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# Computation of Isobaric Vapor-Liquid Equilibrium (VLE) Data of Methyl Tert-Butyl Ether (MTBE) + Acetic Acid (AA) System

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The chemical and biological pathways for acetic acid production involve the separation of acetic acid from water. Azeotropic distillation and liquid-liquid extraction are used to separate acetic acid from water with conventional solvents, as simple distillation is impractical due to the pinch point near the water edge and requires more energy to separate these two components. Methyl tert-butyl ether (MTBE) is a more viable solvent due to its low energy consumption during recovery. To compute isobaric vapor-liquid equilibrium (VLE) data for a binary mixture of methyl tert-butyl ether (MTBE) + acetic acid (AA) system, the group contribution method, UNIFAC was used. The thermodynamic consistency tests such as Redlich and Kister's and Wisniak's L-W were used to check the validity of these data. Wilson, UNIQUAC, and NRTL excess Gibbs energy models were used to determine the binary interaction parameters of these models. VLE data obtained in this work can be used to design the distillation and extraction system to recover and purify MTBE.

**Keywords:** Isobaric VLE data, MTBE, UNIFAC, Thermodynamic consistency tests, Acetic acid separation, Excess Gibbs energy models

## INTRODUCTION

Vinyl acetate, acetic anhydride, and ester production require acetic acid (AA) as a chemical reagent. Acetic acid is used in the manufacture of purified terephthalic acid from which fibers are made in the textile industry, a commodity used as vinegar in the food industry, as an antibacterial agent in the pharmaceutical industry, and in metal acetate preparation in the printing industry [1]. Acetic acid is produced in various ways through biological and chemical processes. The main pathways for the commercial production of acetic acid are methanol carbonylation, acetaldehyde oxidation, ethanol fermentation, and butane and/or naphtha fraction oxidation [2]. Certainly, the methanol carbonylation route is a highly productive and commercially preferred route for the synthesis of acetic acid. In all these processes, the separation of acetic acid from a dilute aqueous solution of acetic acid is required [3]. The dilute aqueous solution typically contains 10-40% acetic acid by weight, which can be economically recovered and recycled by azeotropic distillation, liquid-liquid extraction, or membrane separation processes [4]. When acetic acid is diluted with water, it cannot readily be separated from water. Though acetic acid and water do not form azeotropic mixtures, a pinch point appears on the pure water side of the equilibrium diagram. Hence distillation alone is not sufficient for separating pure acetic acid from a solution of aqueous acetic acid [5-6]. The extraction of diluted acetic acid from water has been studied extensively. Alcohols, acetates, ketones, ethers, and aromatic hydrocarbons have been used as solvents to recover acetic acid. Kurumet *et al.* evaluated more than 34 solvents for acetic acid separation and identified MTBE as the most promising solvent for liquid-liquid extraction based on its selectivity, distribution coefficient, recoverability, density, chemical reactivity, viscosity, freezing point, and vapor pressure [7].

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So far, isobaric vapor-liquid equilibrium (VLE) data for acetic acid (AA) + *p*-xylene [8], acetic acid (AA) + isopropyl acetate [9], acetic acid (AA) + isopropyl alcohol (IPA) [9], acetic acid (AA) + methyl ethyl ketone (MEK) [10], acetic acid (AA) + water [10], acetic acid (AA) + cyclopentyl methyl ether (CPME), acetic acid (AA) + 2-methyltetrahydrofuran (2-MeTHF) [11] and acetic acid (AA) + tetrahydrofuran (THF) [12] are available in the literature. For the separation of MTBE + AA, there is no published VLE data, so it must be determined prior to designing the column. VLE data are crucial to the design of distillation columns.

A modified ebulliometer [13] can be used to determine vapor-liquid equilibrium (VLE) data, but it requires a large quantity of chemicals, sophisticated VLE instrumentation, and analytical instruments. An alternative to experimentally determined VLE data is group contribution methods to predict VLE data, which can be used for preliminary column design [14].

In this article, the UNIQUAC Functional-group Activity Coefficients (UNIFAC) method was used to predict isobaric VLE data for the MTBE + AA binary system. The consistency of predicted VLE data was evaluated by the R-K consistency test and Wisniak's L-W test. Moreover, regression analysis was used to calculate a binary interaction parameter for Van Laar, Wilson, NRTL, and UNIQUAC models.

## MATERIALS AND METHODOLOGY

### VLE Data Prediction Using Group Contribution Methods and Area Test for Thermodynamic Consistency

The group contribution methods are the most reliable for predicting VLE data. The UNIFAC method [15] was used to predict isobaric VLE data for the binary system of MTBE + AA. After appropriate group identification for both compounds, liquid phase non-ideality by means of activity coefficients was estimated for the entire concentration range and *T*-*x*-*y* data were computed. The method described below was followed to obtain VLE at atmospheric pressure for the proposed binary system of MTBE + AA:

The UNIFAC method predicts the activity coefficient at a given temperature ($T$) and composition ($x_1$). This calculation procedure is divided into two parts: combinatorial and residual.

The combinatorial part includes Van der Waals area parameters (Q) and volume parameters (R) which incorporate the size and shape of molecules present, while the residual part includes interaction among groups as shown in Eqs. (2)-(3).

$$\ln\gamma_i = \ln\gamma_{i(com)} + \ln\gamma_{i(res)} \tag{1}$$

$$ln\,\gamma_{i(com)} = ln\frac{\phi_i}{x_i} + \frac{z}{2}q_i\,ln\frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i}\sum_j x_j l_j \tag{2}$$

$$\ln\gamma_{i(res)} = \sum_k v_k^{(i)}\left(\ln\Gamma_k - \ln\Gamma_k^{(i)}\right) \tag{3}$$

Group identification was carried out based on literature analysis and molecular structure of the components involved as shown in Table 1.

After the identification of groups, binary interaction parameters (BIP) for group contribution were reported (Table 2).

Initially, $T$ and $x_1$ were taken inputs, and the $\gamma_1$ and $\gamma_2$ were calculated using group contribution methods. The total pressure is calculated as per Eq. (4) and vapor phase composition is calculated from modified Raoult's Law

**Table 1.** Identified Groups of MTBE and AA for the UNIFAC Method ($V_j^{(i)}$, $R_j$, and $Q_j$ Values from Poling *et al.* [18])

| Compound (i) | Group name | Main group | Secondary group (j) | $V_j^{(i)}$ | $R_j$ | $Q_j$ |
|---|---|---|---|---|---|---|
| MTBE | $CH_3O$ | 13 | 24 | 1 | 1.145 | 1.088 |
| | $CH_3$ | 1 | 1 | 3 | 0.9011 | 0.848 |
| | C | 1 | 4 | 1 | 0.2195 | 0.000 |
| AA | $CH_3$ | 1 | 1 | 1 | 0.9011 | 0.848 |
| | COOH | 20 | 42 | 1 | 1.3013 | 1.224 |

Note: $V_j^{(i)}$ is an integer that represents number of groups of type j present in molecule i, $R_j$, and $Q_j$ are volume and area parameters.

(Eq. (5)) used with an assumption of ideality in the vapor phase. Vapor pressure was calculated using Antoine constants represented in Table 3.

$$P = \sum_i x_i \gamma_i P_i^{sat} \tag{4}$$

$$x_i \gamma_i P_i^{sat} = y_i P \tag{5}$$

Here, the initial values of temperature are not the actual boiling points of the mixture. Therefore, pressure calculated from Eq. (4) shows a deviation from the actual value of 101.325 kPa. Temperature was then regressed to minimize average absolute deviation (AAD) in pressure. For this minimization function was Eq. (6) and the variable was temperature.

$$AAD\ (P) = \frac{1}{n}\sum_i^n \left| P_i^{act} - P_i^{cal} \right| \tag{6}$$

The predicted VLE data are reported in Table 4.

**Table 2.** Binary Interaction Parameters of $a_{nm}$ for MTBE and AA from Poling *et al.* [18]

| Group | $CH_3$ | C | $CH_3O$ | COOH |
|---|---|---|---|---|
| $CH_3$ | 0.00 | 0.00 | 251.50 | 663.50 |
| C | 0.00 | 0.00 | 251.50 | 663.50 |
| $CH_3O$ | 83.36 | 83.36 | 0.00 | 664.60 |
| COOH | 315.30 | 315.30 | -338.50 | 0.00 |

**Table 3.** Antoine Constants for MTBE and AA

| Component | A | B | C | Temperature range (K) | Ref. |
|---|---|---|---|---|---|
| MTBE$^a$ | 6.0703 | -1158.91 | -43.2 | 300.96-411.23 | [19] |
| AA$^b$ | 4.6821 | 1642.54 | -39.8 | 290.26-391.01 | [20] |

$^a\log_{10}(P/kPa) = A + \frac{B}{(T/K)+C}$, $^b\log_{10}(P/bar) = A - \frac{B}{(T/K)+C}$

The excess Gibbs energy vs. composition plot is represented in Fig. 1.

**Table 4.** Predicted VLE Data for MTBE (1) + AA (2) Binary System at 101.325 kPa Using the UNIFAC Method

| T (K) | $x_1$ | $y_1$ | $\gamma_1$ | $\gamma_2$ |
|---|---|---|---|---|
| 391.01 | 0.0000 | 0.0000 | 1.9062 | 1.0000 |
| 378.64 | 0.0500 | 0.3575 | 1.7565 | 1.0020 |
| 370.10 | 0.1000 | 0.5413 | 1.6365 | 1.0074 |
| 363.80 | 0.1500 | 0.6504 | 1.5390 | 1.0158 |
| 358.89 | 0.2000 | 0.7220 | 1.4585 | 1.0268 |
| 354.91 | 0.2500 | 0.7727 | 1.3912 | 1.0403 |
| 351.58 | 0.3000 | 0.8106 | 1.3340 | 1.0562 |
| 348.72 | 0.3500 | 0.8400 | 1.2849 | 1.0745 |
| 346.22 | 0.4000 | 0.8637 | 1.2423 | 1.0956 |
| 344.01 | 0.4500 | 0.8833 | 1.2049 | 1.1196 |
| 342.02 | 0.5000 | 0.8998 | 1.1718 | 1.1471 |
| 340.22 | 0.5500 | 0.9141 | 1.1424 | 1.1788 |
| 338.57 | 0.6000 | 0.9265 | 1.1161 | 1.2155 |
| 337.05 | 0.6500 | 0.9376 | 1.0924 | 1.2586 |
| 335.64 | 0.7000 | 0.9476 | 1.0712 | 1.3098 |
| 334.31 | 0.7500 | 0.9568 | 1.0523 | 1.3717 |
| 333.06 | 0.8000 | 0.9655 | 1.0358 | 1.4477 |
| 331.85 | 0.8500 | 0.9738 | 1.0217 | 1.5434 |
| 330.68 | 0.9000 | 0.9821 | 1.0105 | 1.6668 |
| 329.52 | 0.9500 | 0.9907 | 1.0029 | 1.8308 |
| 328.32 | 1.0000 | 1.0000 | 1.0000 | 2.0574 |

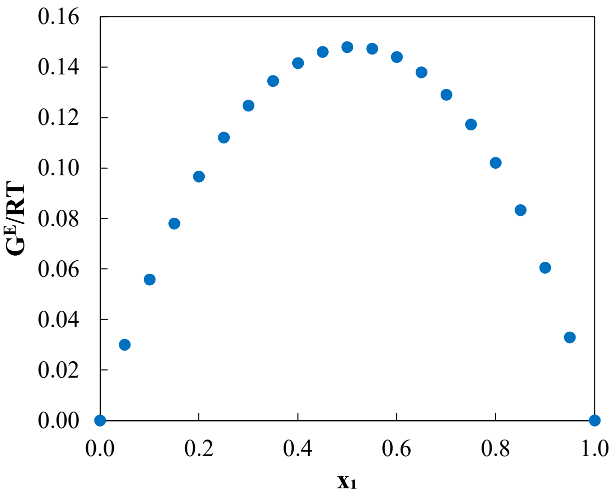

**Fig. 1.** ($G^E/RT$) *vs.* $x_1$ diagram for predicted VLE data by UNIFAC method.

### Thermodynamic Consistency Test

VLE data are thermodynamically consistent if D is less than 10 in the R-K consistency test (Eq. (7)-(8)). The general idea is that if the total area of $\ln \gamma_1/\gamma_2$ *vs.* $x_1$ is zero, then the data passes the test [18]. But a more appropriate way is to calculate the positive area ($A^+$) and negative area ($A^-$) separately and to check the following criteria for consistency check.

$$\int_{x_1=0}^{x_1=1} \ln\left(\frac{\gamma_1}{\gamma_2}\right) dx_1 = -\int_{P(x_1=0)}^{P(x_1=1)} \frac{V^E}{RT} dP + \int_{x_1=0}^{x_1=1} \frac{h^E}{RT^2} dT \quad (7)$$

$$D = 100 \frac{\left|\int_0^1 \ln\frac{\gamma_1}{\gamma_2} dx_1\right|}{\int_0^1 \left|\ln\frac{\gamma_1}{\gamma_2}\right| dx_1} = 100 \frac{\left||A^+| - |A^-|\right|}{|A^+| + |A^-|} \leq 10 \quad (8)$$

According to another consistency test of Wisniak (L-W test) if D is not larger than 3, then the predicted VLE data are thermodynamically consistent [16]. The following equations (Eq. (9)-(11)) were used for the test:

$$L_i = \frac{\sum x_i \Delta s_i^0 \Delta T_i^0}{\sum x_i \Delta s_i^0} - T \quad (9)$$

$$W_i = \frac{g^E}{\sum x_i \Delta s_i^0} - \frac{RT}{\sum x_i \Delta s_i^0} \sum x_i \ln(y_i/x_i) \quad (10)$$

$$\mathrm{D} = 100 \frac{|L-W|}{|L+W|} < 3 \quad (11)$$

The summary of the results of these consistency tests is provided in Table 5.

### Data Reduction Using Excess Gibbs Free Energy Models

Van Laar, Wilson, NRTL, and UNIQUAC models [17-18] were the Excess Gibbs free energy models used to correlate the predicted VLE data. Initially, activity coefficients predicted by the UNIFAC method were fitted to that calculated by Gibbs free energy models by optimizing the BIPs of models. Here the minimization function was as shown in Eq. (12). Then temperature was regressed to minimize pressure deviation with Eq. (6) as the objective function. Correspondingly, average absolute deviation in temperature, AAD (T), and vapor phase composition, AAD (y), were obtained using Eqs. (13)-(14).

**Table 5.** Consistency Test Results for UNIFAC Predicted VLE Data for the Binary System of MTBE (1) + AA (2)

| Test | Criteria | D | Result |
|---|---|---|---|
| Redlich-Kister Area Test | D < 10 | 2.03 | Pass |
| L-W Wisniak Test | D < 3 | 0.00 | Pass |

$$AAD\ (\gamma) = \frac{1}{n}\sum_i^n \left|\gamma_i^{pred} - \gamma_i^{model}\right| \quad (12)$$

$$AAD\ (T) = \frac{1}{n}\sum_i^n \left|T_i^{pred} - T_i^{model}\right| \quad (13)$$

$$AAD\ (y) = \frac{1}{n}\sum_i^n \left|y_i^{pred} - y_i^{model}\right| \quad (14)$$

## RESULT AND DISCUSSION

### Comparison of Model Performance

The plot of activity coefficients predicted by UNIFAC and correlated by Van Laar model is shown in Fig. 2 indicating fairly good fitting except dilution region on both ends. T-x-y and x-y plots for Van Laar, Wilson, NRTL, and UNIQUAC are shown in Figs. 3, 5, 7, 9 and 4, 6, 8, 10 respectively. T-x-y plot indicated easy separation as bubble points and due points are far from each other. The same phenomena are observed in the x-y plot as the equilibrium line is away from x=y lines. As the distance between the x-y equilibrium line and the x=y line increases, the required number of stages for the distillation column will decrease. Models perform differently when it comes to their ability to fit liquid phase non-ideality *i.e.*, activity coefficients. Here, it is very difficult to report the performance of the model in terms of fitting UNIFAC-predicted data just from T-x-y and x-y plots. Therefore deviations as AADs have been reported. The order of higher degree of fitting to lower is in the following sequence: Vaan Laar > UNIQUAC > Wilson > NRTL. The binary interaction parameters obtained from these excess Gibbs energy-based models are reported in Table 6 along with deviations in pressure, temperature, and vapor phase composition. These deviations clearly indicate that each of these models can correlate the data with close proximity. Both thermodynamic consistency tests suggested that the VLE data are consistent and reliable.

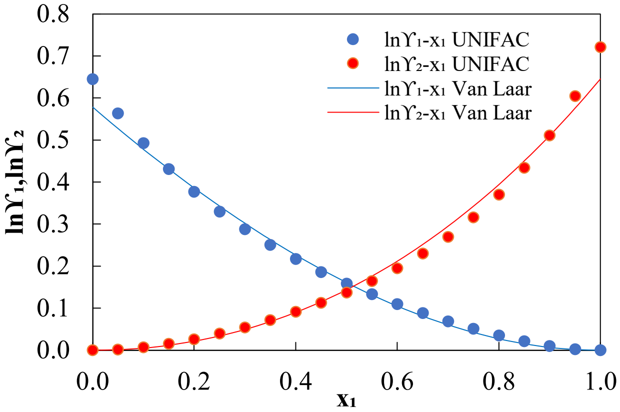

**Fig. 2.** $\ln\gamma_i - x_1$ diagram for VLE data predicted by UNIFAC and correlated by Van Laar model for MTBE (1) + AA (2) system at 101.325 kPa.

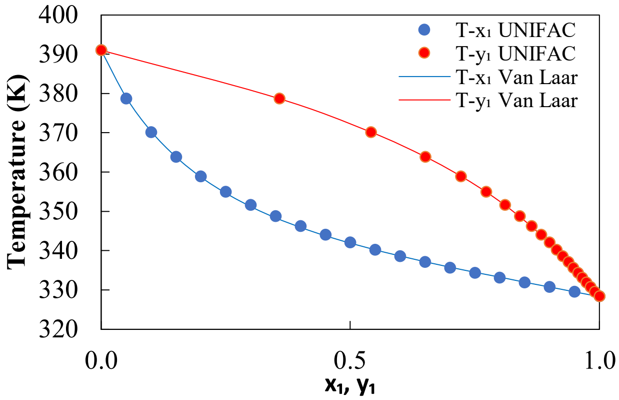

**Fig. 3.** T-x-y diagram for VLE data predicted by UNIFAC and correlated by Van Laar model for MTBE (1) + AA (2) system at 101.325 kPa.

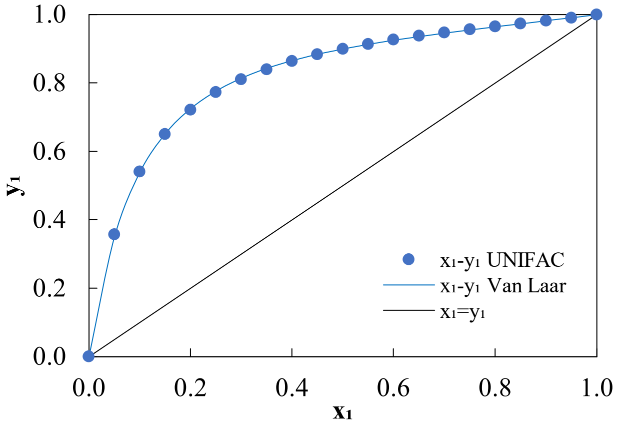

**Fig. 4.** x-y diagram for VLE data predicted by UNIFAC and correlated by Van Laar model for MTBE (1) + AA (2) system at 101.325 kPa.

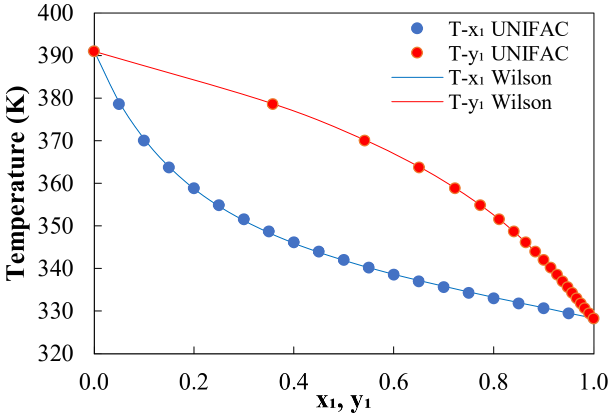

**Fig. 5.** T-x-y diagram for VLE data predicted by UNIFAC and correlated by Wilson model for MTBE (1) + AA (2) system at 101.325 kPa.

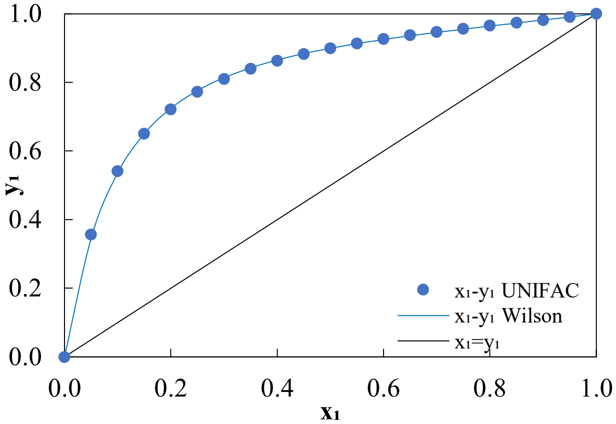

**Fig. 6.** x-y diagram for VLE data predicted by UNIFAC and correlated by Wilson model for MTBE (1) + AA (2) system at 101.325 kPa.

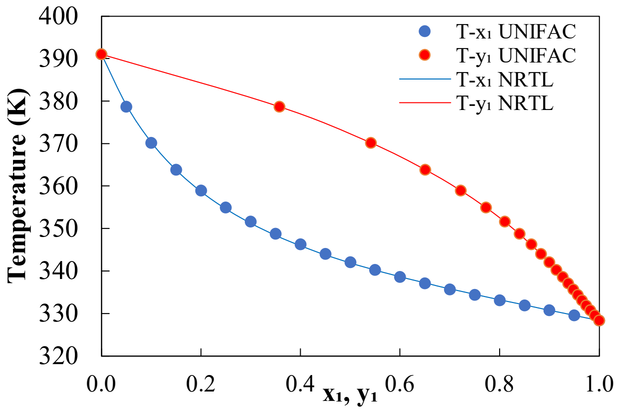

**Fig. 7.** T-x-y diagram for VLE data predicted by UNIFAC and correlated by NRTL model for MTBE (1) + AA (2) system at 101.325 kPa.

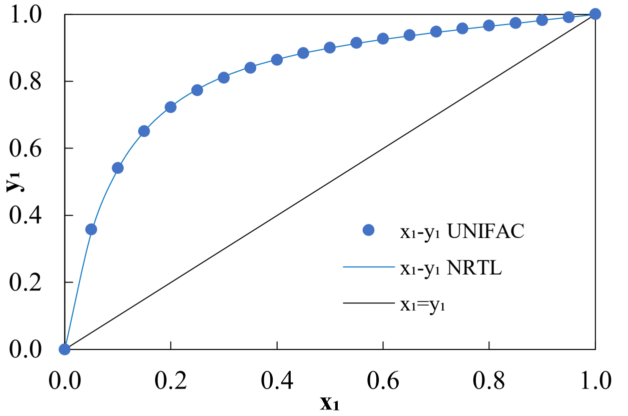

**Fig. 8.** x-y diagram for VLE data predicted by UNIFAC and correlated by NRTL model for MTBE (1) + AA (2) system at 101.325 kPa.

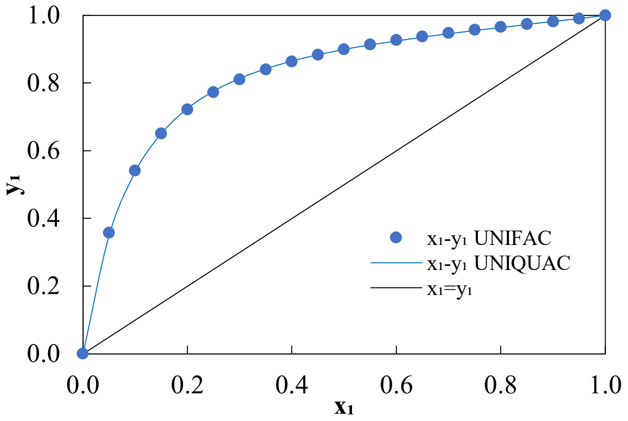

**Fig. 10.** x-y diagram for VLE data predicted by UNIFAC and correlated by UNIQUAC model for MTBE (1) + AA (2) system at 101.325 kPa.

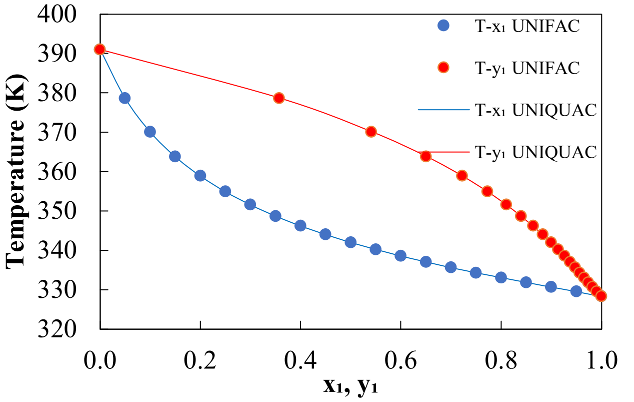

**Fig. 9.** T-x-y diagram for VLE data predicted by UNIFAC and correlated by UNIQUAC model for MTBE (1) + AA (2) system at 101.325 kPa.

## CONCLUSION

In order to design a distillation column for the critical separation of aqueous acetic acid using MTBE as a solvent, VLE data must be obtained. Hence, isobaric VLE data were predicted at atmospheric pressure. Binary interaction parameters (BIPs) were computed for Van Laar, Wilson, NRTL, and UNIQUAC activity coefficient models. The ability to fit the VLE of these models is quite satisfactory. The Van Laar model gives the best fit among all these models. The average absolute deviation (AAD) in temperature, pressure, and vapor phase composition were computed and reported. The R-K area test and the L-W test of Wisniak's L-W test were used to assess the

**Table 6.** Binary Interaction Parameters of Correlated $G^E$ Model

| Model | BIPs (J mol$^{-1}$) | | AAD (P) (kPa) | AAD (T) (K) | AAD (y) |
|---|---|---|---|---|---|
| Van Laar | $A_{12}$<br>0.5782 | $A_{21}$<br>0.6455 | 0.0005 | 0.1732 | 0.0018 |
| Wilson | $\lambda_{12}-\lambda_{11}$<br>-1758.2738 | $\lambda_{21}-\lambda_{22}$<br>3663.5075 | 0.0003 | 0.2131 | 0.0029 |
| NRTL | $g_{12}-g_{22}$<br>1346.2579 | $g_{21}-g_{11}$<br>533.4671 | 0.0005 | 0.1987 | 0.0026 |
| UNIQUAC | $u_{12}-u_{22}$<br>2051.2595 | $u_{21}-u_{11}$<br>-846.8702 | 0.0005 | 0.1853 | 0.0023 |

thermodynamic consistency of the predicted data. There were no thermodynamic inconsistencies in the predicted VLE data. According to the predicted VLE data, the mixture of MTBE + AA acid could be easily separated with ordinary distillation techniques.

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