

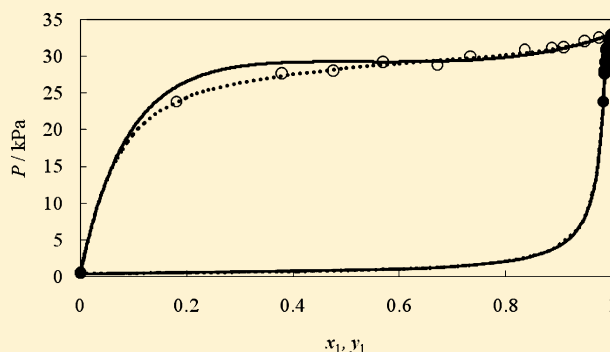
Isothermal Vapor–Liquid Equilibrium Data for the Propan-1-ol + Dodecane System at (323.0, 343.4, 353.2, 363.1, and 369.2) K

C. Narasigadu,[†] S. C. Subramoney,[†] P. Naidoo,[†] C. Coquelet,^{†,‡} D. Richon,^{†,‡} and D. Ramjugernath^{*,†}

[†]Thermodynamics Research Unit, School of Engineering, University of KwaZulu-Natal, Durban, 4041, South Africa

[‡]MINES-ParisTech, CEP/TEP–Centre Energétique et Procédés, 35 rue Saint Honoré, 77305 Fontainebleau, France

ABSTRACT: Isothermal vapor–liquid equilibrium (VLE) data (P – T – x – y) were measured and modeled for the propan-1-ol + dodecane system at (323.0, 343.4, 353.2, 363.1, and 369.2) K. The VLE data were measured using a dynamic–analytic method. The equilibrium cell used is a modified ebulliometer which allows for recirculation of both the liquid and the vapor phases and is capable of measuring systems of high relative volatility. The sampled equilibrium phases were analyzed and quantified using a gas chromatograph with a thermal conductivity detector. The measured experimental data were modeled using the γ – ϕ approach with the nonrandom two-liquid (NRTL) activity coefficient model to account for the liquid phase nonideality and the vapor phase assumed to be ideal. Fitting of the activity coefficient model was undertaken by nonlinear least-squares regression of the experimental data. Thermodynamic consistency testing of the experimental data was undertaken with the Van Ness test, with the data successfully passing the test.



■ INTRODUCTION

The separation of alcohols from water is a commonly encountered problem in industry, especially in the petrochemical industry. One of the methods to effectively remove the alcohols from an aqueous stream is to undertake solvent extraction with a suitable solvent. The separation process therefore comprises of a solvent extraction (liquid–liquid) column followed by a solvent recovery column in which the extractive solvent is separated from the alcohols. If the extractive solvent has a significantly higher boiling point than the alcohols (effectively a very large alcohol to solvent relative volatility), recovery of the solvent from the alcohol can be easily undertaken in a distillation column.

As part of a larger study in our research unit, dodecane was considered as a potential extractive solvent which could effect the separation of alcohols from an aqueous stream. Liquid–liquid equilibrium data for light alcohols with dodecane have already been measured and reported as part of this study.¹ In this paper vapor–liquid equilibrium (VLE) data (P – T – x – y) for one of the alcohol and extractive solvent combinations is reported, namely, the propan-1-ol + dodecane system. Isothermal VLE data were measured at five temperatures ranging from (323.0 to 369.2) K. All measurements were undertaken using an ebulliometer type equilibrium still which has been used extensively^{2–8} in our laboratories, but which was slightly modified to enable accurate measurements for relatively high volatile systems. The measured VLE data were subjected to thermodynamic consistency testing.

P – x data for the propan-1-ol + dodecane system at (342.8 and 352.7) K have been measured⁹ recently in our laboratories

using a static synthetic method. The vapor compositions were computed from the P – T – x data. With P – x data it is not possible to undertake thermodynamic consistency testing of the experimental data, and since we needed P – T – x – y data for preliminary design purposes for propan-1-ol + dodecane, we undertook measurements with a dynamic–analytical method in this study. There are to our knowledge no P – T – x – y data for this system currently available in literature.

The experimental data were correlated with the γ – ϕ approach with the nonrandom two-liquid (NRTL) activity coefficient model to account for the liquid phase nonideality and the vapor phase assumed to be ideal. Comparisons of the data measured in this study with predictions from universal functional activity coefficients (UNIFAC) were also undertaken, as well as a comparison with P – x data for the same system using a static synthetic method.⁹ Finally thermodynamic consistency testing of the data was undertaken using the Van Ness¹⁹ and Danner and Gess¹⁸ tests.

■ EXPERIMENTAL SECTION

Chemicals. The chemicals used in this work were purchased from Merck. The chemicals were used without further purification as careful gas chromatographic (GC) analysis revealed no significant impurities. Table 1 shows the purity of the chemicals as provided by the supplier, as well as the purity verification by GC analysis and refractive index measurement. GC analysis was

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Table 1. Chemical Purity

chemical	GC area fraction	mass fraction purity ^a	measured n_D^b	literature n_D^{12}
1-propanol	0.9997	>0.99	1.3851 ± 0.0001	1.3850
<i>n</i> -dodecane	0.9995	>0.99	1.4218 ± 0.0001	1.4210

^aAs stated by supplier. ^b n_D is the refractive index at $T = 293.15$ K using the Atago RX-7000 α refractometer.

undertaken on a Shimadzu GC-2014 chromatograph fitted with a thermal conductivity detector. Refractive index measurements were undertaken on a Atago RX-7000 α refractometer with a reported uncertainty of 0.0001.

Equipment. VLE measurements were undertaken using a dynamic analytical method on a modified version¹⁰ of an apparatus² which has been used extensively in our laboratories for low pressure VLE measurement. Details on the description and experimental procedure for the unmodified apparatus are available in a previous work.² The experimental procedure for the modified apparatus is identical to that for the unmodified version. The modification was applied to the recirculated streams exiting the liquid and vapor collection chambers whereby they were more intensively mixed using a spiral mixer (see Figure 1).

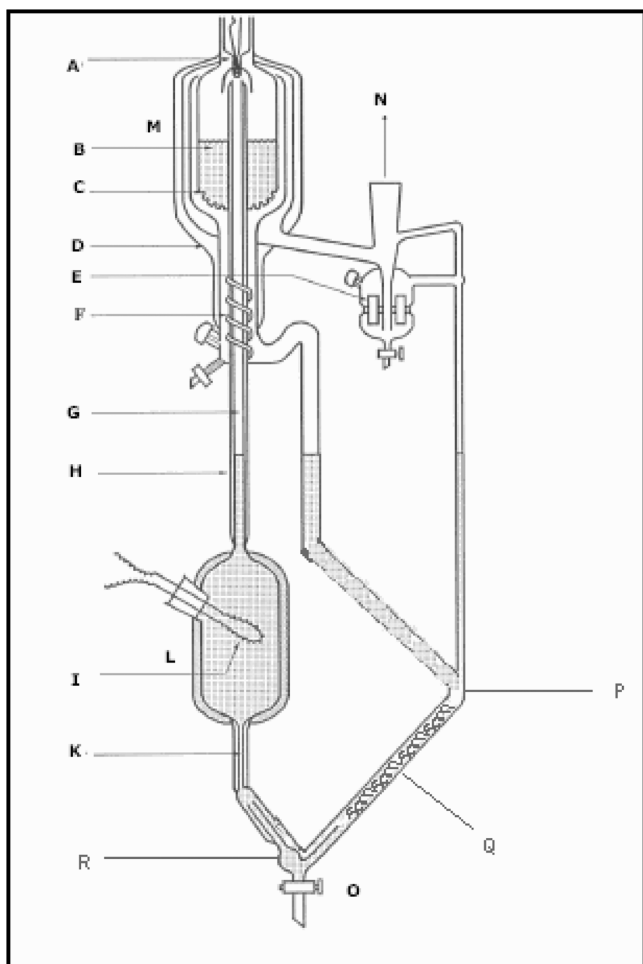


Figure 1. Schematic diagram of the dynamic apparatus. A: temperature sensor; B: stainless steel wire mesh packing; C: equilibrium cell; D: vacuum jacket; E: magnetic stirrer; F: stainless steel spiral; G: Cottrell tube; H: vacuum jacket; I: heating resistance; K: capillary; L: reboiler; M: equilibrium chamber; N: inlet to condenser; O: drain valve; P: mixing tee; Q: glass spiral for mixing; R: mixing chamber.

This improved mixing of the recirculated vapor and liquid phases eliminated the occurrence of flashing which generally occurred when the unmodified apparatus was used for systems of high relative volatility. Systems of high relative volatility are characterized by large concentration differences between the vapor condensate and the liquid return lines. Due to these concentration differences, there are related large differences in the density of the liquid and vapor streams exiting the equilibrium chamber. This large difference in density requires enhanced mixing to create a homogeneous mixture which is returned to the reboiler chamber. Inadequate homogenization of the returning mixture results in flashing and unstable operation of the dynamic still. To enhance the mixing compared to the original design presented in Joseph et al.,² the modified still contains a “mixing tee” into which the liquid and vapor streams are combined. The “mixing tee” has a glass spiral which creates turbulent flow and enhances contact and mixing of the vapor and liquid streams without altering hold-up. To ensure complete homogenization a circular mixing chamber was also added. The stream from the “mixing tee” enters the mixing chamber tangentially which creates a vortex. The principle is similar to that for liquids entering a hydrocyclone. This promotes vigorous agitation and ensures that the mixture entering the reboiler chamber is homogeneous.

A Pt-100 temperature sensor was used to measure the temperature in the equilibrium chamber. The uncertainty in the measured equilibrium temperature is ± 0.1 K. The temperature sensor was calibrated against a Wika CTB 9100 temperature calibration unit. The pressure measurement in the apparatus was via a Wika pressure transducer which had a range from (0 to 101.3) kPa. The pressure transducer was calibrated against a Wika CPH 6000 pressure calibration unit. The calculated maximum uncertainty in the pressure measurement is ± 0.3 kPa.

The equilibrium phase samples were analyzed by gas chromatography using a Shimadzu 2014 GC which was fitted with a thermal conductivity detector. A Zebron ZB-Waxplus capillary GC column which was 30 m in length with a $0.25 \mu\text{m}$ film thickness was used for good separation with helium as the carrier gas. The estimated uncertainty in the composition of the equilibrium phases in terms of mole fraction is ± 0.005 . The estimated uncertainty in the experimental activity coefficients is ± 0.04 . The GC detector was calibrated using the area ratio method outlined by Raal and Mühlbauer.¹¹

Data Reduction. The thermodynamic criteria for VLE result from the equality of the fugacities of the vapor and liquid phases for species in solution. With the vapor phase assumed to be ideal, this reduces to the modified Raoult's law:¹³

$$y_i P = x_i \gamma_i P_i^{\text{sat}} \quad (1)$$

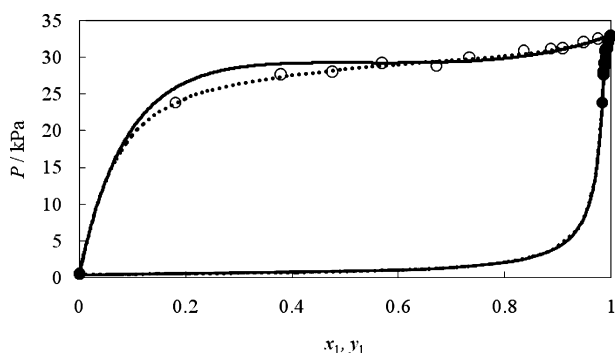
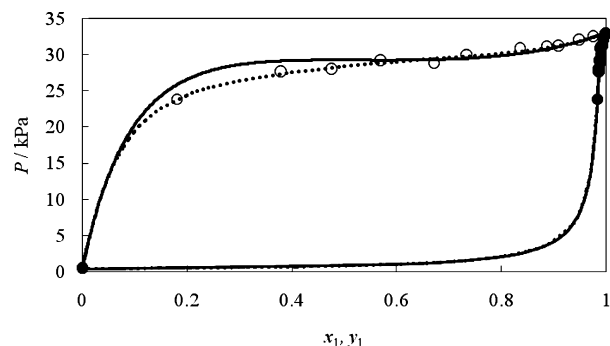
where y is the vapor phase mole fraction, x is the liquid phase mole fraction, γ is the activity coefficient, P^{sat} is the saturation pressure, and i represents species i .

The experimental VLE data were correlated using the NRTL¹⁴ liquid-phase activity coefficient model following the procedure outlined by Smith et al.¹³ The data reduction procedure required the minimization of an objective function. For this study, the minimization of the sum of the squares of the differences between the model and the experimental pressures, as suggested by Van Ness and Abbott,¹⁵ was used as the objective function to correlate the experimental data to

Table 2. Comparison of Literature and Experimental Vapor Pressure Data for Propan-1-ol and Dodecane^a

T/K	1-propanol		dodecane	
	experiment	literature ²⁰	experiment	literature ²⁰
	P/kPa	P/kPa	P/kPa	P/kPa
323.0	12.11	12.08	0.12	0.11
343.4	32.82	33.07	0.46	0.42
353.2	50.82	50.96	0.73	0.73
363.1	76.67	76.63	1.31	1.23
369.2	96.66	97.23	1.76	1.67
rmsd ^b	0.29		0.06	

^a $u(T) = 0.1$ K, $u(P) = 0.3$ kPa. ^bDefined by eq 3.

**Figure 2.** P - x - y diagram for the propan-1-ol (1) + dodecane (2) system at 323.0 K. ●, y_1 , this work; ○, x_1 , this work; ●●, NRTL; —, UNIFAC.**Figure 3.** P - x - y diagram for the propan-1-ol (1) + dodecane (2) system at 343.4 K. ●, y_1 , this work; ○, x_1 , this work; ●●, NRTL; —, UNIFAC.

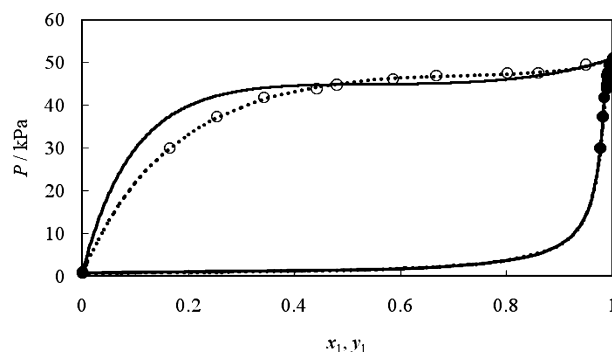
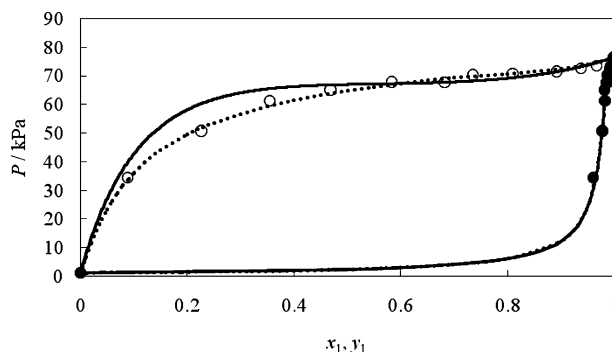
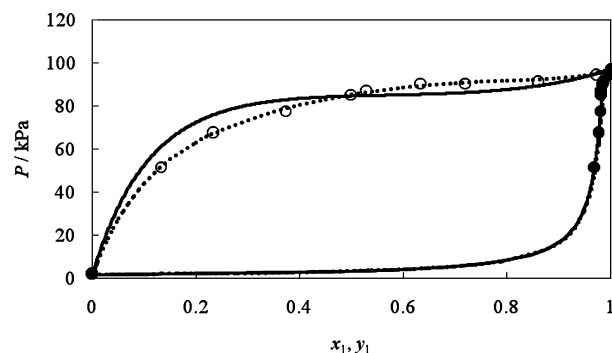
determine model parameters:

$$S = \sum_{k=1}^m (\delta P_k)^2 \quad (2)$$

m is the number of experimental points, and the residual (δP) is the difference between the experimental and the calculated values.

The root-mean-square deviation (rmsd) was calculated to obtain a good measure of the accuracy of the model:

$$\text{rmsd} = \sqrt{\frac{\sum_{k=1}^m (\delta P_k)^2}{m}} \quad (3)$$

**Figure 4.** P - x - y diagram for the propan-1-ol (1) + dodecane (2) system at 353.2 K. ●, y_1 , this work; ○, x_1 , this work; ●●, NRTL; —, UNIFAC.**Figure 5.** P - x - y diagram for the propan-1-ol (1) + dodecane (2) system at 363.1 K. ●, y_1 , this work; ○, x_1 , this work; ●●, NRTL; —, UNIFAC.**Figure 6.** P - x - y diagram for the propan-1-ol (1) + dodecane (2) system at 369.2 K. ●, y_1 , this work; ○, x_1 , this work; ●●, NRTL; —, UNIFAC.

Each isotherm was individually regressed to obtain the NRTL parameters so that the thermodynamic consistency tests could be carried out. However, the experimental data were also regressed simultaneously in a temperature-dependent format to enable phase equilibrium predictions at temperatures that were not measured experimentally. The temperature dependence considered was of the form:

$$\tau_{ij} = a_{ij} + \frac{b_{ij}}{T} \quad (4)$$

where T is in kelvin. For this regression the nonrandomness parameter ($\alpha_{ij} = \alpha_{ji}$) was kept constant at 0.5.

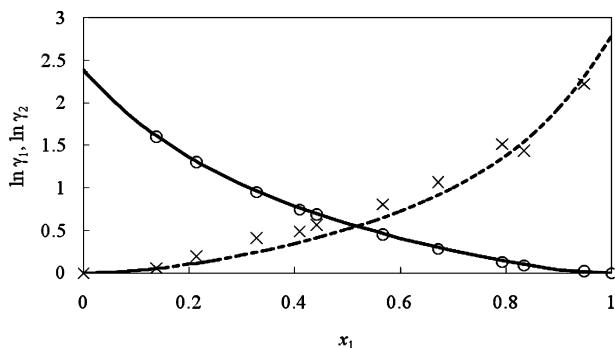


Figure 7. Comparison of the experimental activity coefficients and those calculated from the NRTL model for the propan-1-ol (1) + dodecane (2) system at 323.0 K. O, γ_1 , this work; X, γ_2 , this work; - - -, γ_1 , NRTL; —, γ_2 , NRTL.

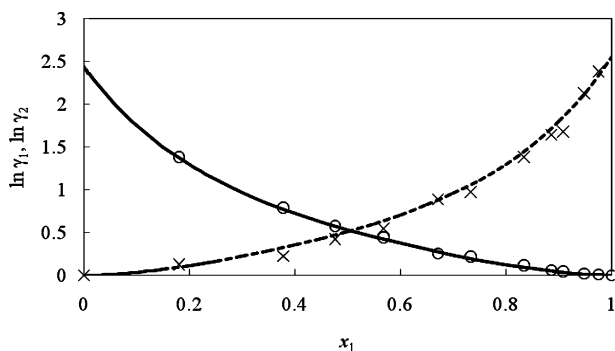


Figure 8. Comparison of the experimental activity coefficients and those calculated from the NRTL model for the propan-1-ol (1) + dodecane (2) system at 343.4 K. O, γ_1 , this work; X, γ_2 , this work; - - -, γ_1 , NRTL; —, γ_2 , NRTL.

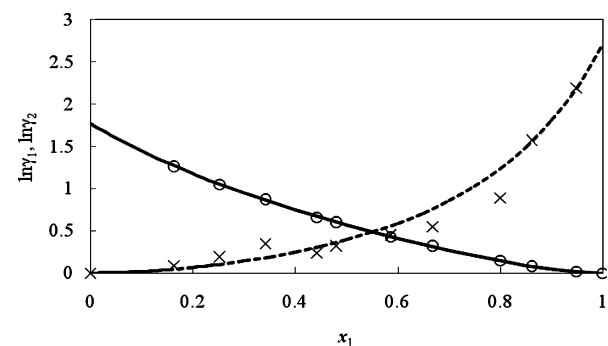


Figure 9. Comparison of the experimental activity coefficients and those calculated from the NRTL model for the propan-1-ol (1) + dodecane (2) system at 353.2 K. O, γ_1 , this work; X, γ_2 , this work; - - -, γ_1 , NRTL; —, γ_2 , NRTL.

The confidence intervals at a 95 % probability were also calculated for the regressed NRTL parameters. To achieve this, the Jacobian was calculated:

$$J_{ij} = \left| \left(\frac{\partial S_i}{\partial \theta_j} \right)_{\theta_p = \theta_{0,p}} \right| \quad (5)$$

m is the number of experimental points, p is the number of regression parameters, $1 \leq i \leq m$, $1 \leq j \leq p$, S_i is the function to be optimized (see eq 2), θ_j represents model parameters, and $\theta_{0,p}$ denotes the optimized model parameters. The covariance

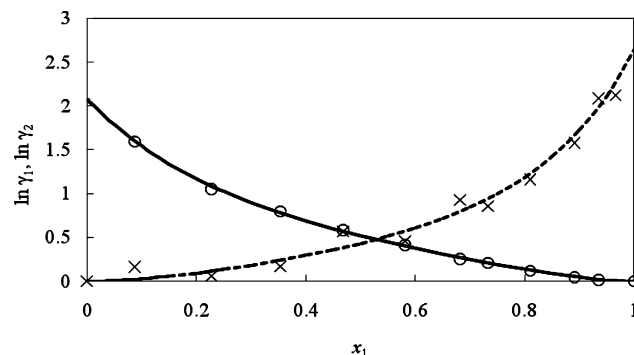


Figure 10. Comparison of the experimental activity coefficients and those calculated from the NRTL model for the propan-1-ol (1) + dodecane (2) system at 363.1 K. O, γ_1 , this work; X, γ_2 , this work; - - -, γ_1 , NRTL; —, γ_2 , NRTL.

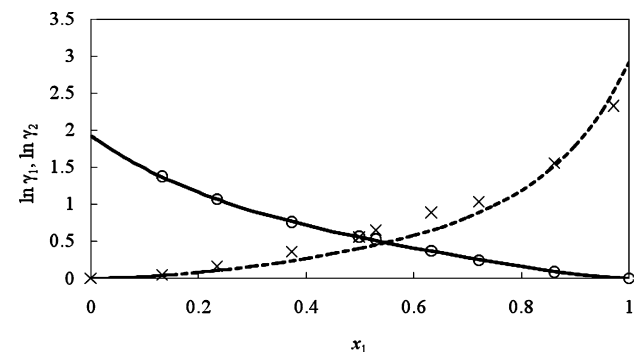


Figure 11. Comparison of the experimental activity coefficients and those calculated from the NRTL model for the propan-1-ol (1) + dodecane (2) system at 369.2 K. O, γ_1 , this work; X, γ_2 , this work; - - -, γ_1 , NRTL; —, γ_2 , NRTL.

matrix was then calculated:

$$C = (J^T J)^{-1} \quad (6)$$

The diagonal elements of the covariance matrix (C_{jj}) were then used to calculate the confidence intervals of the NRTL model parameters:

$$\Delta \theta_j = t_{0.05, \nu} (C_{jj} \sigma_R^2)^{1/2} \quad (7)$$

$$\sigma_R^2 = \frac{S}{m - p} \quad (8)$$

$t_{0.05, \nu}$ is the Student test value for $\nu = m - p$ degrees of freedom and a 95 % probability, and σ_R^2 is the residual variance.

The experimental VLE data were also compared to the UNIFAC¹⁶ model which uses a group-contribution method to predict activity coefficients. The UNIFAC model offers the advantage, provided group contribution parameters are available, of predicting phase equilibrium behavior for many systems that are difficult to measure experimentally. The group-contribution method caters for the combination of small number of subgroups to form large molecules. The UNIFAC model was used in this work to investigate the prediction of VLE behavior for the relatively high volatile system of propan-1-ol and dodecane and compare it to experimental data of this work.

Thermodynamic Consistency Tests. The point test of Van Ness et al.¹⁷ for thermodynamic consistency requires the vapor composition residual (δy) to scatter evenly about the x -axis. Danner

Table 3. Vapor–Liquid Equilibrium Data for the Propan-1-ol (1) + Dodecane (2) System^a

T/K = 323.0					T/K = 343.4				
P/kPa	x_1	y_1	γ_1	γ_2	P/kPa	x_1	y_1	γ_1	γ_2
0.12	0.000	0.000		1.00	0.46	0.000	0.000		1.00
8.42	0.139	0.987	4.93	1.06	23.89	0.181	0.982	3.96	1.13
9.63	0.215	0.988	3.65	1.21	27.65	0.380	0.987	2.19	1.25
10.46	0.329	0.989	2.59	1.49	27.97	0.476	0.987	1.77	1.51
10.60	0.409	0.989	2.12	1.63	29.16	0.570	0.989	1.54	1.71
10.74	0.443	0.989	1.98	1.75	28.85	0.671	0.987	1.29	2.43
10.87	0.569	0.989	1.56	2.25	30.03	0.734	0.989	1.23	2.63
10.92	0.672	0.990	1.33	2.88	30.83	0.835	0.990	1.11	3.95
11.10	0.795	0.990	1.14	4.55	31.25	0.866	0.991	1.07	5.18
11.18	0.835	0.993	1.10	4.19	31.19	0.910	0.993	1.04	5.32
11.73	0.949	0.995	1.02	9.25	32.03	0.949	0.994	1.02	8.35
12.11	1.000	1.000	1.00		32.49	0.975	0.996	1.01	10.73
					32.82	1.000	1.000	1.00	
T/K = 353.2					T/K = 363.1				
P/kPa	x_1	y_1	γ_1	γ_2	P/kPa	x_1	y_1	γ_1	γ_2
0.73	0.000	0.000		1.00	1.31	0.000	0.000		1.00
30.01	0.165	0.978	3.51	1.09	34.65	0.088	0.960	4.92	1.17
37.43	0.253	0.983	2.86	1.20	50.56	0.228	0.979	2.83	1.06
41.92	0.342	0.984	2.37	1.41	61.36	0.354	0.984	2.22	1.18
43.98	0.443	0.988	1.93	1.27	64.98	0.469	0.981	1.77	1.77
44.69	0.481	0.988	1.81	1.37	67.74	0.582	0.987	1.50	1.58
46.14	0.586	0.990	1.53	1.56	67.81	0.683	0.985	1.28	2.53
47.01	0.669	0.991	1.37	1.73	70.19	0.734	0.988	1.23	2.36
47.64	0.801	0.993	1.16	2.43	70.89	0.810	0.989	1.13	3.16
47.65	0.861	0.990	1.08	4.78	71.40	0.891	0.990	1.04	4.79
49.38	0.949	0.993	1.02	8.94	72.76	0.937	0.991	1.00	7.98
50.82	1.000	1.000	1.00		73.65	0.966	0.995	1.00	8.34
					76.67	1.000	1.000	1.00	
T/K = 369.2									
P/kPa	x_1	y_1	γ_1	γ_2					
1.76	0.000	0.000		1.00					
51.72	0.132	0.969	3.93	1.05					
67.40	0.234	0.976	2.91	1.18					
77.69	0.372	0.980	2.11	1.43					
85.30	0.499	0.982	1.74	1.75					
87.28	0.529	0.982	1.68	1.91					
90.44	0.634	0.983	1.45	2.41					
90.46	0.720	0.985	1.28	2.82					
91.08	0.861	0.987	1.08	4.75					
94.32	0.971	0.995	1.00	10.18					
96.66	1.000	1.000	1.00						

^a x_1 and y_1 refer to the mole fraction of propan-1-ol. $u(T) = 0.1$ K, $u(P) = 0.3$ kPa, $u(x_1) = 0.005$, $u(y_1) = 0.005$, $u(\gamma_1) = 0.04$, $u(\gamma_2) = 0.04$.

Table 4. Regressed NRTL Parameters for the Propan-1-ol + Dodecane (2) System

	T/K				
	323.0 ± 0.1	343.4 ± 0.1	353.2 ± 0.1	363.1 ± 0.1	369.2 ± 0.1
τ_{21}	1.573 ± 0.013	1.691 ± 0.016	0.954 ± 0.003	1.396 ± 0.004	1.231 ± 0.003
τ_{12}	2.009 ± 0.012	1.819 ± 0.008	2.088 ± 0.002	1.989 ± 0.004	2.274 ± 0.003
α_{12}	0.450 ± 0.002	0.491 ± 0.002	0.451 ± 0.001	0.544 ± 0.001	0.526 ± 0.001
rmsd	0.07	0.27	0.27	0.94	0.73
δy_1^a	0.001	0.001	0.001	0.002	0.003

^aAverage absolute deviation.

and Gess¹⁸ provided a quantitative criterion for the consistency of VLE data by proposing that the absolute average deviation should be less than 0.01 for the vapor composition residual for the data to

be thermodynamically consistent. Van Ness¹⁹ proposed the direct test (a plot of the residuals $\delta \ln(\gamma_1/\gamma_2)$ versus x_1) and suggested that the extent to which values of this residual fails to scatter about the

Table 5. Regressed Temperature-Dependent NRTL Parameters for the Propan-1-ol + Dodecane (2) System, $\alpha_{ij} = 0.5$

a_{12}	1.164 ± 0.019
a_{21}	-4.253 ± 0.005
b_{12}	276.6 ± 26.3
b_{21}	1991.1 ± 521.8
rmsd	0.07
δy_1^a	0.001

^aAverage absolute deviation.

Table 6. Results of the Van Ness¹⁸ Direct Test for Thermodynamic Consistency for Studied Isotherms of the Propan-1-ol + Dodecane System

T/K	index
323.0 ± 0.1	6
343.4 ± 0.1	4
353.2 ± 0.1	6
363.1 ± 0.1	5
369.2 ± 0.1	6

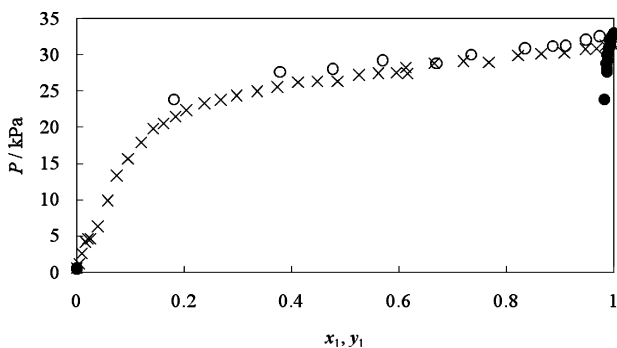


Figure 12. Comparison of the P - x - y diagram for the propan-1-ol (1) + dodecane (2) system for the dynamic apparatus (this work at 343.4 K) and static apparatus (Raal et al.⁹ at 342.8 K). ●, y_1 , this work; ○, x_1 , this work; ×, Raal et al.⁹

zero axis provides a measure of the departure of the data from thermodynamic consistency. Van Ness¹⁹ also developed a quantitative criterion for this test to quantify the degree to which the data departs from consistency by employing an index scale ranging from 1 to 10, where an index of 1 signifies excellent data and 10 very poor data.

RESULTS AND DISCUSSION

The experimental vapor pressures for propan-1-ol and dodecane were measured only at the temperatures for which VLE measurements were undertaken, namely, (323.0, 343.4, 353.2, 363.1, and 369.2) K. Table 2 summarizes the vapor pressure data and compares it to the literature.²⁰ There are some differences between the vapor pressure data measured in this study and that presented in the literature, but the deviations between the data are within the uncertainties of the measurements. The experimental vapor pressures were used in the correlation of VLE data using modified Raoult's law.

The experimental VLE data for the propan-1-ol + dodecane system for isotherms at (323.0, 343.4, 353.2, 363.1, and 369.2) K are presented graphically in Figures 2 to 6, respectively, and listed in Table 3. The experimental activity coefficients and

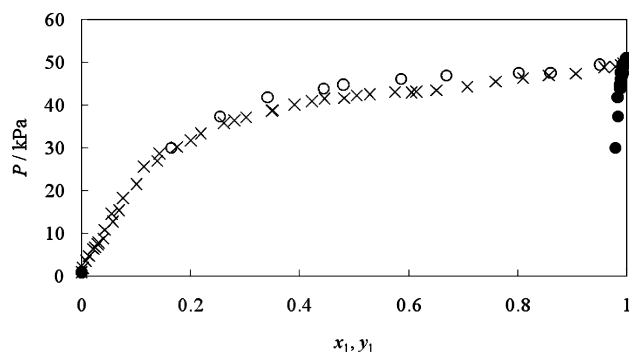


Figure 13. Comparison of the P - x - y diagram for the propan-1-ol (1) + dodecane (2) system for the dynamic apparatus (this work at 353.2 K) and static apparatus (Raal et al.⁹ at 352.7 K). ●, y_1 , this work; ○, x_1 , this work; ×, Raal et al.⁹

those calculated with the NRTL model for isotherms at (323.0, 343.4, 353.2, 363.1, and 369.2) K are presented graphically in Figures 7 to 11, respectively. The regressed NRTL model parameters in temperature-independent forms are reported in Table 4 with their confidence intervals at a 95 % probability. The temperature-dependent form of the NRTL parameters with their confidence intervals at a 95 % probability is reported in Table 5.

The propan-1-ol + dodecane system exhibits a large relative volatility for all isotherms measured, as can be seen by the distance between the P - x and P - y curves in Figures 2 to 6. Due to the large relative volatility that the system exhibits, measurement of experimental VLE data in the propan-1-ol dilute region was extremely difficult even with the modification undertaken to the equipment. The modification did however enable the measurement of data across a reasonable composition range. The experimental data was well-correlated with the modified Raoult's law with the liquid phase nonideality described by the NRTL model. The model could then be used to predict data in the propan-1-ol dilute region. As the system exhibits a large relative volatility across the composition range, separation of dodecane and propan-1-ol can be easily undertaken in a distillation column.

Figures 2 to 6 also show the comparison of the experimental data with the UNIFAC model. Considerable deviation can be seen between the experimental data and the prediction from the UNIFAC model particularly in the propan-1-ol dilute region. Interestingly a region of constant pressure for each isotherm studied can be observed for a mole fraction of propan-1-ol approximately between 0.4 and 0.8. This indicates that a small change in pressure within this region can result in a significant change in composition. Overall it is evident that the NRTL model provides an excellent fit to the experimental data when compared with the prediction of the UNIFAC model.

Figures 7 to 11 show that the NRTL model describes the activity coefficient data well. There is however significant scatter of the experimental data for dodecane. This is not uncommon for systems of high relative volatility as the less volatile component generally displays scatter for the activity coefficient plot.

Thermodynamic consistency testing of the experimental data was undertaken to get an indication of the quality of the data measured. The consistency test is a necessary, but not sufficient, test to determine the quality of experimental data, as it does not conclusively indicate if the measured data are correct. Table 6 indicates that the VLE data satisfy the direct test criteria for thermodynamic consistency. Also, the average absolute value of

Table 7. Comparison of the Regressed NRTL Parameters for the Propan-1-ol + Dodecane (2) System Using Modified Raoult's Law with the NRTL Liquid-Phase Activity Coefficient Model

	$T/K = 343.4 \pm 0.1$	$T/K = 342.8 \pm 0.1$	$T/K = 353.2 \pm 0.1$	$T/K = 352.7 \pm 0.1$
	this work	Raal et al. ⁹	this work	Raal et al. ⁹
τ_{21}	1.691 ± 0.016	0.530 ± 0.086	0.954 ± 0.003	0.583 ± 0.032
τ_{12}	1.819 ± 0.008	1.687 ± 0.130	2.088 ± 0.002	1.638 ± 0.013
α_{12}	0.491 ± 0.002	0.173 ± 0.038	0.451 ± 0.001	0.261 ± 0.014
rmsd	0.27	0.86	0.27	0.87

δy_1 shown in Table 4 is less than 0.01 in mole fraction, which satisfy the consistency criteria suggested by Danner and Gess.¹⁸

The experimental VLE data measured in this work were also compared to data reported by Raal et al.⁹ who used a static apparatus for two isotherms. Comparisons of these data are presented graphically for isotherms at (343.4 and 353.2) K in Figures 12 and 13. The reported data of Raal et al.⁹ were also subjected to VLE regression using modified Raoult's law with the liquid phase nonideality described by the NRTL model. The regression comparison is reported in Table 7 which shows that the NRTL model provides a better fit (lower rmsd) to the experimental data measured in this work (dynamic apparatus).

CONCLUSION

VLE data for the propan-1-ol + dodecane system were measured at (323.0, 343.4, 353.2, 363.1, and 369.2) K using a dynamic-analytical method. The system exhibits a very large relative volatility, and measurements for the system were only possible because of a modification made to an ebulliometer type equilibrium still. The data were correlated using Raoult's law with the NRTL liquid phase activity coefficient model and assuming the vapor phase to be ideal. The NRTL model describes the system well for all studied isotherms. The data satisfied the direct test criteria of Van Ness¹⁹ and point test criteria of Danner and Gess¹⁸ for thermodynamic consistency.

AUTHOR INFORMATION

Corresponding Author

*E-mail: ramjuger@ukzn.ac.za. Tel.: +27 31 260 2969. Fax: +27 31 260 1118.

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Notes

The authors declare no competing financial interest.

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