SUPPORTING INFORMATION

Experimental study and modeling of phase equilibrium of the methanol–tripalmitin system: application to palm oil transesterification with supercritical methanol

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Figure S1

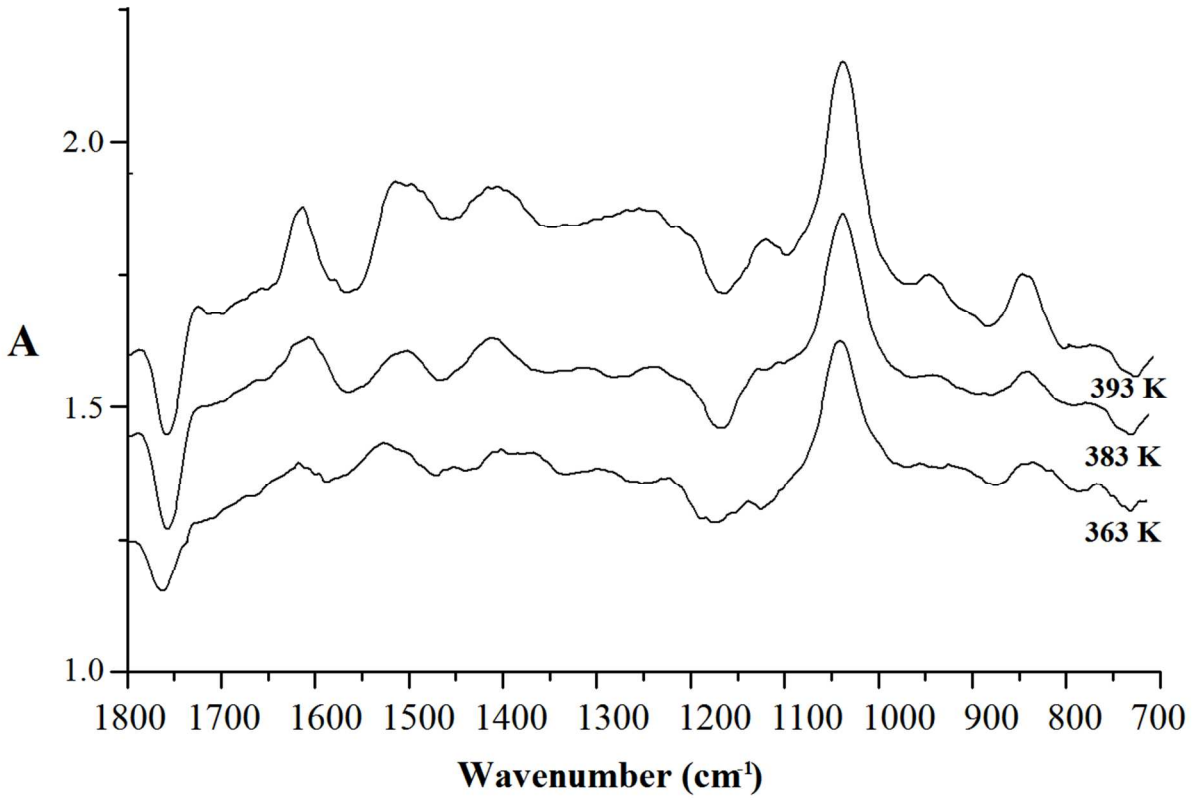

Figure S1. The spectra change in the PO-rich phase with temperature at 1 MPa

Figure S2

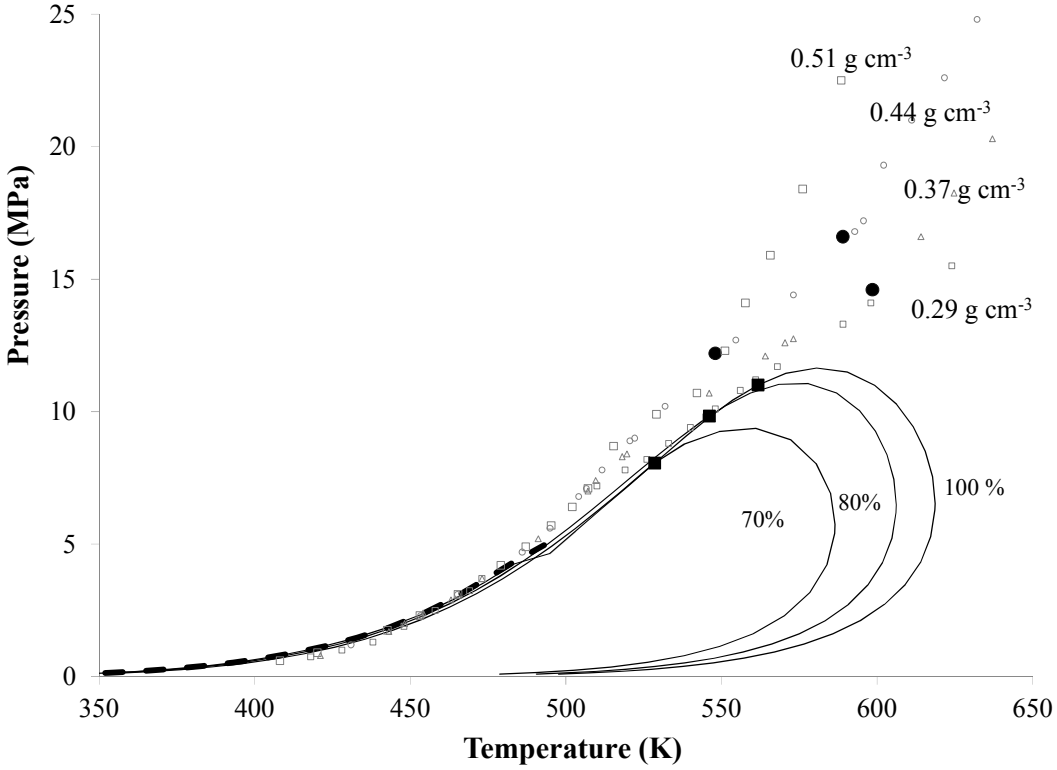

Figure S2. Pressure–temperature (*P–T*) curves for the methanol and sunflower-oil systems with a molar ratio of 40:1; solid circles (●) denote the phase-transition points. Experimental data was obtained from Velez et al.[1]

S1. Calculation of single pseudo-triglyceride

In this work, the PO is represented by a single pseudo-triglyceride with the following molecular structure:

$$[(CH_2COO)_2CHCOO](CH{=}CH)_m(CH_2)_n(CH_3)_3$$

Where m is a degree of unsaturation and n is degree of saturation in a single pseudo-triglyceride. Consequently, the values of n and m can be calculated as following Eq. (S1) and (S2) by using the information from Table S1.

$$n = \sum_{i=1}^{N} n_i x_i , \quad \text{(S1)}$$

$$m = \sum_{i=1}^{N} m_i x_i \quad \text{(S2)}$$

Finally, the pseudo-triglyceride for represent PO is (rounding numbers to the nearest integer numbers):

$$[(CH_2COO)_2CHCOO](CH{=}CH)_{1.5}(CH_2)_{42}(CH_3)_3$$

Table S1. The typical fatty acid composition (mole fractions, x_i) of commercial palm oil (PO) and the number of CH_2 (n_i) and CH=CH (m_i) functional groups.

Fatty acid	mole fraction (x_i)	n_i	m_i
Lauric acid	0.0052	30	0
Myristic acid	0.0104	36	0
Palmitic acid	0.5369	42	0
Palmitoleic acid	0.0010	36	3
Stearic acid	0.0405	48	0
Oleic acid	0.3083	42	3
Linoleic acid	0.0964	36	6
Linolenic acid	0.0009	30	9
	Total	41.52	1.52

Table S2. Experimental and Predicted Mole Fraction of Methanol in PO-Rich Phase (X_{MeOH}) for Phase Equilibrium Data of the Methanol–Tripalmitin Binary System and the Average Absolute Relative Error

Temperature (K)	Pressure (MPa)	Experimental results	Predicted result			
			PR	PR–MHV1–UNIFAC	PR–MHV2–UNIFAC	PR–MHV2–UNIQUAC
363	1	0.403±0.008	0.293	0.172	0.211	0.366
383	1	0.406±0.016	0.342	0.19	0.222	0.4
393	1	0.431±0.017	0.395	0.211	0.232	0.434
363	2	0.373±0.009	0.286	0.167	0.215	0.37
383	2	0.397±0.010	0.334	0.185	0.227	0.405
393	2	0.412±0.015	0.385	0.205	0.238	0.439
363	4	0.357±0.001	0.274	0.157	0.223	0.378
383	4	0.419±0.006	0.319	0.174	0.236	0.413
393	4	0.427±0.053	0.368	0.193	0.248	0.449
		%AARE	16.26	50.89	44.09	5.58

REFERENCES

(1) Velez, A.; Hegel, P.; Mabe, G.; Brignole, E. A. Density and Conversion in Biodiesel Production with Supercritical Methanol. *Ind. Eng. Chem. Res.* **2010,** 49, 7666.