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Fragment-Based Approach for Estimating Thermophysical Properties of Fats and Vegetable Oils for Modeling Biodiesel Production Processes. Li Zong, Sundaram Ramanathan, and Chau-Chyun Chen*

Pages 879, 880, and 883. The *A* constant and the ΔG_{θ}^{vap} constant in Table 4 (page 879), the $\Delta \boldsymbol{G}_{\theta,A}^{vap}$ constant in Table 6, and eq b in Table 5 (page 880), as previously published, are revised. The revision corrects an unfortunate mistake in our handling of pressure units. Also revised are the mole fractions of soybean oil in Table 11 (page 883). We have misread the soybean oil triglyceride composition data of Ndiaye et al.[1] for PPP and SSS.

Table 4. Calculated Physical Constants from Vapor Pressures of Triglycerides

material	carbons	*A*	*B*	ΔH_{θ}^{vap} (J/kmol)	ΔG_{θ}^{vap}(J/kmol)
tributyrin	4:4:4	**12.495**	4250	8.137×10^7	$\mathbf{1.004 \times 10^7}$
tricaproin	6:6:6	**12.945**	4950	9.477×10^7	$\mathbf{2.088 \times 10^7}$
tricaprylin	8:8:8	**14.245**	6060	1.160×10^8	$\mathbf{3.471 \times 10^7}$
tricaprin	10:10:10	**14.205**	6510	1.246×10^8	$\mathbf{4.355 \times 10^7}$
trilaurin	12:12:12	**14.705**	7190	1.377×10^8	$\mathbf{5.371 \times 10^7}$
trimyristin	14:14:14	**14.905**	7720	1.478×10^8	$\mathbf{6.272 \times 10^7}$
tripalmitin	16:16:16	**15.525**	8400	1.608×10^8	$\mathbf{7.220 \times 10^7}$
tristearin	18:18:18	**15.725**	8750	1.675×10^8	$\mathbf{7.776 \times 10^7}$
1-capryl-2-lauryl-3-myristin	10:12:14	**14.025**	6880	1.317×10^8	$\mathbf{5.166 \times 10^7}$
1-lauryl-2-myristyl-3-palmitin	12:14:16	**14.925**	7720	1.478×10^8	$\mathbf{6.261 \times 10^7}$
1-myristyl-2-palmityl-3-stearin	14:16:18	**15.305**	8250	1.579×10^8	$\mathbf{7.058 \times 10^7}$
1-myristyl-2-capryl-3-stearin	14:10:18	**15.005**	7750	1.484×10^8	$\mathbf{6.272 \times 10^7}$
1-myristyl-2-lauryl-3-stearin	14:12:18	**14.965**	7860	1.505×10^8	$\mathbf{6.506 \times 10^7}$
1-palmityl-2-capryl-3-stearin	16:10:18	**15.425**	8090	1.549×10^8	$\mathbf{6.684 \times 10^7}$
1-palmityl-2-lauryl-3-stearin	16:12:18	**15.675**	8360	1.601×10^8	$\mathbf{7.058 \times 10^7}$

Table 5. Relationship between Fragment-Specific Parameters and Carbon Number of Each Fatty Acid Fragment[a]

fragment-specific parameters	trend line equation	R^2	equation number
	Vapor Pressure		
$\Delta H^{vap}_{\theta,A}$ (J/kmol)	$y = 2093479.64x + 31397826.69$	0.988	(a)
$\Delta G^{vap}_{\theta,A}$ (J/kmol)	$\mathbf{y = 1653848.04x + 22009767.68}$	0.994	(b)
	Heat Capacity		
$A_{1,A}$ (J/(kmol K))	$y = 21028.920x - 2485.721$	0.995	(c)
$A_{2,A}$ (J/(kmol K^2))	$y = 31.459476x - 82.038794$	0.946	(d)
	Liquid Enthalpy of Formation		
saturated (kJ/mol)	$y = -59.571x - 1358.7$	0.996	(e)
monounsaturated (kJ/mol)	$y = -76.494x - 815.18$	1.00	(f)
	Solid Enthalpy of Formation		
saturated (kJ/mol)	$y = -76.467x - 1250.8$	0.995	(g)
monounsaturated (kJ/mol)	$y = -85.795x - 752.88$	0.999	(h)
	Liquid Molar Volume		
$B_{1,A}$ (kmol/m^3)	$y = 65.787x^{-0.9251}$	0.999	(i)
$B_{2,A}$ (K^{-1})	$y = 3.6064 \times 10^{-6}x^2 - 7.7353 \times 10^{-5}x + 1.6438 \times 10^{-3}$	0.720	(j)
	Liquid Viscosity		
$C_{1,A}$ (Pa s)	$y = -1.0172x - 45.8525$	0.898	(k)
$C_{2,A}$ (K)	$y = 81.83611x + 2153.99554$	0.943	(l)
$C_{3,A}$ (K)	$y = 0.141996x + 20.545285$	0.896	(m)

[a] Note: In the equations, y represents the fragment-specific parameters in column 1 and x represents the carbon number of each saturated fatty acid fragment. R^2 is R-square values of the trend line equations.

Table 6. Calculated Vapor Pressure Fragment Parameters $\Delta H^{vap}_{\theta,A}$ and $\Delta G^{vap}_{\theta,A}$

fragments	symbols	carbons	$\Delta H^{vap}_{\theta,A}$ (J/kmol)	$\Delta G^{vap}_{\theta,A}$ (J/kmol)
glycerol	Gly-frag		-3.476×10^7	$\mathbf{-7.388 \times 10^7}$
butyric	Bu-frag	C4:0	3.862×10^7	$\mathbf{2.789 \times 10^7}$
caproic	Co-frag	C6:0	4.307×10^7	$\mathbf{3.148 \times 10^7}$
caprylic	Cy-frag	C8:0	5.015×10^7	$\mathbf{3.609 \times 10^7}$
capric	C-frag	C10:0	5.292×10^7	$\mathbf{3.904 \times 10^7}$
lauric	L-frag	C12:0	5.707×10^7	$\mathbf{4.233 \times 10^7}$
myristic	M-frag	C14:0	6.006×10^7	$\mathbf{4.515 \times 10^7}$
palmitic	P-frag	C16:0	6.550×10^7	$\mathbf{4.877 \times 10^7}$
palmitoleic	Po-frag	C16:1	6.550×10^7	$\mathbf{4.877 \times 10^7}$
stearic	S-frag	C18:0	6.800×10^7	$\mathbf{5.088 \times 10^7}$
oleic	O-frag	C18:1	6.800×10^7	$\mathbf{5.088 \times 10^7}$
linoleic	Li-frag	C18:2	6.800×10^7	$\mathbf{5.088 \times 10^7}$
linolenic	Ln-frag	C18:3	6.800×10^7	$\mathbf{5.088 \times 10^7}$
arachidic	A-frag	C20:0	7.327×10^7	$\mathbf{5.509 \times 10^7}$
behenic	B-frag	C22:0	7.745×10^7	$\mathbf{5.839 \times 10^7}$
erucic	E-frag	C22:1	7.745×10^7	$\mathbf{5.839 \times 10^7}$

Table 11. Triglyceride Composition of Soybean Oil[35]

fatty acid chain	triglyceride	mole fraction soybean oil
C16:0	PPP	**0.1221**
C18:0	SSS	**0.0340**
C18:1	OOO	**0.2327**
C18:2	LiLiLi	**0.5425**
C18:3	LnLnLn	**0.0687**

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Literature Cited

(1) Ndiaye, P. M.; Tavares, F. W.; Dalmolin, I.; Dariva, C.; Oliveira, D.; Oliveira, J. V. Vapor Pressure Data of Soybean Oil, Castor Oil, and Their Fatty Acid Ethyl Ester Derivatives. *J. Chem. Eng. Data* **2005**, *50*, 330−333.

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