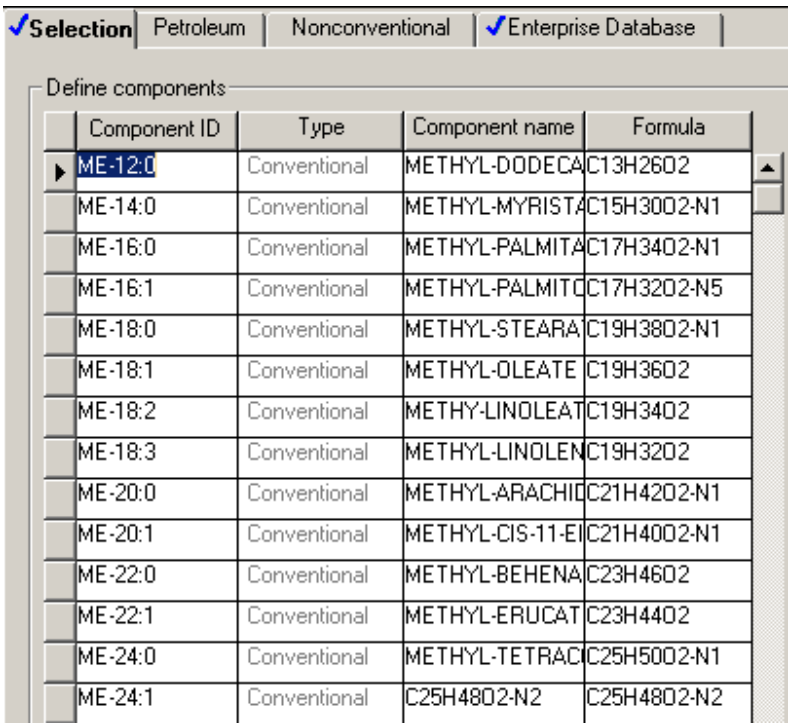
**The following are appendices A, B1 and B2 of our paper, "Integrated Process Modeling and Product Design of Biodiesel Manufacturing", that appears in *the Industrial and Engineering Chemistry Research*, December (2009).**

## Appendix A. An Illustration of How to Access NIST TDE When Applying Aspen Plus to Develop a Biodiesel Process Model

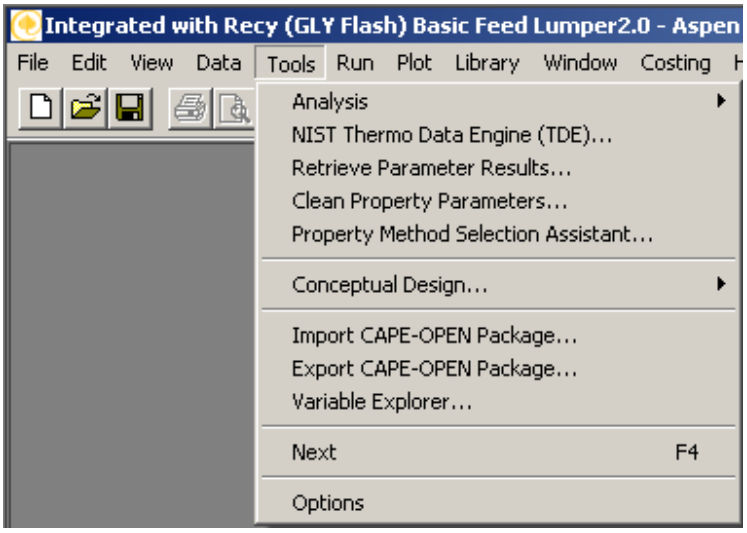
To access NIST TDE Data Engine in Aspen Plus version 2006.5 or V7.0

Step 1. Enter the FAME in the component list

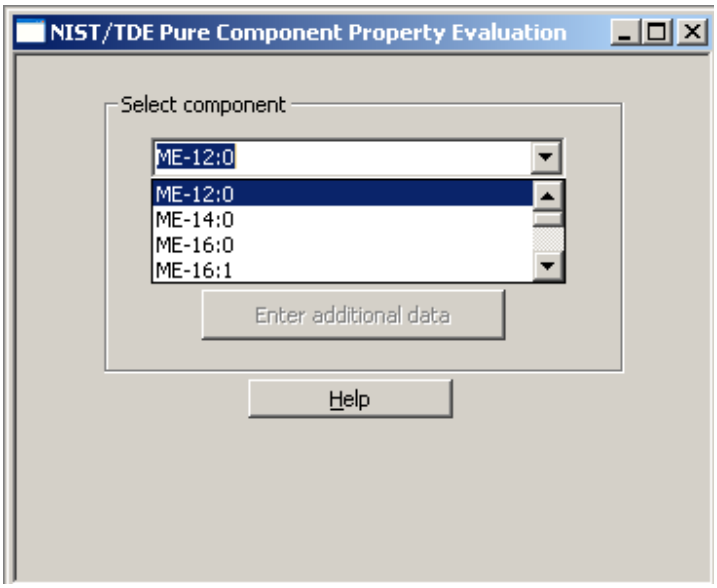



| Component ID | Type | Component name | Formula |
|---|---|---|---|
| ME-12:0 | Conventional | METHYL-DODECA | C13H26O2 |
| ME-14:0 | Conventional | METHYL-MYRISTA | C15H30O2-N1 |
| ME-16:0 | Conventional | METHYL-PALMITA | C17H34O2-N1 |
| ME-16:1 | Conventional | METHYL-PALMITO | C17H32O2-N5 |
| ME-18:0 | Conventional | METHYL-STEARA | C19H38O2-N1 |
| ME-18:1 | Conventional | METHYL-OLEATE | C19H36O2 |
| ME-18:2 | Conventional | METHY-LINOLEAT | C19H34O2 |
| ME-18:3 | Conventional | METHYL-LINOLEN | C19H32O2 |
| ME-20:0 | Conventional | METHYL-ARACHID | C21H42O2-N1 |
| ME-20:1 | Conventional | METHYL-CIS-11-EI | C21H40O2-N1 |
| ME-22:0 | Conventional | METHYL-BEHENA | C23H46O2 |
| ME-22:1 | Conventional | METHYL-ERUCAT | C23H44O2 |
| ME-24:0 | Conventional | METHYL-TETRAC | C25H50O2-N1 |
| ME-24:1 | Conventional | C25H48O2-N2 | C25H48O2-N2 |

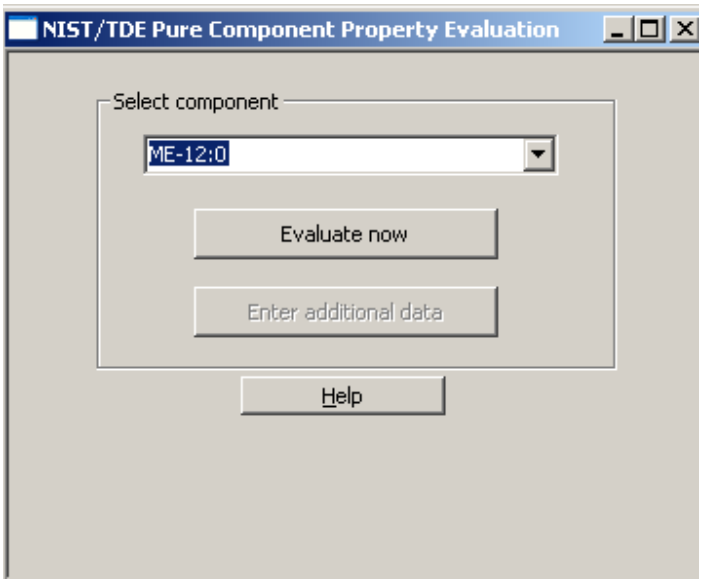
Step 2. Go to "Tools" -> "NIST Thermo Data Engine (TDE)"



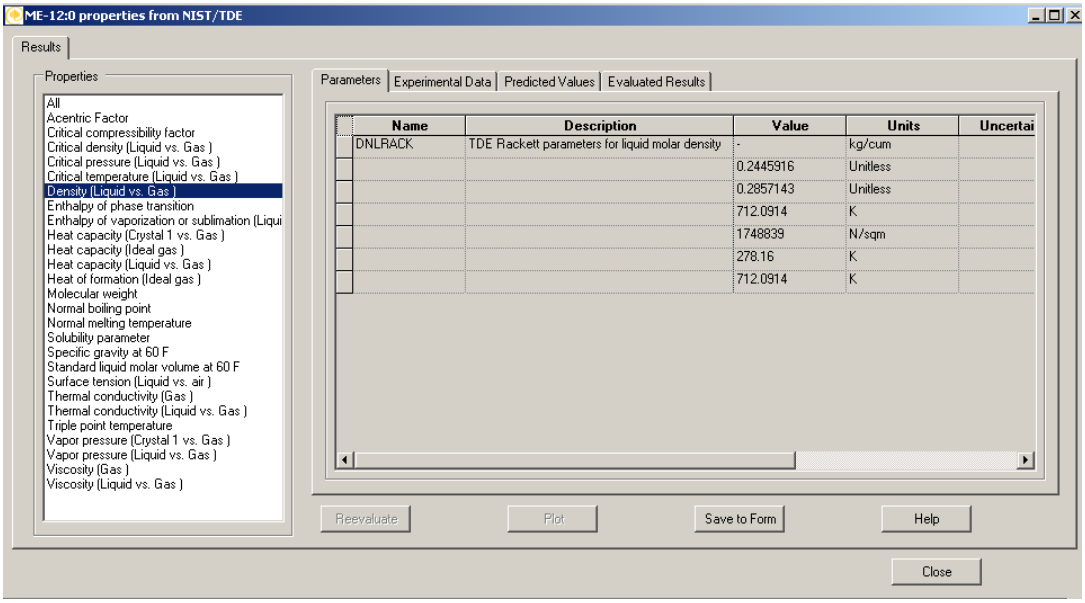

Step 3. Select the component




Step 4. Click “Evaluate now”




Step 5. The user can access the value of a specific property, eq. Liquid Density



## Appendix B Prediction Methods and NIST TDE Equations for Thermophysical Properties

### B.1 Prediction Methods for Thermophysical Properties

***$T_b$, $T_c$, $P_c$, $\omega$: Constantinou and Gani Method*** [29]

Required data: structure

$$T_b\,(K) = 204.359 \times \ln[\sum_k N_k \times tb1k + W \times \sum_j M_j \times tb2j] \quad (B.1)$$

$$T_c\,(K) = 181.128 \times \ln[\sum_k N_k \times tc1k + W \times \sum_j M_j \times tc2j] \quad (B.2)$$

$$P_c\,(bar) = [\sum_k N_k \times pc1k + W \times \sum_j M_j \times pc2j + 0.10022]^{-2} + 1.3705 \quad (B.3)$$

$$\omega = 0.4085 \times \left\{ \ln\left[ \sum_k N_k \times \omega 1k + W \times \sum_j M_j \times \omega 2j + 0.10022 + 1.1507 \right] \right\}^{(1/0.505)} \quad (B.4)$$

where W = 0 when only applying first-order and W = 1 when applying first-order and second-order.

Table B.1. Constantinou and Gani Contributions of $T_b$, $T_c$, $P_c$ for Triglyceride

| C-G | tb1k | tc1k | pc1k | ω |
|---|---|---|---|---|
| $CH_3$ | 0.8849 | 1.6781 | 0.0199 | 0.296 |
| $CH_2$ | 0.9225 | 3.492 | 0.0106 | 0.147 |
| CH | 0.6033 | 4.033 | 0.0013 | -0.071 |
| CH2COO | 3.3953 | 13.8116 | 0.0218 | 0.765 |
| CH=CH | 1.8433 | 7.3691 | 0.0179 | 0.252 |
| CH3COO | 3.636 | 12.5965 | 0.02902 | 0 |
| OH | 3.2152 | 9.7292 | 0.005148 | 0.737 |
| | tb2j | tc2j | pc2j | ω |
| $CH_2$-$CH_m$=CH m = 0, 1; n = | -0.1406 | -0.5231 | 0.003538 | -0.0115 |
| CHOH | -0.5385 | -2.8035 | -0.00439 | 0.03654 |

### *$T_c$: Wilson and Jasperson Method* [29]

Required data: $T_b$ and structure

$$T_c\,(K) = \frac{T_b}{[0.048271 + \sum_k N_k \times \Delta tck + \sum_j M_j \times \Delta tcj]^{0.2}} \tag{B.5}$$

Table B.2. Wilson and Jasperson Contributions of $T_c$ for Triglyceride

| | △tck |
|---|---|
| C | 0.008532 |
| H | 0.002793 |
| O | 0.020341 |
| | △tcj |
| -COO- | -0.015 |

### *$T_b$, $T_c$, $P_c$: Dohrn and Brunner Method A* [34]

Required data: $T_b$ and $V_{L,20}$

$$a_c = \Omega_a \times a^{(1)} \times \left(\frac{b_c}{\Omega_b} \times T_b\right)^{a^{(2)}} \tag{B.6}$$

$$b_c = \Omega_b \times (b^{(1)} \times V_{L,20} \times T_b + b^{(2)}) \tag{B.7}$$

$$T_c(K) = \frac{\Omega_b \times a_c}{\Omega_a \times b_c} \frac{1}{R} \tag{B.8}$$

$$P_c(kPa) = \frac{a_c}{\Omega_a} \left(\frac{\Omega_b}{b_c}\right)^2 \tag{B.9}$$

$$\omega = -\frac{3}{7} \frac{\mathrm{Log}(101.3\,kPa/P_c)}{(T_c/T_b - 1)} - 1 \tag{B.10}$$

where $\Omega_a = 0.45724$, $\Omega_b = 0.0778$, $a^{(1)} = 21.26924$ kJ/kmol-K, $a^{(2)} = 0.913049$, $b^{(1)} = 0.02556188$ $K^{-1}$, $b^{(2)} = 0.168721$ $m^3\,kmol^{-1}$, R = 8.314 kJ/kmol-K, $V_{L,20}$ is liquid density at 20℃

***$T_b$, $T_c$, $P_c$, $\omega$: Dohrn and Brunner Method B*** [34]

Required data: vapor pressure at any temperature ($P^{sat}$ at $T_1$) and $V_{L,20}$

$$a_c = \Omega_a \times a^{(1)} \times \left(\frac{b_c}{\Omega_b} \times T_b\right)^{a^{(2)}} \tag{B.11}$$

$$b_c = \Omega_b \times \left( b^{(1)} \times V_{L,20} \times T_b + b^{(2)} \right) \tag{B.12}$$

$$T_c(K) = \frac{\Omega_b \times a_c}{\Omega_a \times b_c} \frac{1}{R} \tag{B.13}$$

$$P_c(kPa) = \frac{a_c}{\Omega_a} \left(\frac{\Omega_b}{b_c}\right)^2 \tag{B.14}$$

$$\omega = -\frac{3}{7} \frac{\mathrm{Log}(P^{sat} \text{ at } T_1/P_c)}{(T_c/T_1 - 1)} - 1 \tag{B.15}$$

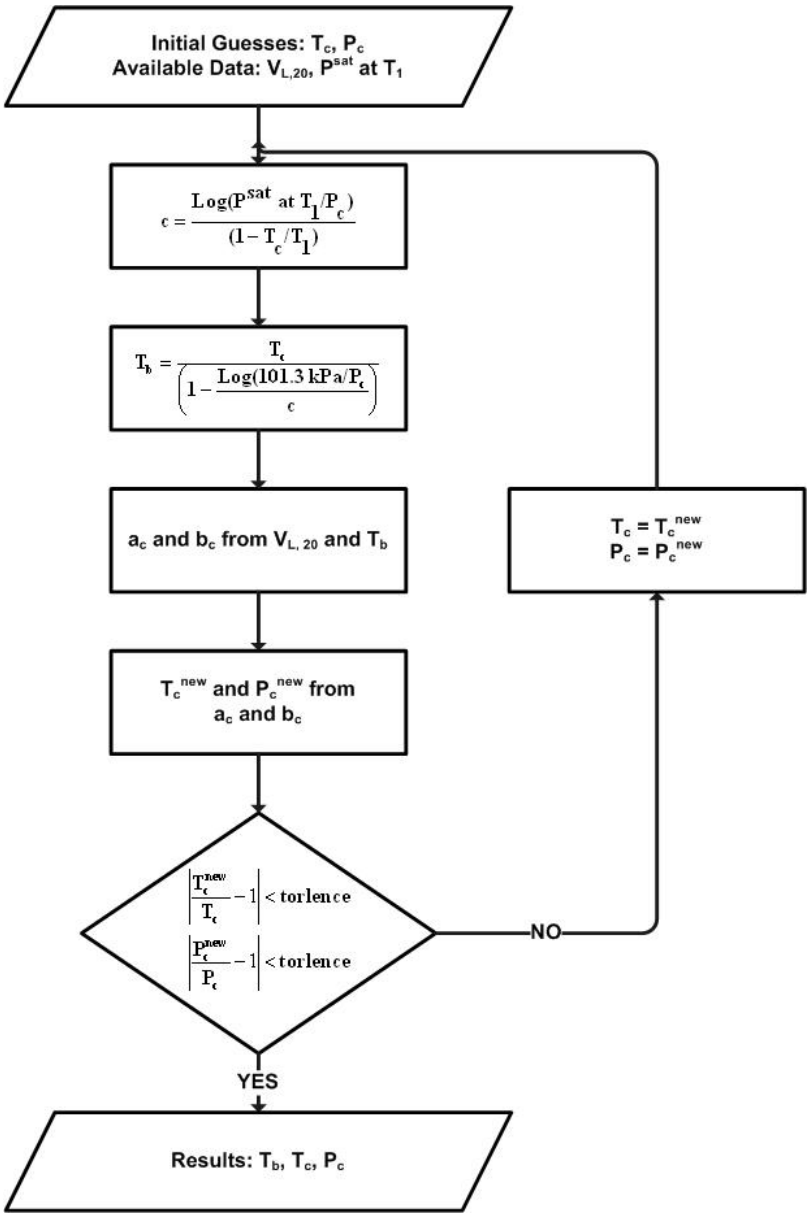



Figure B.1. Iteration step of Dohrn and Brunner Method to predict $T_b$, $T_c$, $P_c$ and$\omega$

Dohrn and Brunner[34] use Joback[29] method to obtain the initial guesses of $T_c$ and $P_c$. Joback method for $T_c$ and $P_c$:

$$\mathbf{T_b\ (K) = 198 + \sum_k N_k \times tbk} \tag{B.16}$$

$$\mathbf{T_c\ (K) = T_b \times \left[ 0.584 + 0.965 \times \left( \sum_k N_k \times tck \right) - \left( \sum_k N_k \times tck \right)^2 \right]^{-1}} \quad \text{(B.17)}$$

$$\mathbf{P_c\ (Bar) = \left[ 0.113 + 0.0032 \times N_{total\ atoms} - \left( \sum_k N_k \times pck \right) \right]^{-2}} \quad \text{(B.18)}$$

Table B.3. Joback Group Contributions of $T_c$ and $P_c$ for Triglyceride

| | tbk | tck | pck |
|---|---|---|---|
| CH3 | 23.58 | 0.0141 | -0.0012 |
| -CH2- | 22.88 | 0.0189 | 0 |
| >CH- | 21.74 | 0.0164 | 0.002 |
| =CH- | 24.96 | 0.0129 | -0.0006 |
| -COO- | 81.1 | 0.0481 | 0.0005 |

***$P_{vap}$: Ambrowse and Walton Method*** [29]

Required data: $T_c$, $P_c$, ω

$$\mathbf{\ln\left(\frac{P_{vap}}{P_c}\right) = f^{(0)}(T_r) + \omega f^{(1)}(T_r) + \omega^2 f^{(2)}(T_r)} \quad \text{(B.19)}$$

$$\mathbf{f^{(0)}(T_r) = \frac{-5.97616 \times \tau + 1.29874 \times \tau^{1.5} - 0.60394 \times \tau^{2.5} - 1.06841 \times \tau^5}{T_r}} \quad \text{(B.20)}$$

$$\mathbf{f^{(1)}(T_r) = \frac{-5.03365 \times \tau + 1.11505 \times \tau^{1.5} - 5.41217 \times \tau^{2.5} - 7.44628 \times \tau^5}{T_r}} \quad \text{(B.21)}$$

$$\mathbf{f^{(2)}(T_r) = \frac{-0.64771 \times \tau + 2.41539 \times \tau^{1.5} - 4.26979 \times \tau^{2.5} + 3.25259 \times \tau^5}{T_r}} \quad \text{(B.22)}$$

$$\mathbf{\tau = 1 - T_r} \quad \text{(B.23)}$$

where $T_r$ is reduced temperature.

***$P_{vap}$: Ceriani and Meirelles Method*** [37]

Required data: Structure

$$\ln(P_{i,vap}, Pa) = \sum_k N_k \times \left( A_{1k} + \frac{B_{1k}}{T^{1.5}} - C_{1k} \times \ln(T) - D_{1k} \times T \right) + \left[ M_i \times \sum_k N_k \times \left( A_{2k} + \frac{B_{2k}}{T^{1.5}} - C_{2k} \times \ln(T) - D_{2k} \times T \right) \right] + Q \quad \text{(B.24)}$$

$$Q = \xi_1 \times q + \xi_2 \quad \text{(B.25)}$$

$$q = \alpha + \frac{\beta}{T^{1.5}} - \gamma \times \ln(T) - \delta \times T \quad \text{(B.26)}$$

$$\xi_1 = f_0 + N_c \times f_1 \quad \text{(B.27)}$$

$$\xi_2 = s_0 + N_{cs} \times s_1 \quad \text{(B.28)}$$

where T is temperature in Kevin, $M_i$ is molecular weight and $A_{1k}$, $B_{1k}$, $C_{1k}$, $D_{1k}$, $A_{2k}$, $B_{2k}$, $C_{2k}$, $D_{2k}$ are group contribution terms. $N_c$ is the total number of carbon atoms in the molecule and $N_{cs}$ is the number of carbons of the substitute fraction. For example, $N_{cs}$ of lauric acid chain, $-OOC-(CH_2)_{10}-CH_3$, is 11.

Table B.4. Ceriani and Meirelles Contributions of Vapor Pressure

| | $A_{1k}$ | $B_{1k}$ | $C_{1k}$ | $D_{1k}$ | $A_{2k}$ | $B_{2k}$ | $C_{2k}$ | $D_{1k}$ |
|---|---|---|---|---|---|---|---|---|
| CH3 | -117.5 | 7232.3 | -22.7939 | 0.0361 | 0.00338 | -63.3963 | -0.00106 | 0.000015 |
| CH2 | 8.4816 | -10987.8 | 1.4067 | -0.00167 | -0.00091 | 6.7157 | 0.000041 | -0.00000126 |
| COOH | 8.0734 | -20478.3 | 0.0359 | -0.00207 | 0.00399 | -63.9929 | -0.00132 | 0.00001 |
| CH=cis | 2.4317 | 1410.3 | 0.7868 | -0.004 | 0 | 0 | 0 | 0 |
| CH=trans | 1.843 | 526.5 | 0.6584 | -0.00368 | 0 | 0 | 0 | 0 |
| COO | 7.116 | 49152.6 | 2.337 | -0.00848 | 0.00279 | 10.0396 | -0.00034 | 0.00000295 |
| OH | 28.4723 | -16694 | 3.257 | 0 | 0.00485 | 0 | 0 | 0 |
| CH2-CH-CH2 | 688.3 | -349293 | 122.5 | -0.1814 | -0.00145 | 0 | 0 | 0 |
| | $f_0$ | $f_1$ | $s_0$ | $s_1$ | | | | |
| Esters | 0.2773 | -0.00444 | -0.4476 | 0.0751 | | | | |
| Acylglycerols | 0 | 0 | 0 | 0 | | | | |
| Fatty Acids | 0.001 | 0 | 0 | 0 | | | | |
| Alcohols | 0.7522 | -0.0203 | 0 | 0 | | | | |
| | $\alpha$ | $\beta$ | $\gamma$ | $\delta$ | | | | |
| | 3.4443 | -499.3 | 0.6136 | -0.00517 | | | | |

***$\rho_L$: Halvorsen Method*** [35] for triglycerides

Required data: $T_c$, $P_c$, $Z_{RA}$ of the fatty acids

$$\rho^{TG} = \frac{\left(\sum \mathbf{x}_i^{FA} \times \mathbf{MW}_i^{FA}\right)}{\mathbf{R} \times \left(\sum \frac{\mathbf{x}_i^{FA} \times \mathbf{T}_{c,i}^{FA}}{\mathbf{P}_{c,i}^{FA}}\right) \times \left(\sum \mathbf{x}_i^{FA} \times \mathbf{Z}_{RA,i}^{FA}\right)^{[1+(1-\mathbf{T}_r)^{2/7}]}} + \mathbf{F_c} \quad \text{(B.29)}$$

$$\mathbf{T_r} = \frac{\mathbf{T}}{\sum \mathbf{x}_i^{FA} \times \mathbf{T}_{c,i}^{FA}} \quad \text{(B.30)}$$

$$\mathbf{MW}^{TG} = 3 \times \sum \mathbf{x}_i^{FA} \times \mathbf{MW}_i^{FA} + 38.0488 \quad \text{(B.31)}$$

$$\mathbf{F_c} = \mathbf{0.0236} + \mathbf{0.000082} \times \left|\mathbf{875} - \mathbf{MW}^{TG}\right| \quad \textbf{when } \mathbf{MW}^{TG} \geq \mathbf{875} \quad \text{(B.32)}$$

$$\mathbf{F_c} = \mathbf{0.0236} + \mathbf{0.000098} \times \left|\mathbf{875} - \mathbf{MW}^{TG}\right| \quad \textbf{when } \mathbf{MW}^{TG} \leq \mathbf{875} \quad \text{(B.33)}$$

where $x_i^{FA}$ is molar fraction of the $i^{th}$ fatty acid chain in the triglyceride molecule, $MW_i^{FA}$ is the molecular weight of the $i^{th}$ fatty acid, $T_{c,i}^{FA}$ is the critical temperature of the $i^{th}$ fatty acid, $P_{c,i}^{FA}$ is the critical pressure of the $i^{th}$ fatty acid and $Z_{RA,i}$ is the Rackett parameter of the $i^{th}$ fatty acid.

Table B.5. Required Parameters for Halvorsen Method of $\rho_L$ Prediction

| Fatty Acid | $T_c$ (K) | $P_c$ (bar) | $Z_{RA}$ |
|---|---|---|---|
| 12:0 | 756.21 | 19.22 | 0.2391 |
| 14:0 | 779.07 | 16.35 | 0.2326 |
| 16:0 | 799.89 | 14.08 | 0.2267 |
| 16:1 | 800.34 | 14.71 | 0.2290 |
| 18:0 | 819.00 | 12.25 | 0.2205 |
| 18:1 | 819.41 | 12.76 | 0.2230 |
| 18:2 | 819.82 | 13.31 | 0.2255 |
| 18:3 | 820.23 | 13.89 | 0.2284 |
| 20:0 | 836.65 | 10.76 | 0.2149 |
| 20:1 | 837.03 | 11.18 | 0.2172 |
| 22:0 | 853.06 | 9.52 | 0.2095 |
| 22:1 | 853.41 | 9.87 | 0.2116 |
| 22:2 | 853.77 | 10.24 | 0.2103 |
| 24:0 | 868.38 | 8.49 | 0.2040 |
| 24:1 | 868.71 | 8.78 | 0.2063 |
| 26:0 | 882.76 | 7.61 | 0.1990 |

Example: find the density of triolein (18:1) at 20℃

Procedure:

1. Triolein is pure triglyceride which is composed of three oleic acid chains (18:1).

2. $$\sum x_i^{FA} \times MW_i^{FA} = 1 \times MW_{18:1}^{FA} = 282.46\ (kg / kmol) = 0.28246\ (kg/mol)$$

3. $$\sum \frac{x_i^{FA} \times T_{c,i}^{FA}}{P_{c,i}^{FA}} = \frac{1 \times T_{18:1}^{FA}}{P_{18:1}^{FA}} = 6.4217\ E - 04\ (K / Pa)$$

4. $$\sum x_i^{FA} \times Z_{RA,i}^{FA} = 1 \times Z_{18:1}^{FA} = 0.223$$ and

$$T_r = \frac{T}{\sum x_i^{FA} \times T_{c,i}^{FA}} = \frac{T}{1 \times T_{c,18:1}^{FA}} = \frac{293.15}{819.41} = 3.5776E - 01$$

5. $$\left(\sum x_i^{FA} \times Z_{RA,i}^{FA}\right)^{[1+(1-T_r)^{2/7}]} = \left(1 \times Z_{18:1}^{FA}\right)^{[1+(1-T_r)^{2/7}]} = 5.9437E - 02$$

6. $$MW^{TG} = 3 \times \sum x_i^{FA} \times MW_i^{FA} + 38.0488 = 3 \times (1 \times 282.46) + 38.0488$$
$$= 885.4288\ (kg/kmol)$$

7 $$F_c = 0.0236 + 0.000082 \times \left|875 - MW^{TG}\right| = 2.4455E - 02\ (g/cm^3) = 2.4455E01\ (kg/m^3)$$

$$\rho^{TG}\left(\frac{kg}{m^3}\right) = \frac{\left(\sum x_i^{FA} \times MW_i^{FA}\right)}{R \times \left(\sum \frac{x_i^{FA} \times T_{c,i}^{FA}}{P_{c,i}^{FA}}\right) \times \left(\sum x_i^{FA} \times Z_{RA,i}^{FA}\right)^{[1+(1-T_r)^{2/7}]}} + F_c$$

8. $$= \frac{0.28246\left(\frac{kg}{mol}\right)}{8.314\left(\frac{Pa - m^3}{K - mol}\right) \times 6.4217E - 04\left(\frac{K}{Pa}\right) \times 5.9437E - 02} + 2.455E01\left(\frac{kg}{m^3}\right)$$
$$= 914.66\ \frac{kg}{m^3}$$

9. The experimental value is 912.6 kg/m$^3$ and the ARD is 0.23%.

***$C_{P,L}$: Morad Method*** [36] for triglycerides

Required data: $T_c$, ω of the fatty acids

$$C_{P,L}^{TG} = C_{p,mix}^{IG} + R \times \left( \begin{array}{l} 1.45 + 0.45 \times (1 - T_r)^{-1} + \\ 0.25 \times \omega_{mix} \times \left[ \left( 17.11 + 25.2 \times \frac{(1 - T_r)^{1/3}}{T_r} + \frac{1.742}{(1 - T_r)} \right) \right] \end{array} \right) \quad \text{(B.34)}$$

$$T_r = \frac{T}{\sum x_i^{FA} \times T_{c,i}^{FA}} \quad \text{(B.35)}$$

$$C_{p,mix}^{IG} = \sum x_i^{FA} \times C_{p,i}^{IG,FA} \quad \text{(B.36)}$$

$$\omega_{mix} = \sum x_i^{FA} \times \omega_i^{FA} \quad \text{(B.37)}$$

$$MW_{mix} = \sum x_i^{FA} \times MW_i^{FA} \quad \text{(B.38)}$$

$$MW^{TG} = 3 \times \sum x_i^{FA} \times MW_i^{FA} + 38 \quad \text{(B.39)}$$

$$F_c = -0.2386 - 0.0005 \times \left| 850 - MW^{TG} \right| \quad \text{when } MW^{TG} \geq 850 \quad \text{(B.40)}$$

$$F_c = -0.3328 + 0.0001 \times \left| 850 - MW^{TG} \right| \quad \text{when } MW^{TG} \leq 850 \quad \text{(B.41)}$$

where R=1.987 Cal/K-mol and the unit of heat capacity is Cal/K-mol. Table B. 6 lists the required parameters of fatty acids.

Table B.6. Required Parameters for Morad Method of $C_{P,L}$ Prediction

| Fatty Acid | Tc (K) | ω | MW |
|---|---|---|---|
| 12:0 | 756.21 | 0.8422 | 200.32 |
| 14:0 | 779.07 | 0.9760 | 228.37 |
| 16:0 | 799.88 | 1.1087 | 256.42 |
| 16:1 | 800.34 | 1.0524 | 254.41 |
| 18:0 | 819.00 | 1.2369 | 284.48 |
| 18:1 | 819.14 | 1.1850 | 282.46 |
| 18:2 | 819.82 | 1.1294 | 280.45 |
| 18:3 | 820.23 | 1.0724 | 278.43 |

$C_{p,i}^{IG,FA}$ is idea gas heat capacity of fatty acid. Morad et al.[36] use Rihani method[76] to estimate $C_{p,i}^{IG,FA}$ :

$$\mathbf{C_p^{IG,FA}} = \sum \mathbf{N_k} \times \mathbf{a_k} + \sum \mathbf{N_k} \times \mathbf{b_k} \times \mathbf{T} + \sum \mathbf{N_k} \times \mathbf{c_k} \times \mathbf{T^2} + \sum \mathbf{N_k} \times \mathbf{d_k} \times \mathbf{T^3} \quad \text{(B.42)}$$

where $N_k$ is the number of the given functional groups. The unit of $\mathbf{C_p^{IG,FA}}$ is Cal/K-mol.

Table B.7. Rihani Contributions of Ideal Gas Heat Capacity for Fatty Acid

| | $a_k$ | $b_k$ | $c_k$ | $d_k$ |
|---|---|---|---|---|
| CH3 | 6.0870E-01 | 2.1433E-02 | -8.5200E-06 | 1.1350E-09 |
| CH2 | 3.9450E-01 | 2.1363E-02 | -1.1970E-05 | 2.5960E-09 |
| CH | -3.5232E+00 | 3.4158E-02 | -2.8160E-05 | 8.0150E-09 |
| -CH=CH- cis | -3.1210E+00 | 3.8060E-02 | -2.3590E-05 | 5.5040E-09 |
| -CH=CH- trans | 9.3770E-01 | 2.9904E-02 | -1.7490E-05 | 3.9180E-09 |
| -COOH | 1.4055E+00 | 3.4632E-02 | -2.5570E-05 | 6.8860E-09 |
| -COO- | 2.7350E+00 | 1.0751E-02 | 6.6700E-06 | -9.2300E-09 |

***$\triangle H_{vap}$：Vetere method combined with Watson relation*** [29]

Required data: $T_b$, $T_c$, $P_c$

$$\Delta H_{vap,b} = R \times T_b \frac{(1-T_{br})^{0.38}\left(\ln P_c - 0.513 + \frac{0.5066}{P_c T_{br}^{\ 2}}\right)}{1 - T_{br} + \ln T_{br}\left(1-(1-T_{br})^{0.38}\right)} \quad \text{(B.43)}$$

$$\Delta H_{vap} = \Delta H_{vap,b}\left(\frac{1-T_r}{1-T_{br}}\right)^{0.38} \quad \text{(B.44)}$$

where $\Delta H_{vap,b}$ is heat of vaporization at normal boiling point, $T_r$ is reduced temperature, and $T_{br}$ is reduced temperature at normal boiling point

## B.2 NIST TDE Equations for Thermophysical Property

$V_L$: NIST Rackett Equation [28]

$$V_L = \frac{R \times T_c}{P_c \times Z_{RA}^{-\left[1+\left(1-\frac{T}{T_c}\right)^{C_2}\right]}} \tag{B.45}$$

Table B.8. The Parameters of NIST Rackett Equation for FAME

| NIST TDE Rackett Equation ($m^3$/mol) | C1 ($Z_{RA}$) | C2 | C3 ($T_c$, K) | C4 ($P_c$, Pa) | C5 | C6 |
|---|---|---|---|---|---|---|
| C12:0 | 0.2445916 | 0.2857143 | 712 | 1748839 | 278 | 712 |
| C14:0 | 0.2353773 | 0.2857143 | 718 | 1448599 | 292 | 718 |
| C16:0 | 0.2227887 | 0.2857143 | 749 | 1205875 | 303 | 749 |
| C16:1 | 0.2071558 | 0.2857143 | 734 | 1279721 | 240 | 734 |
| C18:0 | 0.2298488 | 0.2857143 | 770 | 1178960 | 312 | 770 |
| C18:1 | 0.2225078 | 0.2857143 | 751 | 1124671 | 253 | 751 |
| C18:2 | 0.2226222 | 0.2857143 | 773 | 1162805 | 234 | 773 |
| C18:3 | 0.224261 | 0.2857143 | 774 | 1202626 | 110 | 774 |
| C20:0 | 0.1967211 | 0.2857143 | 767 | 1036965 | 319 | 767 |
| C20:1 | 0.2138194 | 0.2857143 | 767 | 990082 | 636 | 767 |
| C22:0 | 0.1841152 | 0.2857143 | 785 | 901921 | 326 | 785 |
| C22:1 | 0.2122916 | 0.2857143 | 784 | 881791 | 110 | 784 |
| C24:0 | 0.183291 | 0.2857143 | 804 | 821192 | 332 | 804 |
| C24:1 | 0.2010567 | 0.2857143 | 802 | 822329 | 678 | 802 |
| Parameter | C1 | C2 | C3 | C4 | C5 | C6 |
| Description | $Z_{RA}$ | - | $T_c$ | $P_c$ | $T_{lower}$ | $T_{upper}$ |
| Unit | N/A | N/A | K | Pa | K | K |

$V_L$: NIST ThermoML Equation [28]

$$V_L = \sum_{i=1}^{C_5} C_i \times T^{n-1} \tag{B.46}$$

Table B.9. The Parameters of NIST ThermoML Equation for $V_L$

| Parameter | Symbol | Unit |
|---|---|---|
| C1 | - | $kmol/m^3$ |
| C2 | - | $kmol/m^3$-K |
| C3 | - | $kmol/m^3$-$K^2$ |
| C4 | - | $kmol/m^3$-$K^3$ |
| C5 | - | Unitless |
| C6 | $T_{lower}$ | K |
| C7 | $T_{upper}$ | K |

$C_{P, IG}$: NIST Aly-Lee Equation [28]

$$\mathbf{C_{P,IG} = C_1 + C_2 \times \left( \frac{C_3/T}{Sinh(C_3/T)} \right)^2 + C_4 \times \left( \frac{C_5/T}{Cosh(C_5/T)} \right)^2} \quad \text{(B.47)}$$

Table B.10. The Parameters of NIST Aly-Lee Equation for $C_{P, IG}$ for FAME

| NIST Aly-Lee Equation (J / kmol-K) | C1 | C2 | C3 | C4 | C5 | C6 | C7 |
|---|---|---|---|---|---|---|---|
| C12:0 | 240063.9 | 542541.1 | -819 | 121697.8 | 0 | 200 | 980 |
| C14:0 | 205454.4 | 805594.2 | -574 | -442429.9 | 650 | 200 | 980 |
| C16:0 | 230137.9 | 910125.1 | -574 | -497826.1 | -650 | 200 | 980 |
| C16:1 | 234231.9 | 895310.9 | -588 | -512600 | -664 | 200 | 980 |
| C18:0 | 267382.2 | 563286.7 | -569 | 596005.8 | -1600 | 200 | 980 |
| C18:1 | 269559.9 | 532189.6 | -577 | 616279.7 | -1617 | 200 | 980 |
| C18:2 | 261554.1 | 984480.8 | -1271 | 490798 | -556 | 200 | 980 |
| C18:3 | 265702.7 | 972734.7 | -614 | -599483.1 | -687 | 200 | 980 |
| C20:0 | 278834.7 | 1117297 | -1214 | 609431 | -536 | 200 | 980 |
| C20:1 | 282797.7 | 1102514 | -1240 | 579972.5 | -545 | 200 | 980 |
| C22:0 | 299203.3 | 1224641 | 564 | -674861.1 | -641 | 200 | 980 |
| C22:1 | 307461.3 | 1206798 | 1237 | 638488.9 | -544 | 200 | 980 |
| C24:0 | 345378.1 | 741693.7 | 568 | 774619.4 | -1600 | 200 | 980 |
| C24:1 | 347594 | 710543.1 | 574 | 794868.1 | -1613 | 200 | 980 |
| Parameter | C1 | C2 | C3 | C4 | C5 | C6 | C7 |
| Description | - | - | - | - | - | $T_{lower}$ | $T_{upper}$ |
| Unit | J/kmol-K | J/kmol-K | K | J/kmol-K | K | K | K |

$C_{P, L}$: NIST ThermoML Equation [28]

$$\mathbf{C_{P,L} = \sum_{i=1}^{C_3} C_i \times T^{n-1}} \quad \text{(B.48)}$$

Table B.11. The Parameters of NIST ThermoML Equation for $C_{P,L}$

| Parameter | Symbol | Unit |
|---|---|---|
| C1 | - | J/kmol-K |
| C2 | - | J/kmol-K$^2$ |
| C3 | - | Unitless |
| C4 | $T_{lower}$ | K |
| C5 | $T_{upper}$ | K |

$C_{P,L}$: NIST TDE Equation [28]

$$C_{P,L} = \frac{C_5}{1-\frac{T}{C_6}} + \sum_{i=1}^{C_7} C_i \times \left(1-\frac{T}{C_6}\right)^{n-1} \quad \text{(B.49)}$$

Table B.12. The Parameters of NIST TDE Equation for $C_{P,L}$ for FAME

| NIST TDE Equation (J/kmol-K) | C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 | C9 |
|---|---|---|---|---|---|---|---|---|---|
| C12:0 | 508414.7 | -1413.503 | 4.966722 | -0.004025 | 8804.63 | 712 | 4 | 278 | 698 |
| C14:0 | 974844.7 | -4513.728 | 12.42177 | -0.009581 | 11780.11 | 718 | 4 | 292 | 704 |
| C16:0 | 767706.7 | -2508.638 | 7.655214 | -0.005827 | 10693.47 | 749 | 4 | 303 | 734 |
| C16:1 | 472441.6 | -168.3002 | 1.95041 | -0.001492 | 7765.68 | 734 | 4 | 240 | 719 |
| C18:0 | 689451.7 | -1677.292 | 6.066038 | -0.004698 | 10924.92 | 770 | 4 | 312 | 755 |
| C18:1 | 466346.9 | 120.4442 | 1.566388 | -0.00124 | 7728.59 | 761 | 4 | 253 | 746 |
| C18:2 | 471973.1 | -38.21093 | 1.788936 | -0.001336 | 7519.56 | 773 | 4 | 234 | 758 |
| C18:3 | 498535.9 | -209.9461 | 1.964523 | -0.001379 | 7539.46 | 774 | 4 | 250 | 759 |
| C20:0 | 910960 | -2927.919 | 9.154863 | -0.007013 | 13838.95 | 767 | 4 | 319 | 750 |
| C20:1 | 526862.5 | 76.54091 | 1.84262 | -0.001448 | 8310.67 | 767 | 4 | 250 | 750 |
| Parameter | C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 | C9 |
| Description | - | - | - | - | - | $T_c$ | | $T_{lower}$ | $T_{upper}$ |
| Unit | J/kmol-K | J/kmol-K | J/kmol-K | J/kmol-K | J/kmol-K | K | N/A | K | K |

$P_{vap}$: NIST Wagner Equation [28]

$$\ln(P_{vap}) = \ln(P_c) + \left( \begin{array}{l} C_1 \times \left(1-\frac{T}{C_6}\right) + C_2 \times \left(1-\frac{T}{C_6}\right)^{1.5} \\ + C_3 \times \left(1-\frac{T}{C_6}\right)^{2.5} + C_4 \times \left(1-\frac{T}{C_6}\right)^{5} \end{array} \right) \Bigg/ \left(\frac{T}{C_6}\right) \quad \text{(B.50)}$$

Table B.13. The Parameters of NIST Wagner Equation for $P_{vap}$ for FAME

| NIST Wagner Equation (Bar) | C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 |
|---|---|---|---|---|---|---|---|---|
| C12:0 | -9.694324 | 2.509544 | -4.402982 | -9.230351 | 14.3745 | 712 | 278 | 712 |
| C14:0 | -10.32312 | 0.2486618 | -0.272116 | -15.16169 | 14.1861 | 718 | 292 | 718 |
| C16:0 | -10.98844 | 4.20676 | -8.735103 | -5.583598 | 14.0027 | 749 | 303 | 749 |
| C16:1 | -11.50495 | 4.414073 | -9.852489 | -5.443423 | 14.0622 | 734 | 240 | 734 |
| C18:0 | -11.01778 | 3.60513 | -9.883088 | -2.333603 | 13.9801 | 770 | 312 | 770 |
| C18:1 | -11.90171 | 5.368385 | -10.61564 | -5.806015 | 13.933 | 761 | 253 | 761 |
| C18:2 | -11.17148 | 4.445311 | -9.284593 | -5.08707 | 13.9664 | 773 | 234 | 773 |
| C18:3 | -10.5887 | 2.436575 | -6.783611 | -7.340778 | 14 | 774 | 200 | 774 |
| C20:0 | -12.79261 | 6.579309 | -14.06263 | -4.254656 | 13.8518 | 767 | 319 | 767 |
| C20:1 | -12.46868 | 5.523578 | -12.0696 | -5.475907 | 13.8055 | 767 | 200 | 767 |
| C22:0 | -13.41457 | 5.666122 | -13.2316 | -8.207159 | 13.7123 | 785 | 326 | 785 |
| C22:1 | -12.9095 | 6.159538 | -13.16899 | -5.268222 | 13.6897 | 784 | 200 | 784 |
| C24:0 | -13.15767 | 6.335366 | -13.74519 | -5.33026 | 13.6185 | 804 | 332 | 804 |
| C24:1 | -13.28506 | 6.719306 | -14.09176 | -5.100378 | 13.6199 | 802 | 200 | 802 |
| Parameter | C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 |
| Description | - | - | - | - | ln ($P_c$) | $T_c$ | $T_{lower}$ | $T_{upper}$ |
| Unit | N/A | N/A | N/A | N/A | ln (Bar) | K | K | K |

$\triangle H_{vap}$: NIST Watson Equation [28]

$$\ln(\Delta H_{vap}) = C_1 + \sum_{i=2}^{C_6} C_i \times \left(\frac{T}{C_5}\right)^{i-2} \times \ln\left(1 - \frac{T}{C_5}\right) \quad \text{(B.51)}$$

Table B.14. The Parameters of NIST Watson Equation for $\triangle H_{vap}$ for FAME

| NIST Watson Equation (J / kmol) | C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 |
|---|---|---|---|---|---|---|---|---|
| C12:0 | 18.71476 | 1.562579 | -1.321583 | 0.2647786 | 712 | 4 | 278 | 712 |
| C14:0 | 19.11147 | 2.941289 | -3.70431 | 1.327995 | 718 | 4 | 292 | 718 |
| C16:0 | 18.36144 | -0.701121 | 2.342368 | -1.24532 | 749 | 4 | 303 | 749 |
| C16:1 | 19.10368 | 2.33551 | -2.86149 | 1.05891 | 734 | 4 | 240 | 734 |
| C18:0 | 18.34189 | -0.918448 | 2.425747 | -1.143153 | 770 | 4 | 312 | 770 |
| C18:1 | 18.67553 | 0.0416939 | 1.315343 | -0.907716 | 761 | 4 | 253 | 761 |
| C18:2 | 19.07527 | 2.26599 | -2.78663 | 1.03997 | 773 | 4 | 234 | 773 |
| C18:3 | 18.49942 | -0.978716 | 3.4717 | 2.2344 | 753 | 4 | 255 | 753 |
| Parameter | C1 | C2 | C3 | C4 | C5 | C6 | C7 | C8 |
| Description | - | - | - | - | $T_c$ | - | $T_{lower}$ | $T_{upper}$ |
| Unit | N/A | N/A | N/A | N/A | K | N/A | K | K |