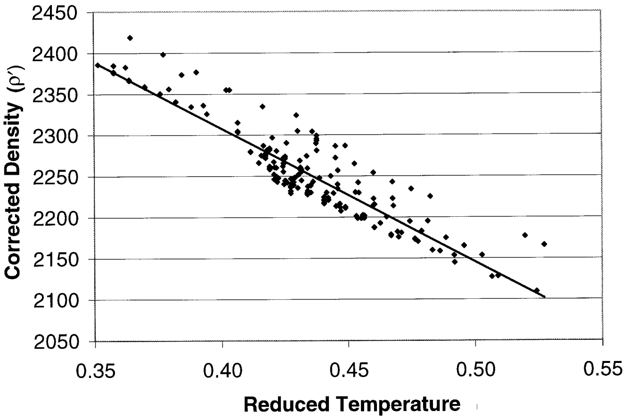

FIG. 3. Generalized correlation of the density of vegetable oil fatty acids based on critical density.

$$U = \frac{\Delta H}{T^{1/2}} \qquad [17]$$

Also, the velocity of sound in a liquid is given by the relation

$$U = U_g (V/v_f)^{1/3} \qquad [18]$$

where U_g is the velocity of sound in gas, and v_f is molal-free-volume.

By combining Equations 16, 17, and 18, the following relation can be obtained:

$$\eta^{1/2} = \frac{K}{U^{1/3}} \qquad [19]$$

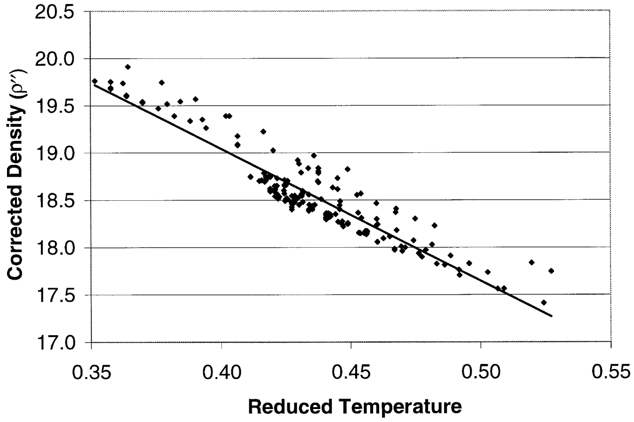

FIG. 4. Generalized correlation of the density of vegetable oil fatty acids based on molecular weight.

Finally, Equation 19 can be written as:

$$\rho = A' + \frac{B'}{\eta^{1/2}} \qquad [20]$$

which retains the first two terms in the expansion and relates viscosity to the density of the oils. Equation 13 was used to estimate the density of vegetable oils corresponding to the temperature of the viscosity data. The use of Equation 20 resulted in a linear fit for each oil with a calculated R^2 value in the range of 0.984–0.998. In the attempt to find one linear equation for all of the oils, ρ in Equation 20 was replaced with ρ′ from Equation 13. The resulting equation is:

$$\rho' = C + \frac{D}{\eta^{1/2}} \qquad [21]$$

TABLE 2
Comparison of Experimental and Calculated Densities of Fatty Acids[a]

			Equation 13		Equation 14		Modified Rackett	
Fatty acid	Points	*T* Range (K)	AAD%	MAD%	AAD%	MAD%	AAD%	MAD%
Caproic	14	288.2–353.2	2.38	3.20	1.85	2.78	0.23	0.50
Caprylic	24	293.2–353.2	0.39	0.83	0.36	0.86	0.15	0.45
Capric	30	303.2–383.2	0.49	0.88	0.35	0.74	0.14	0.40
Lauric	26	318.2–383.2	0.78	1.28	0.59	1.10	0.33	0.79
Myristic	19	329.2–383.2	0.59	0.86	0.51	0.78	0.10	0.21
Palmitic	14	335.2–383.2	0.29	0.58	0.37	0.69	0.10	0.34
Palmitoleic	1	288.2	0.12	0.12	0.55	0.55	0.15	0.15
Margaric	7	333.2–353.2	0.08	0.16	0.29	0.40	0.03	0.07
Stearic	13	341.2–394.3	0.58	1.12	0.27	0.88	0.11	0.29
Oleic	25	288.2–383.2	0.66	1.23	1.11	1.89	0.18	0.58
Linoleic	1	283.2	0.67	0.67	1.91	1.91	0.02	0.02
Linolenic	3	291.2–293.2	1.09	1.25	3.12	3.28	0.30	0.46
Arachidic	1	373.2	1.30	1.30	0.74	0.74	0.06	0.06
Behenic	2	363.2–373.2	1.71	2.12	0.82	1.24	0.38	0.74
Erucic	9	310.9–383.2	2.48	2.79	2.35	2.72	0.38	0.60
Lignoceric	1	373.2	3.03	3.03	1.84	1.84	0.38	0.28
Overall	190	288.2–394.3	0.80		0.77		0.20	

[a] See Table 1 for abbreviations.

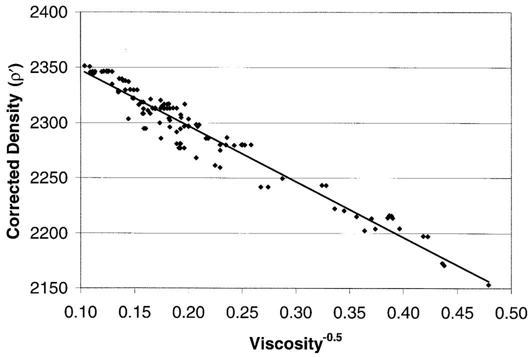

FIG. 5. A relationship between the density and viscosity of vegetable oils.

TABLE 3
Comparison of Predicted and Experimental Viscosities of Oils[a]

Oil	Points	*T* range (K)	AAD%	MAD%
Sunflower	9	293.2–372.1	10.7	22.1
Palm	6	313.2–333.2	26.1	30.3
Cottonseed	6	293.2–372.1	12.4	21.4
Corn	12	293.2–383.2	7.4	17.8
Rapeseed	17	293.2–383.2	11.2	15.6
Peanut	7	293.2–333.2	6.4	13.3
Soybean	23	293.2–383.2	10.4	30.8
Coconut	19	298.2–383.2	32.2	46.8
Olive	10	293.2–372.1	13.3	26.0
Linseed	6	293.2–372.1	7.0	19.2
Sesame	2	293.2–323.2	14.3	19.3
Overall	117	293.2–383.2	14.6	

[a] See Table 1 for abbreviations.

Figure 5 is a plot of Equation 21. In Equation 21 the constant *C* equals –513 and *D* equals 2405. Table 3 shows the accuracy of the predicted results from Equation 21. The absolute average deviation for the 117 points examined is 14.6%. This is comparable to 15.2% calculated using Equation 10, as proposed by Dutt and Prasad (5). Regression analysis of Equation 21 and Equation 10, in the prediction of viscosity, gave R^2 values of 0.915 and 0.899, respectively. An examination of Table 3 shows greater inaccuracy occurred in the case of oils with lower molecular weights. An advantage of Equation 21 is that viscosity can be calculated from density data, which are somewhat easier to obtain experimentally than viscosity data, particularly for highly viscous oils. In the absence of this viscosity data, Equation 21 can predict the viscosity of a vegetable oil from its density with reasonable accuracy.

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