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Isobaric vapor–liquid equilibrium for the three binary systems of C_{14}–C_{16} *n*-alkane + methyl myristate at 5.00 kPa

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ABSTRACT

In this work, new isobaric vapor–liquid equilibrium (VLE) data for the three binary mixtures (*n*-tetradecane + methyl myristate), (*n*-pentadecane + methyl myristate) and (*n*-hexadecane + methyl myristate) have been determined at 5.00 kPa by a Rose still. The three binary systems exhibit positive deviations and do not have an azeotropic point. All the experimental data were confirmed to be thermodynamic consistent using the van Ness method. The NRTL, UNIQUAC, and Wilson activity coefficient models were applied to regress the experimental VLE data and the new binary interaction parameters for the three models were obtained. The correlated values of the three models were compared with the measured data, the average absolute deviations of the temperatures and the vapor compositions for all the systems were less than 0.23 K and 0.0024, respectively. Therefore, the three activity coefficient models are suitable for all the three binary systems.

1. Introduction

Since the traditional fossil energy resources dry up day by day and the environmental concerns are worsening, it is very eager to take immediate action for a sustainable future [1,2]. Biodiesel, produced from transesterification of vegetable oils or animal fats, is fatty acid ester mixtures and presents the promising alternative substitute to fossil energy due to its renewable and low-emission characters [3,4]. However, the long-term engine tests using biodiesel as fuels showed ignition delay and higher carbon built up, which suggested that biodiesel is not suitable well to use directly in the existing diesel engines. Fortunately, biodiesel is miscible with fossil-based diesel in any proportion and the blended fuel of biodiesel with diesel exhibits the excellent combustion performance and prevents the engine failure [5].

During the exploitation, transport, and storage of diesel/biodiesel blended fuel, the vapor–liquid equilibrium data of mixtures involving in fatty acid methyl ester (biodiesel) and alkane (diesel) are very essential to accurately understand the boiling point and volatility of the blended fuel [6]. Some VLE data for the mixtures containing fatty acid methyl ester and alkane have been reported in the published paper. Luo et al. [7] determined the VLE data for four binary systems of C_{11}–C_{14} *n*-alkane + methyl dodecanoate at subatmospheric pressure. Schwarz el at. [8] reported the phase equilibrium data for the binary mixtures (propane + methyl decanoate) and (propane + methyl docosanoate) at high pressure. A survey of literatures showed that there was no published work on the VLE data for the binary mixtures of (alkane + methyl myristate).

In this work, the vapor–liquid equilibrium data for the three binary systems of C_{14}–C_{16} *n*-alkane + methyl myristate were determined at 5.00 kPa by a Rose still. The measured VLE data were verified with the van Ness method to check thermodynamic consistency. Furthermore, the non-random two-liquid (NRTL), universal quasi-chemical activity coefficient (UNIQUAC), and Wilson model were applied to regress the measured data and the corresponding parameters were obtained.

2. Experiments

2.1. Materials

All the reagents used in this study were obtained from J&K Scientific, China. Table 1 presented the information of the four chemicals, including the suppliers, the purity and CAS#. All

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Table 1
Materials description.

Chemical	*n*-Tetradecane	*n*-Pentadecane	*n*-Hexadecane	Methyl myristate
Source	J&K Scientific, China	J&K Scientific, China	J&K Scientific, China	J&K Scientific, China
CAS #	629-59-4	629-62-9	544-76-3	124-10-7
Final purity (wt%)	≥99.0	≥99.0	≥99.0	≥99.0
Measurement method[a]	GC-FID	GC-FID	GC-FID	GC-FID
Purification method	None	None	None	None

[a] In this work.

chemicals were used without further purification. The purities of all the components have been confirmed by GC-FID.

2.2. Apparatus and procedure

A modified Rose still was used to determine the experimental VLE data and the detailed procedures were described in our reported literatures [9,10]. In order to obtain the phase equilibrium rapidly, the intimate contact was maintained for the vapor and the liquid phases through the continuous dynamic circulation between the two phases in each experimental run. The system assumed to reach equilibrium state when the temperature was kept constant for more than 60 min. The system's pressure was kept at 5.00 kPa, which were controlled by needle valve in each experiment.

The digital vacuum gauge (Testo552, Testo, Germany) was used to determine the pressure. And, the temperature was determined by a precise mercury thermometer (Tianjin Glass Instrument Factory). The standard uncertainty of pressure and temperature were ±0.01 kPa and ±0.02 K, respectively.

2.3. Analysis

The compositions of the equilibrium liquid and vapor samples (cooled to liquid) were determine using Purkinje General GC-1100 equipped with FID and a DB-5HT chromatographic column (30m 0.25 mm 0.10 μm). The temperature of injector and FID were set at 250 °C and 270 °C, respectively. The high-purity nitrogen (mass fraction 0.99999) was employed as carrier gas at a constant flow

Table 2
Experimental and calculated VLE data of three binary systems of *n*-tetradecane(1) + methyl myristate(2), *n*-pentadecane(1) + methyl myristate(2) and *n*-hexadecane(1) + methyl myristate(2) at 5.00 kPa.[a]

No.	x_1	T (K)				y_1				γ_1	γ_2
		exp	NRTL	UNIQUAC	Wilson	exp	NRTL	UNIQUAC	Wilson		
n-Tetradecane(1) + methyl myristate(2) system											
1	1	425.67	425.55	425.55	425.55	1	1	1	1	1	
2	0.9113	426.85	427.26	427.26	427.26	0.9790	0.9775	0.9775	0.9776	1.021	1.188
3	0.8047	429.05	429.48	429.48	429.49	0.9500	0.9477	0.9477	0.9477	1.031	1.158
4	0.6837	431.84	432.24	432.24	432.25	0.9105	0.9085	0.9085	0.9084	1.046	1.126
5	0.5345	435.99	436.19	436.19	436.2	0.8447	0.8468	0.8469	0.8467	1.064	1.102
6	0.4725	438.2	438.1	438.1	438.11	0.8107	0.8143	0.8144	0.8141	1.066	1.075
7	0.3332	442.8	443.1	443.1	443.11	0.7153	0.7170	0.7170	0.7168	1.132	1.049
8	0.2497	446.45	446.88	446.88	446.88	0.6320	0.6311	0.6311	0.6310	1.175	1.033
9	0.1881	450.07	450.24	450.24	450.23	0.5435	0.5449	0.5449	0.5450	1.185	1.019
10	0.1278	454.05	454.11	454.11	454.09	0.4252	0.4312	0.4312	0.4315	1.194	1.017
11	0.063	458.95	459.13	459.13	459.12	0.2520	0.2571	0.2571	0.2575	1.224	1.016
12	0.0246	462.55	462.69	462.69	462.68	0.1107	0.1140	0.1140	0.1143	1.231	1.010
13	0	465.35	465.35	465.35	465.35	0	0	0	0		1
n-Pentadecane(1) + methyl myristate(2) system											
1	1	440.41	440.38	440.38	440.38	1	1	1	1	1	
2	0.9434	441.22	441.23	441.23	441.23	0.9761	0.9752	0.9752	0.9753	1.002	1.111
3	0.8474	442.65	442.75	442.74	442.75	0.9325	0.9310	0.9311	0.9310	1.010	1.094
4	0.7132	444.84	445.03	445.01	445.03	0.8643	0.8623	0.8627	0.8623	1.025	1.066
5	0.6026	446.82	447.12	447.11	447.13	0.7973	0.7965	0.7971	0.7963	1.040	1.058
6	0.5126	449.05	449.03	449.02	449.03	0.7363	0.7339	0.7346	0.7337	1.041	1.023
7	0.3821	451.8	452.11	452.1	452.11	0.6240	0.6232	0.6237	0.6230	1.073	1.028
8	0.2493	455.73	455.85	455.86	455.85	0.4672	0.4737	0.4738	0.4736	1.071	1.024
9	0.1282	460.11	459.97	459.97	459.96	0.2807	0.2863	0.2862	0.2864	1.077	1.004
10	0.0439	463.2	463.29	463.3	463.29	0.1136	0.1116	0.1114	0.1116	1.146	1.002
11	0	465.35	465.35	465.35	465.35	0	0	0	0		1
n-Hexadecane(1) + methyl myristate(2) system											
1	1	454.24	454.21	454.21	454.21	1	1	1	1	1	
2	0.9299	454.65	454.65	454.65	454.65	0.9473	0.9462	0.9462	0.9462	1.017	1.152
3	0.8059	455.41	455.5	455.51	455.5	0.8515	0.8515	0.8515	0.8515	1.022	1.131
4	0.7055	456.17	456.28	456.28	456.28	0.7710	0.7738	0.7738	0.7738	1.027	1.116
5	0.572	457.29	457.45	457.45	457.45	0.6620	0.6656	0.6655	0.6656	1.040	1.080
6	0.4562	458.56	458.61	458.61	458.61	0.5598	0.5640	0.5639	0.5640	1.053	1.054
7	0.3745	459.43	459.53	459.53	459.53	0.4818	0.4859	0.4859	0.4859	1.062	1.034
8	0.2581	460.86	461.01	461.01	461.01	0.3607	0.3619	0.3619	0.3619	1.096	1.018
9	0.1966	461.72	461.88	461.87	461.88	0.2879	0.2885	0.2885	0.2885	1.114	1.013
10	0.119	463.09	463.1	463.09	463.1	0.1827	0.1860	0.1861	0.1860	1.111	1.006
11	0.0542	464.21	464.22	464.22	464.22	0.0874	0.0897	0.0897	0.0897	1.122	1.003
12	0	465.2	465.24	465.24	465.24	0	0	0	0		1

[a] Standard uncertainties μ are $\mu(T) = 0.02$ K, $\mu(x_1) = \mu(y1) = 0.001$ and $\mu(P) = 0.01$ kPa. x_1 is the mole fraction of *n*-alkane in the liquid phase; y_1 is the mole fraction of *n*-alkane in the vapor phase; T is the equilibrium temperature; γ_1 and γ_2 are the activity coefficients of *n*-alkane and methyl myristate, respectively.