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# Vapor–liquid equilibria of the binary mixtures 2-butanone + *t*-pentanol, *t*-pentanol + butyl acetate and 2-propanol + diethyl ketone at 101.3 kPa

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## Abstract

Vapor–liquid equilibria have been measured at 101.3 kPa for three binary mixtures of 2-butanone + *t*-pentanol, *t*-pentanol + butyl acetate and 2-propanol + diethyl ketone. The isobaric $T$–$x$–$y$ data have been reported and the thermodynamic consistency has been examined. Calculations of the non-ideality of the vapor phase have been made with the second virial coefficients determined by the Tsonopoulos correlation. Various activity coefficient models have been used to correlate the experimental data. Satisfactory results have been obtained and optimally fitted binary parameters are presented. © 1999 Elsevier Science B.V. All rights reserved.

*Keywords:* Data; Vapor–liquid equilibria; Mixture

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## 1. Introduction

Phase equilibrium data are essential for the design of separation processes. VLE data have been measured in our laboratory for binary and ternary mixtures [1,2]. The VLE data of three binary mixtures of 2-butanone + *t*-pentanol, *t*-pentanol + butyl acetate and 2-propanol + diethyl ketone have been measured at 101.3 kPa in this study. To our knowledge, these data have not been presented in the literature except for the binary mixture of *t*-pentanol + butyl acetate. An all-glass recirculating still was employed and the equilibrium temperatures and compositions of the coexisting vapor and liquid phases were measured. Various thermodynamic consistency tests were examined for these systems. The experimental data were then correlated by various activity coefficient models.

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## 2. Experimental section

### 2.1. Chemicals

All the chemicals were high-purity grade purchased from Merck. All chemicals were used without further purification. No detectable impurities were found in the gas chromatography (GC) analyses. The purities of all chemicals were better than 99.5 mass%. The pure component properties were measured, and comparisons with literature data are shown in Table 1. The refractive indices of the pure components were measured at $(293.15 \pm 0.1)$ K by an Abbe refractometer, Atago 3T, with an accuracy of $\pm 0.0001$. The densities of the pure components were measured at $(293.15 \pm 0.01)$ K using an Anton Paar DMA 60/602 density meter with an accuracy of $\pm 1.0 \times 10^{-5}$ g cm$^{-3}$.

### 2.2. Apparatus and procedures

The apparatus used was an all-glass recirculating still described by Paul [3]. This equipment has a side-heating unit which ensures complete mixing of the liquid mixtures. This design also prevents liquid drop entrainment and partial condensation of the vapor phase. A digital quartz thermometer (DMT-610, Tokyo Electrical, Japan), with an accuracy of $\pm 0.01$ K, was used to measure the equilibrium temperatures. The pressure in the still was measured by a mercury barometer. The pressure oscillates slightly which can be observed with a dibutyl phthalate manometer. The experimental temperatures were taken at this constant pressure of 101.3 kPa. The accuracy of the pressure control was within $\pm 0.05\%$.

In each experiment, the liquid mixture was heated in the recirculating still at a fixed pressure of 101.3 kPa. Equilibrium was usually reached after 1 h, when the temperatures of the liquid and vapor phases were constant and their difference was within $\pm 0.02$ K. Samples of the equilibrium phases were then taken at small volumes and were analyzed in a gas chromatograph.

A Shimadzu GC, type 8A, equipped with a thermal conductivity detector, was used to determine the equilibrium compositions. The GC column was made of a 3 m length stainless steel tube of 3 mm diameter and was packed with Porapak Q. The GC response peaks were integrated using a Shimadzu C-R3A integrator. The temperature of the injection port of the GC was maintained at 503.15 K. The oven temperature of the GC was at 483.15 K. Helium gas with a purity of 99.9% was used and the carrier gas flow rate was 30 cm$^3$/min. The GC was calibrated using mixtures of known compositions

Table 1
Comparison of the measured normal boiling temperatures, refractive indices, and densities of pure fluids in this work with literature data. The numbers in parentheses are the normal boiling temperatures calculated from the Antoine equation

| Component | $T_b$ (K) | | $n_D$ (293.15 K) | | $\rho$ (293.15 K) (g cm$^{-3}$) | | GC purity (mass%) |
|---|---|---|---|---|---|---|---|
| | experimental | literature [14] | experimental | literature [14] | experimental | literature [14] | |
| 2-Butanone | 352.76 | 352.79 (352.73) | 1.3788 | 1.3788 | 0.8053 | 0.8049 | > 99.5 |
| *t*-Pentanol | 375.11 | 375.15 (375.41) | 1.4049 | 1.4049 | 0.8088 | 0.8090 | > 99.7 |
| Butyl acetate | 399.14 | 399.15 (399.04) | 1.3940 | 1.3942 | 0.8821 | 0.8813 | > 99.9 |
| 2-Propanol | 355.39 | 355.41 (355.38) | 1.3773 | 1.3772 | 0.7854 | 0.7855 | > 99.9 |
| Diethyl ketone | 374.80 | 374.85 [13] (375.10) | 1.3924 | 1.3923 | 0.8147 | 0.8143 | > 99.7 |

for each binary system. The relationship between peak area and composition was determined for each binary mixture. In the VLE experiments, more than three analyses were made for each liquid or vapor sample, respectively. With these repeated procedures, the accuracy of the equilibrium composition measurements was within ±0.001 mole fraction.

## 3. Results and discussion

VLE have been measured at 101.3 kPa for 2-butanone + *t*-pentanol, *t*-pentanol + butyl acetate and 2-propanol + diethyl ketone. The results are shown in Tables 2–4, respectively. The liquid phase activity coefficients $\gamma_t$ were calculated by the classical equation:

$$\gamma_i = \left(\hat{\phi}_i y_i P\right) / \left\{ x_i P_i^{\mathrm{sat}} \phi_i^{\mathrm{sat}} \exp\left[ V_i^{\mathrm{L}} \left( P - P_i^{\mathrm{sat}} \right) / RT \right] \right\} \quad (1)$$

where $\phi$ is the fugacity coefficient and $x$ and $y$ are the equilibrium mole fractions in the liquid and vapor phases, respectively. $P^{\mathrm{sat}}$ is the saturated vapor pressure, and $V^{\mathrm{L}}$ is the saturated liquid molar volume.

Table 2
Experimental VLE data for 2-butanone (1) + *t*-pentanol (2) at 101.3 kPa

| $T$ (K) | $x_1$ | $y_1$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|
| 352.76 | 1.0000 | 1.0000 | 1.0000 | |
| 353.66 | 0.9356 | 0.9657 | 1.0014 | 1.2309 |
| 354.37 | 0.8848 | 0.9381 | 1.0060 | 1.2056 |
| 354.92 | 0.8429 | 0.9151 | 1.0124 | 1.1849 |
| 355.09 | 0.8329 | 0.9094 | 1.0128 | 1.1803 |
| 355.98 | 0.7819 | 0.8801 | 1.0157 | 1.1538 |
| 356.49 | 0.7526 | 0.8625 | 1.0179 | 1.1422 |
| 357.04 | 0.7195 | 0.8424 | 1.0223 | 1.1288 |
| 357.72 | 0.6787 | 0.8165 | 1.0285 | 1.1159 |
| 358.22 | 0.6506 | 0.7981 | 1.0330 | 1.1067 |
| 358.76 | 0.6185 | 0.7762 | 1.0395 | 1.0992 |
| 359.53 | 0.5774 | 0.7471 | 1.0468 | 1.0870 |
| 360.11 | 0.5491 | 0.7259 | 1.0509 | 1.0788 |
| 360.92 | 0.5061 | 0.6927 | 1.0618 | 1.0693 |
| 361.63 | 0.4733 | 0.6659 | 1.0685 | 1.0600 |
| 362.31 | 0.4400 | 0.6369 | 1.0772 | 1.0550 |
| 362.89 | 0.4152 | 0.6139 | 1.0815 | 1.0502 |
| 363.80 | 0.3741 | 0.5759 | 1.0960 | 1.0403 |
| 364.35 | 0.3501 | 0.5499 | 1.1323 | 1.0388 |
| 366.55 | 0.2602 | 0.4499 | 1.1359 | 1.0275 |
| 368.38 | 0.1941 | 0.3629 | 1.1651 | 1.0198 |
| 370.23 | 0.1331 | 0.2699 | 1.1986 | 1.0143 |
| 371.37 | 0.1011 | 0.2129 | 1.2054 | 1.0116 |
| 372.08 | 0.0811 | 0.1749 | 1.2103 | 1.0111 |
| 373.30 | 0.0460 | 0.1049 | 1.2368 | 1.0108 |
| 375.11 | 0.0000 | 0.0000 | | 1.0000 |

Table 3
Experimental VLE data for *t*-pentanol (1) + butyl acetate (2) at 101.3 kPa

| $T$ (K) | $x_1$ | $y_1$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|
| 375.11 | 1.0000 | 1.0000 | 1.0000 | |
| 376.25 | 0.9389 | 0.9681 | 1.0004 | 1.0579 |
| 376.51 | 0.9208 | 0.9584 | 1.0006 | 1.0551 |
| 376.71 | 0.9068 | 0.9508 | 1.0011 | 1.0535 |
| 377.11 | 0.8799 | 0.9359 | 1.0013 | 1.0509 |
| 377.51 | 0.8536 | 0.9211 | 1.0018 | 1.0472 |
| 377.72 | 0.8398 | 0.9132 | 1.0021 | 1.0455 |
| 377.98 | 0.8239 | 0.9040 | 1.0023 | 1.0432 |
| 378.55 | 0.7878 | 0.8825 | 1.0032 | 1.0397 |
| 378.96 | 0.7626 | 0.8671 | 1.0040 | 1.0371 |
| 379.24 | 0.7453 | 0.8563 | 1.0049 | 1.0358 |
| 380.01 | 0.6998 | 0.8271 | 1.0067 | 1.0309 |
| 381.14 | 0.6358 | 0.7836 | 1.0103 | 1.0254 |
| 381.92 | 0.5955 | 0.7544 | 1.0114 | 1.0217 |
| 384.08 | 0.4896 | 0.6704 | 1.0172 | 1.0143 |
| 386.45 | 0.3858 | 0.5752 | 1.0247 | 1.0082 |
| 387.37 | 0.3486 | 0.5371 | 1.0280 | 1.0068 |
| 388.31 | 0.3129 | 0.4981 | 1.0304 | 1.0052 |
| 389.32 | 0.2757 | 0.4546 | 1.0333 | 1.0044 |
| 390.71 | 0.2276 | 0.3939 | 1.0379 | 1.0032 |
| 392.06 | 0.1839 | 0.3336 | 1.0428 | 1.0022 |
| 393.36 | 0.1450 | 0.2749 | 1.0469 | 1.0013 |
| 395.26 | 0.0919 | 0.1857 | 1.0525 | 1.0004 |
| 396.31 | 0.0648 | 0.1355 | 1.0551 | 1.0001 |
| 397.35 | 0.0387 | 0.0838 | 1.0587 | 1.0001 |
| 399.14 | 0.0000 | 0.0000 | | 1.0000 |

The fugacity coefficient was calculated using the virial equation of state truncated at the second virial term. The second virial coefficient was determined from the correlation equation according to Tsonopoulos [4]. The critical constants were taken from the literature [5]. At the low pressure condition, the ratio of the fugacity coefficients in Eq. (1) is very close to unity. The vapor pressures of the pure compounds were expressed by the Antoine equation:

$$\log P_i^{\mathrm{sat}}(\mathrm{kPa}) = a_i - b_i / [T(\mathrm{K}) + c_i] \tag{2}$$

The constants $a$, $b$ and $c$ in Eq. (2) were taken from the literature [6]. Values for the various pure fluids are shown in Table 5. The liquid molar volumes were calculated by the Rackett equation [7]. The calculated activity coefficients for each binary mixture are also listed in Tables 2–4. All binary mixtures show positive deviations. The activity coefficients were used in thermodynamic consistency test where the method of Kojima et al. [8] was employed. The method includes both the point test and the integral test and has been used in literature to examine the experimental data. In the Kojima's point test, a parameter $\delta$ is defined as:

$$\delta = 100 \sum_{j=1}^{n} |\delta_j| / n \tag{3}$$

Table 4
Experimental VLE data for 2-propanol (1) + diethyl ketone (2) at 101.3 kPa

| $T$ (K) | $x_1$ | $y_1$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|
| 355.39 | 1.0000 | 1.0000 | 1.0000 | |
| 355.40 | 0.9655 | 0.9735 | 1.0071 | 1.4564 |
| 355.73 | 0.8812 | 0.9114 | 1.0209 | 1.3903 |
| 355.97 | 0.8465 | 0.8865 | 1.0248 | 1.3644 |
| 356.15 | 0.8023 | 0.8560 | 1.0376 | 1.3325 |
| 356.30 | 0.7715 | 0.8355 | 1.0477 | 1.3083 |
| 356.60 | 0.7327 | 0.8125 | 1.0613 | 1.2600 |
| 356.97 | 0.6895 | 0.7842 | 1.0742 | 1.2307 |
| 357.23 | 0.6540 | 0.7620 | 1.0904 | 1.2058 |
| 357.69 | 0.6182 | 0.7370 | 1.0975 | 1.1875 |
| 358.18 | 0.5745 | 0.7090 | 1.1165 | 1.1583 |
| 358.57 | 0.5359 | 0.6865 | 1.1431 | 1.1282 |
| 359.75 | 0.4478 | 0.6252 | 1.1955 | 1.0877 |
| 360.41 | 0.4062 | 0.5921 | 1.2199 | 1.0762 |
| 361.10 | 0.3684 | 0.5633 | 1.2494 | 1.0585 |
| 361.95 | 0.3246 | 0.5275 | 1.2896 | 1.0412 |
| 362.86 | 0.2845 | 0.4892 | 1.3229 | 1.0313 |
| 364.41 | 0.2254 | 0.4255 | 1.3787 | 1.0193 |
| 366.05 | 0.1749 | 0.3604 | 1.4255 | 1.0117 |
| 367.83 | 0.1304 | 0.2896 | 1.4501 | 1.0093 |
| 368.67 | 0.1075 | 0.2526 | 1.4940 | 1.0086 |
| 370.08 | 0.0784 | 0.1960 | 1.5203 | 1.0073 |
| 371.68 | 0.0482 | 0.1310 | 1.5728 | 1.0059 |
| 373.47 | 0.0199 | 0.0584 | 1.6082 | 1.0054 |
| 374.80 | 0.0000 | 0.0000 | | 1.0000 |

the summation is over all the data points where:

$$\delta_j = \partial(\Delta G_m/RT)/\partial x_1 - \ln(\gamma_1/\gamma_2) - \varepsilon \tag{4}$$

The free energy change on mixing $\Delta G_m$ is calculated by the summation of the activity for each component in a mixture. The $\epsilon$ term is related to the heat of mixing in a constant pressure experiment. An estimated value about 0.03 was used for $\epsilon$ in this study which is in the range

Table 5
Pure component properties used in this work. The critical constants and acentric factors were taken from Ref. [5]. The parameters in the vapor pressure equation ($\log P_i^{sat}$ (kPa) $= a_i - b_i/[T$ (K) $+ c_i]$) were taken from Ref. [6]

| Component | $T_c$ (K) | $P_c$ (kPa) | $\omega$ | $a$ | $b$ | $C$ |
|---|---|---|---|---|---|---|
| 2-Butanone | 535.50 | 4154 | 0.324 | 6.22518 | 1286.794 | −47.766 |
| *t*-Pentanol | 545.15 | 3880 | 0.483 | 6.07488 | 1075.367 | −111.143 |
| Butyl acetate | 579.15 | 3110 | 0.410 | 6.13505 | 1355.816 | −70.705 |
| 2-Propanol | 508.31 | 4764 | 0.669 | 6.61939 | 1225.439 | −89.774 |
| Diethyl ketone | 560.95 | 3739 | 0.350 | 6.14917 | 1309.653 | −59.032 |

Table 6
Consistency test results of the binary VLE experimental data

| Method of test | Criterion of consistency | 2-butanone (1)+ *t*-pentanol (2) | *t*-pentanol (1)+ butyl acetate (2) | 2-propanol (1)+ diethyl ketone (2) |
|---|---|---|---|---|
| *Kojima method* | | | | |
| (a) point test | $\delta < 5$ | 3.49 (+) | 3.10 (+) | 2.30 (+) |
| (b) area test | $A < 3$ | 2.49 (+) | 3.00 (+) | 2.21 (+) |
| (c) infinite dilution test | $I_1 < 30$ | 26.68 (+) | 4.47 (+) | 8.60 (+) |
| | $I_2 < 30$ | 13.39 (+) | 7.02 (+) | 4.28 (+) |

suggested by Kojima et al. [8]. According to Kojima et al. [8], $\delta$ should be less than 5 for thermodynamically consistent data. For the Kojima's area test, a parameter $A$ is defined as:

$$A = 100\left[\int_0^1 \ln(\gamma_1/\gamma_2)\mathrm{d}x_1 + \int_0^1 (\varepsilon)\mathrm{d}x_1\right] \tag{5}$$

The criterion for the area test is that $A$ must be less than 3. Kojima et al. [8] also proposed the infinite dilution test. In this test, the following terms were calculated at the infinite dilution conditions:

$$I_1 = 100\left|\left[\left(\frac{G^{\mathrm{E}}}{x_1x_2RT}\right)_{x_1=0} - \left(\ln\frac{\gamma_1}{\gamma_2}\right)_{x_1=0}\right]\bigg/\left(\ln\frac{\gamma_1}{\gamma_2}\right)_{x_1=0}\right| \tag{6}$$

$$I_2 = 100\left|\left[\left(\frac{G^{\mathrm{E}}}{x_1x_2RT}\right)_{x_2=0} - \left(\ln\frac{\gamma_2}{\gamma_1}\right)_{x_2=0}\right]\bigg/\left(\ln\frac{\gamma_2}{\gamma_1}\right)_{x_2=0}\right| \tag{7}$$

In order to satisfy the thermodynamic consistency, both $I_1$ and $I_2$ values should be less than 30. Van Ness [9] also suggested a thermodynamic consistency test method. The activity coefficients deter-

Table 7
Correlation parameters and absolute average deviations in boiling temperature ($\Delta T$) and vapor-phase mole fraction ($\Delta y$) for the binary mixtures

| Equations | $A_{12}$ (cal mol$^{-1}$) | $A_{21}$ (cal mol$^{-1}$) | $\alpha_{12}$ | $\Delta y_1$ | $\Delta T$ (K) |
|---|---|---|---|---|---|
| *2-butanone (1) + t-pentanol (2)* | | | | | |
| Wilson | −137.440 | 352.947 | | 0.0028 | 0.117 |
| NRTL | 222.665 | −44.436 | 0.2 | 0.0013 | 0.104 |
| UNIQUAC | −188.429 | 283.989 | | 0.0012 | 0.119 |
| *t-pentanol (1) + butyl acetate (2)* | | | | | |
| Wilson | −10.583 | 109.502 | | 0.0006 | 0.033 |
| NRTL | −67.893 | 118.509 | 0.2 | 0.0002 | 0.010 |
| UNIQUAC | −113.801 | 125.695 | | 0.0001 | 0.012 |
| *2-propanol (1) + diethyl ketone (2)* | | | | | |
| Wilson | 88.586 | 257.430 | | 0.0024 | 0.079 |
| NRTL | 310.121 | 98.437 | 0.2 | 0.0055 | 0.188 |
| UNIQUAC | 53.611 | 26.937 | | 0.0028 | 0.092 |

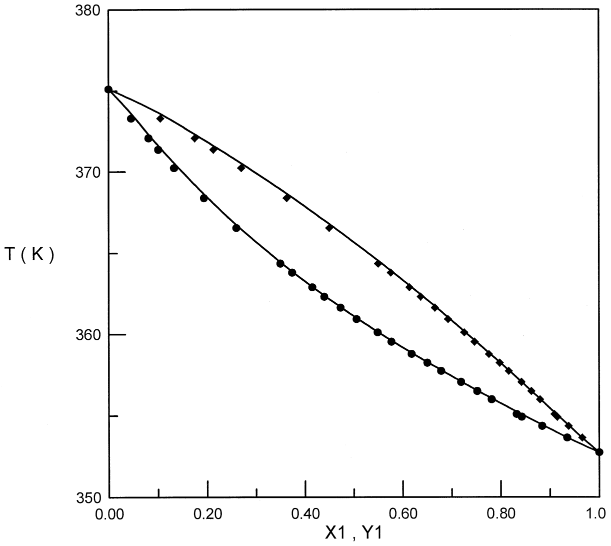

Fig. 1. $T-x-y$ Curve for 2-Butanone (1) + *t*-Pentanol (2) at 101.3 kPa. (—) NRTL Model. Experimental Data: (●) Liquid Phase; (♦) Vapor Phase.

mined from the experiment were fitted by an excess Gibbs free energy function. At each experimental point, the residual between the calculated and experimental activity coefficient ratios was evaluated. The root mean square (RMS) deviations for the residual values were then determined. According to Van Ness [9], the RMS value should be as small as possible. The thermodynamic consistency test results using the Kojima's method are shown in Table 6. It is demonstrated that all three binary

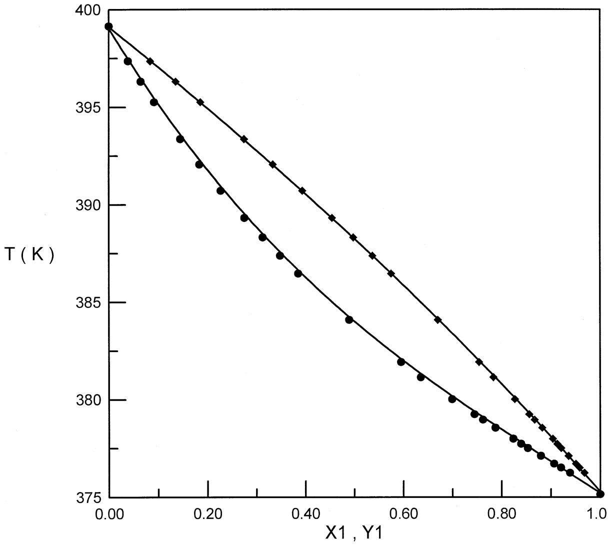

Fig. 2. $T-x-y$ Curve for *t*-Pentanol (1) + Butyl Acetate (2) at 101.3 kPa. (—) NRTL Model. Experimental Data: (●) Liquid Phase; (♦) Vapor Phase.

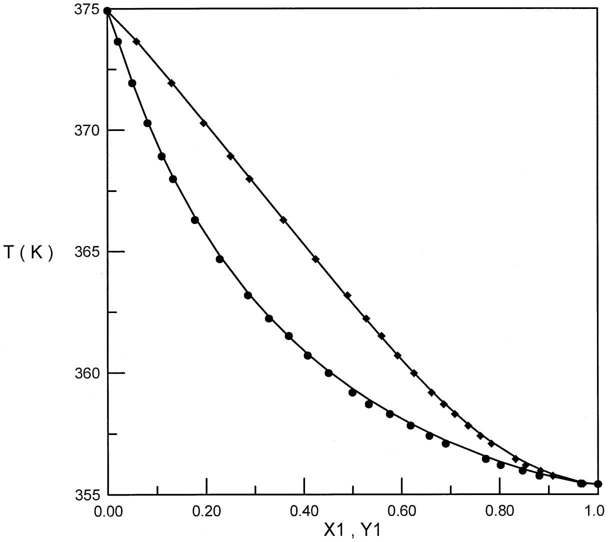

Fig. 3. $T-x-y$ Curve for 2-Propanol (1) + Diethyl Ketone (2) at 101.3 kPa. (—) NRTL Model. Experimental Data: (●) Liquid Phase; (◆) Vapor Phase.

systems satisfy the requirements for the various consistency test methods. We also have examined the consistency test using the method of Van Ness with the NRTL model. The RMS errors for all three systems range from 0.01 to 0.05. These results also indicate that the experimental data are satisfactory.

The experimental results were then used to obtain the binary parameters in various activity coefficient models. The Wilson [10], NRTL [11] and UNIQUAC [12] models were used in the regressions. The expressions for the activity coefficients for each model are listed in the literature [13]. The following objective function was minimized in the regressions:

$$Q = \sum_{N} \sum_{i} \left( \frac{\gamma_i^{\mathrm{exp}} - \gamma_i^{\mathrm{cal}}}{\gamma_i^{\mathrm{exp}}} \right)^2 \tag{8}$$

The regression results are shown in Table 7. The deviations in vapor phase compositions and equilibrium temperatures are reasonably small, and it is indicated that all three activity coefficient models are suitable to represent the binary experimental data. The $T$–$x$–$y$ diagrams of these binary systems are shown in Figs. 1–3, respectively. No azeotrope was found for these binary systems. To our knowledge, no isobaric VLE data at 101.3 kPa has been given in the literature for binary mixtures of 2-butanone + *t*-pentanol and 2-propanol + diethyl ketone. VLE data at 101.3 kPa for the binary mixture of *t*-pentanol + butyl acetate have been presented by Gmehling et al. [13]. Only six data points were given with appreciable deviations from correlation. Our experimental data show better thermodynamic consistency as well as correlation results using various activity coefficient models.

## 4. Conclusion

Vapor–liquid equilibria of three binary mixtures of 2-butanone + *t*-pentanol, *t*-pentanol + butyl acetate and 2-propanol + diethyl ketone were measured at 101.3 kPa. The results of all binary mixtures satisfy the requirements for various thermodynamic consistency tests. Three activity coefficient models have been employed to correlate the experimental data. The correlation results are satisfactory and the deviations in vapor phase compositions and equilibrium temperatures are reasonably small.

## 5. List of symbols

| | |
|---|---|
| $A$ | parameter in the Kojima's area test |
| $a, b, c$ | parameters in the vapor pressure equation |
| $G$ | Gibbs free energy |
| $I$ | parameter in the Kojima's infinite dilution test |
| $n$ | number of data points |
| $P$ | pressure |
| $Q$ | objective function |
| $R$ | gas constant |
| $T$ | temperature |
| $V$ | volume |
| $x, y$ | mole fractions |
| *Greek letters* | |
| $\delta$ | parameter in the Kojima's point test |
| $\gamma$ | activity coefficient |
| $\phi$ | fugacity coefficient |
| *Subscripts* | |
| $i$ | component $i$ |
| m | mixture property |
| *Superscripts* | |
| cal | calculated data |
| E | excess property |
| exp | experimental data |
| L | liquid phase |
| sat | saturated property |
| V | vapor phase |

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## References

[1] C.C. Chen, M. Tang, Y.P. Chen, Vapor–liquid equilibria of binary and ternary mixtures of cyclohexane, 3-methyl-2-butanone and octane at 101.3 kPa, J. Chem. Eng. Data 41 (1996) 557–561.

[2] K.W. Cheng, C.Y. Chen, M. Tang, Y.P. Chen, Vapor–liquid equilibria of binary mixtures cyclopentane + isopropyl acetate, isopropyl acetate + hexane and cyclopentane + methyl methacrylate at 101.3 kPa, J. Chem. Eng. Data 42 (1997) 754–757.
[3] R.N. Paul, Study of vapor–liquid equilibrium in improved equilibrium still, J. Chem. Eng. Data 21 (1976) 165–169.
[4] C. Tsonopoulos, An empirical correlation of second virial coefficients, AIChE J. 20 (1974) 263–272.
[5] T.E. Daubert, R.P. Danner, Physical and thermodynamic properties of pure chemicals. Data Compilation, Hemisphere Publishing, NY, 1989.
[6] M.S. Richard, M. Stanislaw, Handbook of the Thermodynamics of Organic Compounds, Elsevier, Amsterdam, 1987.
[7] C.F. Spencer, R.P. Danner, Improved equation for prediction of saturated liquid density, J. Chem. Eng. Data 17 (1972) 236–241.
[8] K. Kojima, H.M. Moon, K. Ochi, Thermodynamic consistency test of vapor–liquid equilibrium data. Methanol–water, benzene-cyclohexane and ethyl methyl ketone–water, Fluid Phase Equilibria 56 (1990) 269–284.
[9] H.C. Van Ness, Thermodynamics in the treatment of vapor/liquid equilibrium (VLE) data, Pure and Applied Chemistry 67 (1995) 859–872.
[10] G.M. Wilson, Vapor–liquid equilibrium: XI. A new expression for the excess free energy of mixing, J. Am. Chem. Soc. 86 (1964) 127–130.
[11] H. Renon, J.M. Prausnitz, Local compositions in thermodynamic excess functions for liquid mixtures, AIChE J. 14 (1968) 135–144.
[12] D.S. Abrams, J.M. Prausnitz, Statistical thermodynamics of liquid mixtures: a new expression for the excess Gibbs free energy of partly or completely miscible systems, AIChE J. 21 (1975) 116–128.
[13] J. Gmehling, U. Onken, W. Arlt, P. Grenzheuzer, U. Weidlich, B. Kolbe, J. Rarey-Nies, Vapor–liquid equilibrium data collection, Chemistry Data Series, Vol. 1, DECHEMA, Frankurt, Germany, 1979.
[14] TRC Data Base for Chemistry and Engineering. Thermodynamic Research Center, Texas A&M University, College Station, TX, 1993.