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Isobaric Vapor−Liquid Equilibria of Heptane + 1-Butanol and Heptane + 1-Pentanol Systems at (53.3 and 91.3) kPa

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Isobaric vapor−liquid equilibrium (VLE) data have been determined at (53.3 and 91.3) kPa for the binary mixtures of heptane + 1-butanol and heptane + 1-pentanol. The VLE data of binary systems were found to be thermodynamically consistent. In addition, the experimental VLE data were correlated by using the Wilson, nonrandom two-liquid (NRTL), and universal quasi-chemical (UNIQUAC) activity coefficient models for the liquid phases. The binary interaction parameters of the activity coefficient models have been determined and reported. A comparison of model performances has been made by using the criterion of the average absolute deviation (AAD) in boiling-point and vapor-phase composition. The obtained results indicate that the used activity coefficient models satisfactorily correlate the VLE data of the studied systems.

Introduction

Considering environmental protection strategies, production costs, and different requests for the industrial production of chemicals involves purification and recovery of the products, byproducts, and unreacted raw materials. The presence of some specific groups, particularly polar groups (oxygen, nitrogen), in most liquid mixtures of organic components forms nonideal systems. The separation of nonideal mixtures especially azeotropic mixtures is a topic of great practical and industrial interest.[1,2] Distillation is clearly the dominating separation process, accounting for more applications than all of the other separation processes, such as extraction, adsorption, crystallization, and membrane-based technologies. For the development of efficient distillation processes for the non-ideal mixtures, there is a great need for vapor−liquid equilibrium (VLE) data.[3,4]

In recent years it has become increasingly important to develop new thermodynamic research on the VLE of mixtures formed by hydrocarbons and oxygenated additives (ethers and alkanols) to unleaded gasoline. There are various models to estimate the VLE of non-ideal systems, but for new systems especially in the final design step the necessary VLE data needs to be determined experimentally.[5−7]

In this work, to improve our knowledge of the phase behavior of alkanes with 1-butanol and 1-pentanol mixtures, we measured isobaric VLE data for the (heptane + 1-butanol) and (heptane + 1-pentanol) systems at (53.3 and 91.3) kPa. The obtained VLE data of binary systems and the activity coefficients were found to be thermodynamically consistent. The experimental data were correlated with using the Wilson,[8] nonrandom two-liquid (NRTL),[9] and universal quasi-chemical (UNIQUAC)[10] equations for the liquid-phase activity coefficients. The correlated parameters of the models are given.

Experimental Section

Materials. All materials were supplied by Merck. The purity of the pure components was checked on the basis of its refractive index at 293.15 K. The refractive index was measured using a thermostatically controlled Abbe refractometer (Atago 1T/4T) equipped with a digital thermometer, with an uncertainty of ± 0.05 °C, with an uncertainty of ± 0.0001 n_D. The measured physical properties are listed in Table 1 along with values from the literature.[11,12] Boiling point measurements were obtained by using a Fischer boiling-point measurement. The estimated uncertainty in the boiling point measurements was 0.05 K. The materials were used directly without further purification.

Table 1. Normal Boiling Temperature and Refractive Index of the Chemicals[a]

	heptane	1-butanol	1-pentanol
T_b^{lit}/K	371.55	390.88	411.13
T_b^{exp}/K	371.65	390.95	411.10
n_D^{lit}	1.3877	1.3993	1.4100
n_D^{exp}	1.3876	1.3992	1.4101

[a] T_b and n_D data are taken from Lide[11] and Dean,[12] respectively.

Apparatus and Procedure. In the dynamic equilibrium still the binary mixture was brought to a boil under controlled pressure. The pressure was fixed and held constant by using a vacuum pump. In each VLE experiment, the vapor and liquid mixture was separated in the equilibrium glass cell, and the vapor phase was condensed and returned to the boiling cell. The composition of the boiling liquid and the vapor changed with time until a steady state was achieved. The system was kept at the boiling point at least for 20 min to ensure that the steady state was reached. Then, samples of liquid and condensate were taken for analysis. The equilibrium compositions were determined by the refractometry method. The refractive index measurements were done by an Abbe refractometer (Atago 1T/4T). The refractometer was frequently calibrated by using double-distilled water. Water was circulated into the instrument through a thermostatically controlled bath maintained constant to ± 0.01 °C. At least three analyses were made for each sample. The measured refractive index data of the binary mixtures of heptane + 1-butanol and heptane + 1-pentanol at 293.15 K are reported in Table 2. The maximum deviations from the average value were less than 0.1 %. The uncertainties of the pressure, equilibrium composition measurements, and temperature were ± 0.1 kPa, ± 0.006 mol fraction, and ± 0.05 K, respectively. The vapor pressures of the pure components were measured with the same recirculating still.

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Table 2. Experimental Refractive Index of [Heptane (1) + 1-Butanol (2)] and [Heptane (1) + 1-Butanol (2)] Binary Mixtures at 293.15 K

heptane (1) + 1-butanol (2)		heptane (1) + 1-pentanol (2)	
x_2	n_D	x_2	n_D
0.000	1.3876	0.000	1.3876
0.112	1.3889	0.075	1.3893
0.190	1.3898	0.160	1.3912
0.284	1.3909	0.284	1.3940
0.371	1.3919	0.351	1.3955
0.465	1.3930	0.462	1.3980
0.500	1.3934	0.582	1.4007
0.586	1.3944	0.684	1.4030
0.681	1.3955	0.773	1.4051
0.759	1.3964	0.898	1.4078
0.828	1.3972	1.000	1.4101
0.922	1.3983		
1.000	1.3992		

Table 3. Experimental Vapor Pressures at Different Temperatures

1-butanol		1-pentanol		heptane	
P/kPa	T/K	P/kPa	T/K	P/kPa	T/K
120.1	395.80	113.3	414.65	108.8	374.00
105.3	391.95	101.9	411.35	100.8	371.35
84.9	386.05	94.5	409.00	92.7	368.55
72.8	381.90	81.3	404.60	78.7	363.15
61.2	377.30	69.3	400.05	65.3	357.25
52.5	373.45	56.9	394.70	55.3	352.35
42.8	368.60	49.2	390.75	48.9	348.55
33.5	362.95	40.0	385.65	41.3	343.75
29.3	359.45	35.3	382.40	36.9	340.55
25.3	356.35	31.2	379.35	32.3	336.85
				29.9	335.20
				27.1	332.90

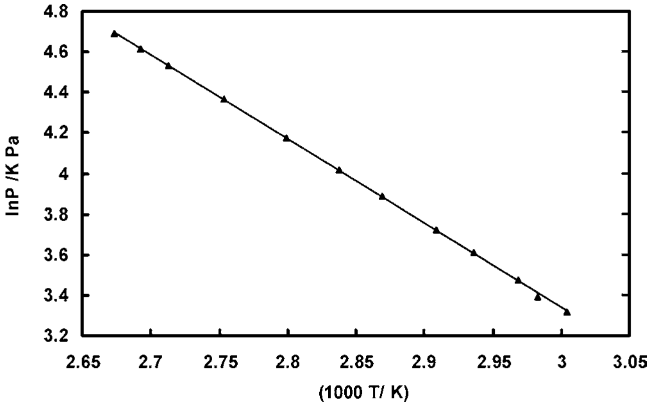

Figure 1. Experimental vapor pressure data at different temperatures for heptane. Solid line calculated from the Wagner equation.

Results and Discussion

Vapor Pressure. The experimental vapor pressures measured in this work are given in Table 3. The measured vapor pressure data was compared with those obtained by the Wagner equation, which is expressed in the following form:[13]

$$\ln P_{\text{vpr}} = (a\tau + b\tau^{1.5} + c\tau^{2.5} + d\tau^{5})/T_{\text{r}} \qquad (1)$$

where $\tau = (1 - T_{\text{r}})$ and a, b, c, and d are constant parameters. T_{r} and P_{vpr} are the reduced temperature and the reduced vapor pressure, respectively. Table 4 shows the Wagner constant parameters, critical pressure, and critical temperature of the pure chemicals from the literature.[14,15] The measured heptane vapor pressure and the predicted one by the Wagner equation are presented in Figure 1. As shown in Figure 1, the obtained heptane vapor-pressure data was well-matched with the Wagner equation. The percent average absolute deviation (AAD %) between the obtained vapor pressure data and those correlated by Wagner equation was 0.37 %, 0.19 %, and 0.13 % for 1-butanol, 1-pentanol, and heptane, respectively.

Isobaric VLE. VLE were measured at (53.3 and 91.3) kPa for the (heptane + 1-butanol) and (heptane + 1-pentanol) binary systems. The obtained results are shown in Tables 5 and 6. VLE data include vapor- and liquid-phase compositions, temperature, and liquid-phase activity coefficients. The thermodynamic consistency of the experimental data was checked by means of the Herington[16] and Redlich and Kister[17,18] test methods. According to the test method criteria, the VLE data were of acceptable quality. The experimental liquid-phase activity coefficient of component i was evaluated by the following equation:

$$\gamma_i = \frac{y_i P}{x_i P_i^{\text{sat}}} \qquad (2)$$

where y_i, x_i, P, and P_i^{sat} are respectively the gas-phase mole fraction, the liquid-phase mole fraction, the total pressure, and the saturated pressure of component i. Equation 2 was used to calculate the experimental liquid-phase activity coefficient assuming that the vapor phase behaves as an ideal gas at low experimental pressures ($P_{\text{r}} < 0.03$).

The Wilson, NRTL, and UNIQUAC activity-coefficient models were used for the VLE calculations of the studied binary systems by a bubble temperature calculation procedure.[19] The binary interaction parameters of the models studied were determined on the basis of the simplex method[20] by minimization of the following objective function (OF):

$$\text{OF} = \sum_{i=1}^{N} \sum_{j=1}^{2} \left[\left(\frac{\gamma_j - \gamma_j^{\text{cal}}}{\gamma_j}\right)^2\right]_i \qquad (3)$$

where N is number of data points and γ_j and γ_j^{cal} are the experimental and calculated activity coefficients of the jth component. The AADs in the boiling temperatures and vapor-phase mole fractions were calculated as a measure of the agreement between the experimental data and the calculated values. The AAD was defined in the following form:

$$\text{AAD} = \frac{1}{N}\sum_{i=1}^{N} |x_i - x_i^{\text{cal}}| \qquad (4)$$

The obtained interaction parameters for the Wilson, NRTL, and UNIQUAC activity coefficient models and the calculated AAD for the boiling temperature and vapor-phase mole fraction are shown in Tables 7 and 8.

Figures 2 and 3 are the temperature–composition phase diagrams at 53.3 kPa for the binary systems of (heptane + 1-butanol) and (heptane + 1-pentanol), respectively.

Table 4. Parameters of the Wagner Equation,[14] Equation 1, and the Critical Pressure and Temperature of Pure Chemicals[15]

component	a	b	c	d	P_c/bar	T_c/K
heptane	−8.14882	0.79590	−3.1836	−3.8130	45.30	604.00
1-butanol	−8.40615	2.23010	−8.2486	−0.7110	44.24	563.05
1-pentanol	−8.98005	3.91624	−9.9081	−2.1910	39.09	588.15

Table 5. Experimental VLE Data for the Heptane (1) + 1-Butanol (2) System

x_1	y_1	T/K	γ_1	γ_2	x_1	y_1	T/K	γ_1	γ_2
		$P = 53.3$ kPa					$P = 91.3$ kPa		
0.000	0.000	373.85		1.000	0.000	0.000	387.75		1.000
0.005	0.036	373.25	3.725	0.992	0.005	0.040	386.85	4.383	1.005
0.012	0.090	371.90	3.854	0.997	0.016	0.102	385.55	3.893	0.997
0.026	0.176	369.85	3.686	0.995	0.028	0.185	383.15	4.234	1.001
0.062	0.335	365.35	3.418	1.006	0.059	0.322	379.65	3.907	0.983
0.081	0.400	363.50	3.320	1.002	0.092	0.412	376.10	3.535	1.015
0.108	0.469	360.95	3.148	1.021	0.131	0.491	373.40	3.202	1.020
0.136	0.522	358.80	2.986	1.044	0.166	0.549	371.20	3.006	1.030
0.193	0.605	356.10	2.656	1.043	0.223	0.614	369.00	2.673	1.036
0.246	0.657	353.65	2.452	1.084	0.322	0.679	365.70	2.266	1.133
0.310	0.690	352.35	2.137	1.138	0.420	0.710	364.15	1.859	1.235
0.377	0.721	351.15	1.910	1.199	0.487	0.725	364.05	1.681	1.376
0.441	0.741	350.50	1.714	1.282	0.542	0.738	363.65	1.556	1.497
0.503	0.759	349.95	1.567	1.379	0.604	0.741	363.30	1.418	1.735
0.570	0.771	349.55	1.425	1.540	0.670	0.742	363.25	1.282	2.080
0.638	0.780	349.35	1.298	1.773	0.701	0.752	363.15	1.245	2.130
0.709	0.790	349.15	1.190	2.130	0.744	0.765	363.05	1.197	2.464
0.745	0.796	349.05	1.145	2.377	0.775	0.776	363.05	1.166	2.674
0.759	0.801	349.00	1.134	2.451	0.784	0.782	363.05	1.162	2.709
0.792	0.806	349.00	1.094	2.765	0.819	0.797	363.15	1.130	2.995
0.805	0.810	349.00	1.081	2.896	0.832	0.805	363.25	1.121	3.080
0.852	0.827	349.10	1.040	3.448	0.868	0.815	363.50	1.079	3.683
0.890	0.847	349.25	1.013	4.093	0.909	0.834	363.90	1.041	4.720
0.915	0.866	349.35	1.004	4.621	0.947	0.861	364.55	1.012	6.580
0.945	0.896	349.85	0.990	5.369	0.969	0.890	365.75	0.985	8.478
0.969	0.930	350.30	0.986	6.304	0.983	0.935	366.65	0.992	8.809
0.983	0.957	350.75	0.985	6.912	0.992	0.969	367.75	0.986	8.512
1.000	1.000	351.45	1.000		1.000	1.000	368.45	1.000	

Table 6. Experimental VLE Data for the Heptane (1) + 1-Pentanol (2) System

x_1	y_1	T/K	γ_1	γ_2	x_1	y_1	T/K	γ_1	γ_2
		$P = 53.3$ kPa					$P = 91.3$ kPa		
0.000	0.000	393.20		1.000	0.000	0.000	408.15		1.000
0.006	0.057	391.65	2.280	1.011	0.008	0.057	406.85	2.570	0.989
0.012	0.112	390.35	2.271	0.995	0.020	0.107	405.40	2.680	0.996
0.020	0.183	388.25	2.293	0.995	0.026	0.180	403.45	2.700	0.985
0.044	0.323	384.15	2.325	0.995	0.052	0.314	398.25	2.625	1.019
0.073	0.460	379.00	2.354	0.996	0.090	0.460	393.80	2.510	0.983
0.105	0.585	373.85	2.370	1.101	0.136	0.570	389.25	2.305	0.981
0.163	0.692	368.20	2.348	0.999	0.188	0.673	383.40	2.304	1.003
0.252	0.794	361.80	2.166	1.150	0.282	0.758	378.25	1.999	1.032
0.346	0.841	357.35	2.063	1.050	0.375	0.804	374.15	1.789	1.145
0.433	0.870	354.30	1.853	1.124	0.450	0.840	371.45	1.688	1.192
0.519	0.887	353.15	1.637	1.255	0.545	0.851	370.25	1.463	1.413
0.578	0.895	352.75	1.489	1.407	0.599	0.870	369.45	1.392	1.454
0.624	0.900	352.50	1.388	1.563	0.650	0.875	368.90	1.313	1.635
0.674	0.902	352.15	1.289	1.794	0.694	0.880	368.55	1.249	1.829
0.726	0.906	351.95	1.197	2.110	0.740	0.888	368.30	1.192	2.025
0.787	0.909	351.70	1.113	2.701	0.802	0.898	368.20	1.114	2.447
0.855	0.917	351.50	1.049	3.568	0.861	0.910	368.10	1.055	3.089
0.912	0.930	351.25	1.009	4.795	0.919	0.920	367.95	1.004	4.757
0.947	0.947	351.15	0.995	5.749	0.950	0.949	367.75	1.008	5.720
0.955	0.952	351.15	0.992	6.073	0.960	0.954	367.85	0.992	6.391
0.980	0.971	351.25	0.987	7.099	0.980	0.969	367.95	0.992	7.416
0.989	0.983	351.35	0.986	7.579	0.990	0.983	368.10	0.994	7.708
1.000	1.000	351.50	1.000		1.000	1.000	368.45	1.000	

The temperature−composition phase diagrams at 91.3 kPa for the binary systems of (heptane + 1-butanol) and (heptane + 1-pentanol) are shown in Figures 4 and 5, respectively. As presented in the figures, the studied binary systems show a minimum boiling azeotrope. The azeotropic composition for the systems was obtained by determining the x_1 values that make the difference ($x_1 - y_1$) zero. The corresponding azeotropic temperature was computed from the experimental result around the azeotropic point, using the x_1 value previously determined. The azeotropic compositions and temperatures were reported in Table 9. The comparisons of the experimental results with those calculated by the Wilson, NRTL, and UNIQUAC activity coefficient models are shown in Figures 6 and 7. According to these figures and the calculated AAD reported in Tables 7 and

Table 7. Correlation Parameters and AADs in Boiling Temperatures and Vapor-Phase Mole Fractions for the System Heptane (1) + 1-Butanol (2)

model	$A_{12}{}^a$	$A_{21}{}^a$	$(1/N)\sum_{i=1}^{N} \lvert y_i - y_i^{\text{cal}}\rvert$	$(1/N)\sum_{i=1}^{N} \lvert T_i - T_i^{\text{cal}}\rvert$
			$P = 53.3$ kPa	
NRTL	324.89	1104.94	0.002	0.18
Wilson	108.73	1504.49	0.002	0.09
UNIQUAC	790.23	−263.11	0.003	0.27
			$P = 91.3$ kPa	
NRTL	399.28	1274.80	0.006	0.32
Wilson	83.23	1864.75	0.002	0.10
UNIQUAC	921.44	−298.64	0.004	0.41

[a] The binary adjustable parameters for various models are as follows: NRTL, $A_{ij} = (g_{ij} - g_{jj})$; Wilson, $A_{ij} = (\lambda_{ij} - \lambda_{ii})$; UNIQUAC, $A_{ij} = (u_{ij} - u_{jj})$. The uncertainties of the parameters are all ± 0.01.

Table 8. Correlation Parameters and AADs in Boiling Temperatures and Vapor-Phase Mole Fractions for the System 1-Heptane (1) + 1-Pentanol (2)

model	$A_{12}{}^{a}$	$A_{21}{}^{a}$	$(1/N)\sum_{i=1}^{N} \lvert y_i - y_i^{\text{cal}} \rvert$	$(1/N)\sum_{i=1}^{N} \lvert T_i - T_i^{\text{cal}} \rvert$
		$P = 53.3$ kPa		
NRTL	−26.331	1605.810	0.002	0.03
Wilson	−84.220	1982.605	0.001	0.12
UNIQUAC	842.964	−304.132	0.001	0.24
		$P = 91.3$ kPa		
NRTL	−51.078	1504.870	0.001	0.04
Wilson	−142.801	2074.335	0.002	0.10
UNIQUAC	993.544	−392.104	0.004	0.41

[a] The binary adjustable parameters for various models are as follows: NRTL, $A_{ij} = (g_{ij} - g_{jj})$; Wilson, $A_{ij} = (\lambda_{ij} - \lambda_{ii})$; UNIQUAC, $A_{ij} = (u_{ij} - u_{jj})$. The uncertainties of the parameters are all ± 0.01.

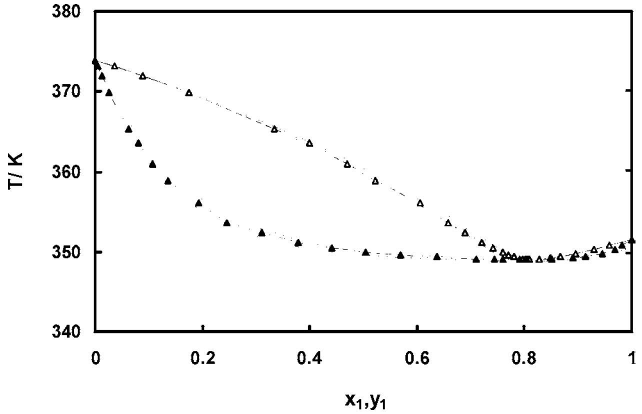

Figure 2. *T*−*x*−*y* diagram for heptane (1) + 1-butanol (2) at 53.3 kPa: ▲, experimental liquid-phase mole fractions, x_1; △, experimental vapor-phase mole fractions, y_1; —, NRTL equation; - - -, Wilson equation; — —, UNIQUAC equation.

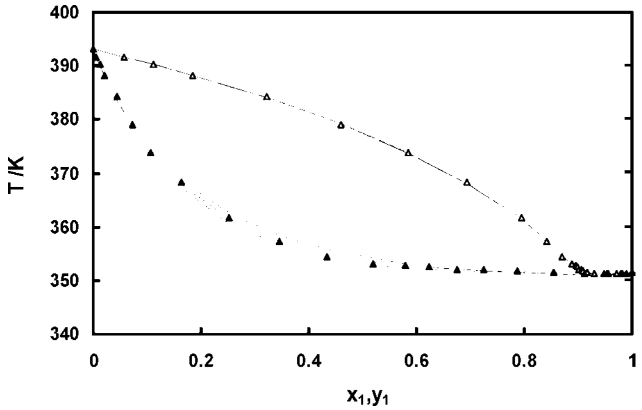

Figure 3. *T*−*x*−*y* diagram for heptane (1) + 1-butanol (2) at 91.3 kPa: ▲, experimental liquid-phase mole fractions, x_1; △, experimental vapor-phase mole fractions, y_1; —, NRTL equation; - - -, Wilson equation; — —, UNIQUAC equation.

Table 9. Azeotropic Compositions and Temperatures

P/kPa	*x*	*T*/K
	Heptane (1) + 1-Butanol (2)	
53.3	0.812	349.00
91.3	0.775	363.05
	Heptane (1) + 1-Pentanol (2)	
53.3	0.947	351.15
91.3	0.919	367.95

8, the activity coefficient models are generally satisfactory in VLE data representation for the studied binary systems.

The reduced excess molar Gibbs energy, (G_m^E/RT), was calculated from:

$$\frac{G_m^E}{RT} = x_1 \ln \gamma_1 + x_2 \ln \gamma_2 \tag{5}$$

The experimental reduced excess molar Gibbs energy for the studied binary mixtures is compared with those calculated by the NRTL model at (53.3 and 91.3) kPa. The obtained results as a function of liquid composition for [heptane (1) + 1-butanol (2)] and [heptane (1) + 1-pentanol (2)] binary mixtures are

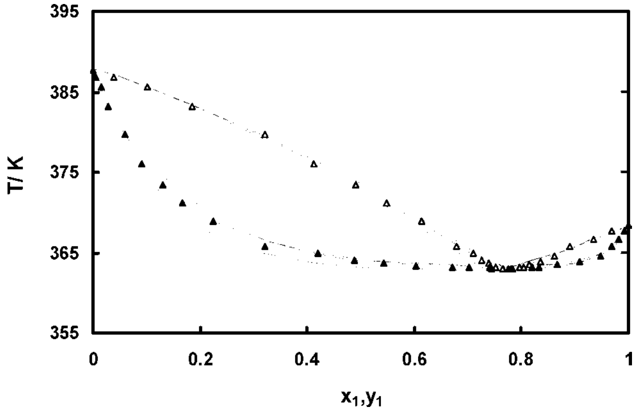

Figure 4. *T*−*x*−*y* diagram for heptane (1) + 1-pentanol (2) at 53.3 kPa: ▲, experimental liquid-phase mole fractions, x_1; △, experimental vapor-phase mole fractions, y_1; —, NRTL equation; - - -, Wilson equation; — —, UNIQUAC equation.

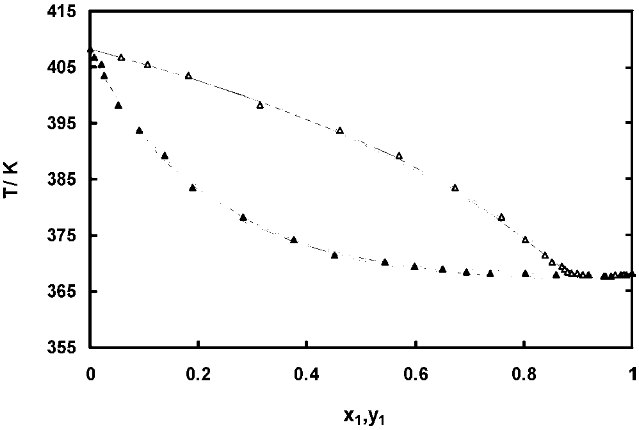

Figure 5. *T*−*x*−*y* diagram for heptane (1) + 1-pentanol (2) at 53.3 kPa: ▲, experimental liquid-phase mole fractions, x_1; △, experimental vapor-phase mole fractions, y_1; —, NRTL equation; - - -, Wilson equation; — —, UNIQUAC equation.

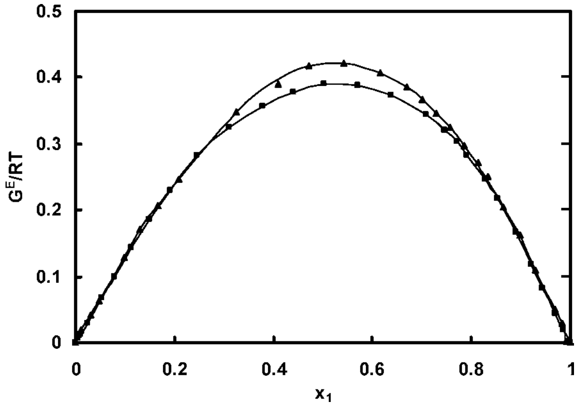

Figure 6. Excess molar Gibbs energy, G_m^E, for the binary mixture heptane (1) + 1- butanol (2). ■ and ▲ are the experimental points at (53.3 and 91.3) kPa, respectively. Solid curves are calculated by the NRTL equation.

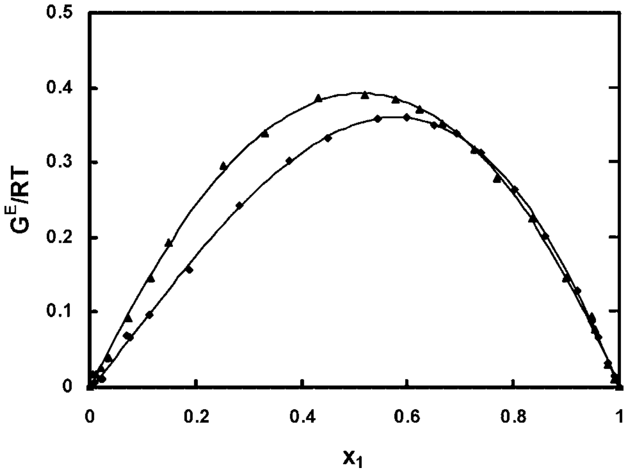

Figure 7. Excess molar Gibbs energy, G_m^E, for the binary mixture heptane (1) + 1-pentanol (2). ■ and ▲ are the experimental points at (53.3 and 91.3) kPa, respectively. Solid curves are calculated by the NRTL equation.

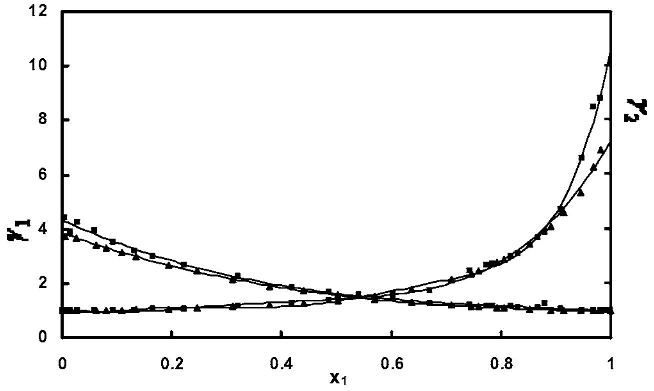

Figure 8. Experimental data and the fitting curves for the correlative NRTL model of γ_i, for the binary mixture heptane (1) + 1-butanol (2). ■ and ▲ are the experimental data points at (53.3 and 91.3) kPa, respectively.

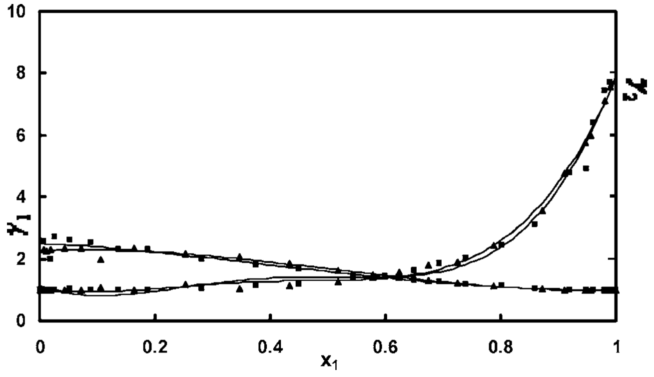

Figure 9. Experimental data and the fitting curves for the correlative NRTL model of γ_i, for the binary mixture heptane (1) + 1-pentanol (2). ■ and ▲ are the experimental data points at (53.3 and 91.3) kPa, respectively.

presented in Figures 6 and 7, respectively. A positive deviation from ideal behavior was observed for these two systems. The experimental γ_1 and γ_2 are compared with those calculated with the NRTL model, which is shown in Figures 8 and 9. According to these figures, the activity coefficient data was successfully correlated by the NRTL model.

Conclusion

Isobaric VLE data were determined experimentally for [heptane (1) + 1-butanol (2)] and [heptane (1) + 1-pentanol (2)] binary systems at (53.3 and 91.3) kPa. The studied systems exhibited a positive deviation from ideal behavior. Thus, a minimum boiling azeotrope occurred in the entire system. The obtained VLE data were examined by thermodynamic consistency tests. By the analysis of the Herington and Redlich and Kister tests, the VLE data were of acceptable quality. The VLE data were correlated by the Wilson, NRTL, and UNIQUAC activity coefficient models. The interaction parameters of three activity coefficient models were obtained and reported. The obtained results showed that all three models were generally satisfactory, while the NRTL and Wilson models gave a slightly better result than UNIQUAC model.

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