Prediction of Vapor-Liquid Equilibrium of Binary Systems Linalool + Eugenol, Linalool + β-Caryophyllene, and Eugenol + β-Caryophyllene at Pressures of 30 and 60 kPa using the UNIFAC Method

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**Abstract.** Cinnamon leaf essential oil and its components, namely linalool, eugenol, and β-caryophyllene, are used as basic ingredients for making perfume, flavorings, cosmetics, and raw materials for the pharmaceutical industry. To separate the components of cinnamon leaf essential oil, several methods can be used, namely distillation, extraction, etc. Separating cinnamon leaf essential oil using distillation under vacuum pressure is an easier process to separate its components because the boiling point decreases so it does not require high temperatures. However, the design and simulation of the distillation process requires knowledge of the vapor-liquid equilibrium data of the components to be separated as a result of the extraction process. This research aims to obtain vapor-liquid equilibrium prediction data for the binary systems linalool + eugenol, linalool + β-caryophyllene, and eugenol + β-caryophyllene at pressures of 30 and 60 kPa using the UNIFAC method. T-x-y diagrams are obtained for the three binary systems studied. In all three binary systems, a decrease in pressure causes a decrease in the equilibrium temperature. It was found that the best pressure for the separation of the linalool + eugenol and linalool + β-caryophyllene binary systems was 60 kPa. Therefore, it can be concluded that in both binary systems, high vacuum pressure does not always produce the most optimal separation process. In addition, the eugenol + β-caryophyllene binary system exhibits azeotropic behavior so it cannot be separated by simple distillation.

# INTRODUCTION

Cinnamon (*Cinnamomum zeylanicum* Blume), an endemic plant known as "Kurundu" in Sri Lanka, belongs to the *Cinnamomum* genus of the Lauraceae plant family. This plant is also found in southern India, China, Burma and Indonesia [1]. Cinnamon is cultivated mainly to produce essential oils extracted from the leaves and bark which are used as ingredients for making perfumes, cosmetics, flavorings and raw materials for the pharmaceutical industry [2].

For the synthesis, design, and optimization of distillation processes, a reliable knowledge of the vapor-liquid equilibrium behavior is necessary. Because experimental data are often not available, at least for process synthesis, group contribution methods can be used for the prediction of the required vapor-liquid equilibria [3]. The UNIFAC (UNIQUAC Functional Group Activity Coefficients) group contribution method has proven to be a fast and reliable method for predicting liquid phase activity coefficients in nonelectrolyte, nonpolymeric mixtures at low to moderate pressures. It has become a valuable tool and widely used in practical chemical engineering applications, most notably in phase equilibrium calculations in cases where little or no relevant experimental information is available [4][5]. In the past several decades, the UNIFAC group contribution method has become very popular. As a result, UNIFAC has been integrated into most commercial process simulators [3]. The success and the range of applicability of the UNIFAC group contribution method depends on the availability and the reliability of certain parameters. The parameters needed for the use of UNIFAC are group volumes (Rk), group surface areas (Qk), and group interaction parameters (amn and anm) [3][6][7][8].

The fundamental idea of a solution-of-groups model is to utilize existing phase equilibrium data for predicting phase equilibria of systems for which no experimental data are available. In concept, the UNIFAC method follows the ASOG (Analytical Solution of Groups) method, wherein activity coefficients in mixtures are related to interactions between structural groups in the components. These structural groups have their own group volume parameters (Rk) and group surface area parameters (Qk), also the interactions between them have their own group interaction parameters (amn and anm). The essential features are suitable reduction of experimentally obtained activity-coefficient data to yield parameters characterizing interactions between pairs of structural groups in nonelectrolyte systems and use of those parameters to predict activity coefficients for other systems that have not been studied experimentally but that contain the same functional groups. The molecular activity coefficient is separated into two parts, namely combinatorial and residual. Combinatorial, provides the contribution due to differences in molecular size and shape, is influenced by group volume parameters (Rk) and group surface area parameters (Qk) meanwhile residual, provides the contribution due to molecular interactions, is influenced by group surface area parameters (Qk) and group interaction parameters (amn and anm) [9].

This research was carried out by reviewing several previous studies on vapor-liquid equilibrium, including Deng et al. [10] examined the vapor-liquid equilibrium of the binary systems linalool + 1-propanol and linalool + 1-butanol at pressures of 20, 30, 40, 50, and 60 kPa. The corrected vapor-liquid equilibrium data have been correlated using the UNIQUAC equation with temperature-dependent binary parameters to model the liquid phase and the virial equation of state to model the vapor phase. The results obtained are vapor-liquid equilibrium data and correlation parameters for the binary systems linalool + 1-propanol and linalool + 1-butanol at pressures of 20, 30, 40, 50, and 60 kPa. Garcia-Abarrio et al. [11] examined the vapor-liquid equilibrium of the linalool + ethanol binary system at pressures of 26.66, 40.00 and 53.33 kPa. Three activity coefficient models, namely, Wilson, NRTL and UNIQUAC were used to correlate the experimental data and to check their thermodynamic consistency. The results obtained are vapor-liquid equilibrium data and correlation parameters for the linalool + ethanol binary system at pressures of 26.66, 40.00 and 53.33 kPa. Hidayatulloh et al. [12] examined the vapor-liquid equilibrium of the binary system ethanol + eugenol at pressures of 400 and 760 mmHg. The vapor-liquid equilibrium data of the binary system is correlated with the Wilson, NRTL and UNIQUAC models to obtain binary parameters. The reliability of these models was tested by comparing with experimental results using Root Mean Square Deviation (RMSD). For the system and operating conditions studied, the Wilson, NRTL and UNIQUAC models are very suitable and provide satisfactory results based on RMSD values. The results obtained are vapor-liquid equilibrium data and correlation parameters for the ethanol + eugenol binary system at pressures of 400 and 760 mmHg. Huang et al. [13] investigated the vapor-liquid equilibrium of the binary systems β-caryophyllene + dipentene and dipentene + α-pinene as well as the ternary system β-caryophyllene + dipentene + α-pinene at a pressure of 100.7 kPa. The vapor-liquid equilibrium data of the binary systems was correlated using the Margules, Non-Random Two-Liquid (NRTL), Wilson, and Universal Quasi Chemical (UNIQUAC) activity coefficient models. The Wilson model parameters obtained from the binary systems are used to predict the vapor-liquid equilibrium data of the ternary system. The results obtained are vapor-liquid equilibrium data and correlation parameters for the binary systems β-caryophyllene + dipentene and dipentene + α-pinene as well as the ternary system β-caryophyllene + dipentene + α-pinene at a pressure of 100.7 kPa. Yao et al. [14] investigated the vapor-liquid equilibrium of the binary systems p-cymene + β-caryophyllene, 3-carene + β-caryophyllene, and 3-carene + p-cymene as well as the ternary system β-caryophyllene + p-cymene + 3-carene in pressure 101.33 kPa. Vapor-liquid equilibrium data for binary systems are correlated using Wilson, NRTL, and UNIQUAC activity coefficient models with small deviations. The ternary system vapor liquid equilibrium data was also correlated using the Wilson, NRTL and UNIQUAC models. The results obtained are vapor-liquid equilibrium data and correlation parameters for the binary systems p-cymene + β-caryophyllene, 3-carene + β-caryophyllene, and 3-carene + p-cymene as well as the ternary system β-caryophyllene + p-cymene + 3-carene at a pressure of 101.33 kPa.

Essential oil from cinnamon leaves contains 29 components with 3 main components having the highest levels, namely eugenol at 76.74%, β-caryophyllene at 3.47%, and linalool at 2.77% [1]. The purification processes commonly used are extraction and distillation. However, the design and simulation of the distillation process requires knowledge of the vapor-liquid equilibrium data of the mixture of components to be separated as a result of the extraction process [12]. However, data regarding the vapor-liquid equilibrium between linalool, eugenol, and β-caryophyllene are still missing. Therefore, in this study, predictions of the vapor-liquid equilibrium of the binary systems linalool + eugenol, linalool + β-caryophyllene, and eugenol + β-caryophyllene at pressures of 30 and 60 kPa were carried out using the UNIFAC method to determine whether there was an influence of variations in the applied vacuum pressure. The three binary systems studied are then depicted in a T-x-y diagram.

# RESEARCH METHODS

The vapor-liquid equilibrium prediction method used in this research is the UNIFAC method. This method is carried out by dividing each compound into its constituent groups. Then, the activity coefficient is calculated using the UNIFAC equation. Then, T (temperature) is calculated using bubble T calculations. After that, y (vapor fraction) is calculated using modified Raoult's law.

In this research, the UNIFAC equation is used to obtain the activity coefficient. There are two parameters of the activity coefficient, namely combinatorial and residual. Combinatorial (C) is a pure component parameter to calculate differences in molecular shape and size. Residual (R) combines two binary parameters for each pair of molecules to calculate molecular interactions. The following are the equations used in calculating the prediction of vapor-liquid equilibrium of binary systems using the UNIFAC method [15]:

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Notes:

γi = Activity coefficient of component i

γiC = Combinatorial contribution to the activity coefficient of component i

γiR = Residual contribution to the activity coefficient of component i

ri = Relative molecular volume

qi = Relative molecular surface area

vk(i) = Number of groups of type k in component i

Rk = Group volume parameters

Qk = Group surface area parameters

amk = Group interaction parameters

xi = Liquid phase mole fraction of component i

T = Temperature

# RESULTS AND DISCUSSION

In this study, predicted data for the vapor-liquid equilibrium of the binary systems linalool + eugenol, linalool + β-caryophyllene, and eugenol + β-caryophyllene at pressures of 30 and 60 kPa were obtained using the UNIFAC method. The group identification parameters for each component are shown in Table 1, as well as the group interaction parameters for each component are shown in Table 2 with the group interaction parameters between the same main group are set equal to zero. The calculation results of the predicted vapor-liquid equilibrium of the binary systems linalool + eugenol, linalool + β-caryophyllene, and eugenol + β-caryophyllene at pressures of 30 and 60 kPa using the UNIFAC method are shown in Table 3 to Table 5. T-x-y diagram of the predicted vapor-liquid equilibrium of the binary systems linalool + eugenol, linalool + β-caryophyllene, and eugenol + β-caryophyllene at pressures of 30 and 60 kPa using the UNIFAC method are shown in Figure 1 to Figure 3.

**TABLE 1.** Group Identification Parameters of Linalool, Eugenol, and β-Caryophyllene [9]

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Component** | **Name** | **Main Group** | **Secondary Group** | **vk** | **Rk** | **Qk** | **ri** | **qi** |
| Linalool | CH3 | 1 | 1 | 3 | 0.9011 | 0.848 | 7.5056 | 6.676 |
| CH2 | 1 | 2 | 2 | 0.6744 | 0.540 |
| C | 1 | 4 | 1 | 0.2195 | 0.000 |
| CH2=CH | 2 | 5 | 1 | 1.3454 | 1.176 |
| CH=C | 2 | 8 | 1 | 0.8886 | 0.676 |
| OH | 5 | 14 | 1 | 1.0000 | 1.200 |
| Eugenol | CH2=CH | 2 | 5 | 1 | 1.3454 | 1.176 | 6.3843 | 4.924 |
| ACH | 3 | 9 | 3 | 0.5313 | 0.400 |
| AC | 3 | 10 | 1 | 0.3652 | 0.120 |
| ACCH2 | 4 | 12 | 1 | 1.0396 | 0.660 |
| ACOH | 8 | 17 | 1 | 0.8952 | 0.680 |
| CH3O | 13 | 24 | 1 | 1.1450 | 1.088 |
| β-Caryophyllene | CH3 | 1 | 1 | 3 | 0.9011 | 0.848 | 9.1945 | 7.364 |
| CH2 | 1 | 2 | 5 | 0.6744 | 0.540 |
| CH | 1 | 3 | 2 | 0.4469 | 0.228 |
| C | 1 | 4 | 1 | 0.2195 | 0.000 |
| CH2=C | 2 | 7 | 1 | 1.1173 | 0.988 |
| CH=C | 2 | 8 | 1 | 0.8886 | 0.676 |

Notes:

vk = The number of species belonging to the same group

Rk = Group volume parameters

Qk = Group surface area parameters

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **a** | | **k** | | | | | | |
| **1** | **2** | **3** | **4** | **5** | **8** | **13** |
| **m** | **1** | 0.0 | 86.02 | 61.13 | 76.50 | 986.5 | 1333 | 251.5 |
| **2** | -35.36 | 0.0 | 38.81 | 74.15 | 524.1 | 526.1 | 214.5 |
| **3** | -11.12 | 3.446 | 0.0 | 167.0 | 636.1 | 1329 | 32.14 |
| **4** | -69.70 | -113.6 | -146.8 | 0.0 | 803.2 | 884.9 | 213.1 |
| **5** | 156.4 | 457.0 | 89.60 | 25.82 | 0.0 | -259.7 | 28.06 |
| **8** | 275.8 | 217.5 | 25.34 | 244.2 | -451.6 | 0.0 | -162.9 |
| **13** | 83.36 | 26.51 | 52.13 | 65.69 | 237.7 | -178.5 | 0.0 |

**TABLE 2.** Group Interaction Parameters of Linalool, Eugenol, and β-Caryophyllene [9]

**TABLE 3.** Calculation Results for Vapor-Liquid Equilibrium Predictions for the Linalool (1) + Eugenol (2) Binary System at Pressures of 30 and 60 kPa using the UNIFAC Method

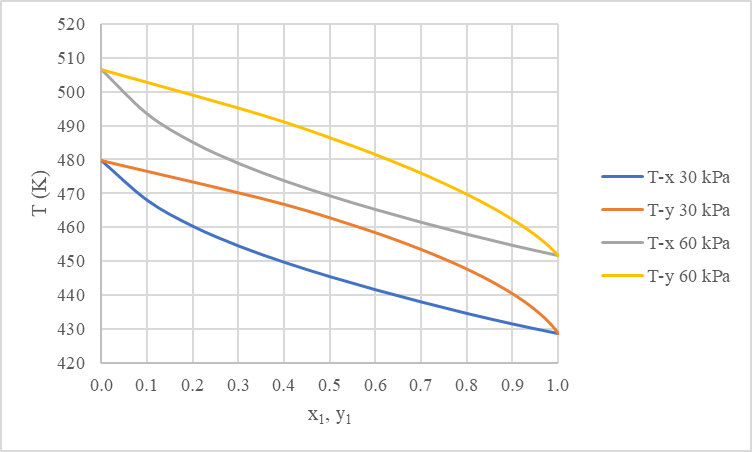
|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **P = 30 kPa** | | | **P = 60 kPa** | | | |
| **T (K)** | **x1** | **y1** | **T (K)** | **x1** | **y1** |
| 479.68 | 0.0000 | 0.0000 | 506.47 | 0.0000 | 0.0000 |
| 468.00 | 0.1000 | 0.3656 | 493.39 | 0.1000 | 0.3434 |
| 460.35 | 0.2000 | 0.5573 | 485.02 | 0.2000 | 0.5276 |
| 454.55 | 0.3000 | 0.6795 | 478.78 | 0.3000 | 0.6482 |
| 449.75 | 0.4000 | 0.7667 | 473.67 | 0.4000 | 0.7367 |
| 445.52 | 0.5000 | 0.8331 | 469.21 | 0.5000 | 0.8061 |
| 441.66 | 0.6000 | 0.8852 | 465.17 | 0.6000 | 0.8626 |
| 438.05 | 0.7000 | 0.9264 | 461.41 | 0.7000 | 0.9091 |
| 434.68 | 0.8000 | 0.9585 | 457.88 | 0.8000 | 0.9469 |
| 431.56 | 0.9000 | 0.9827 | 454.59 | 0.9000 | 0.9771 |
| 428.74 | 1.0000 | 1.0000 | 451.58 | 1.0000 | 1.0000 |

**TABLE 4.** Calculation Results for Vapor-Liquid Equilibrium Predictions for the Linalool (1) + β-Caryophyllene (2) Binary System at Pressures of 30 and 60 kPa using the UNIFAC Method

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **P = 30 kPa** | | | **P = 60 kPa** | | | |
| **T (K)** | **x1** | **y1** | **T (K)** | **x1** | **y1** |
| 480.68 | 0.0000 | 0.0000 | 507.13 | 0.0000 | 0.0000 |
| 457.72 | 0.1000 | 0.5349 | 484.21 | 0.1000 | 0.4984 |
| 448.23 | 0.2000 | 0.6827 | 473.82 | 0.2000 | 0.6554 |
| 443.13 | 0.3000 | 0.7515 | 468.02 | 0.3000 | 0.7314 |
| 439.85 | 0.4000 | 0.7943 | 464.23 | 0.4000 | 0.7793 |
| 437.43 | 0.5000 | 0.8271 | 461.42 | 0.5000 | 0.8157 |
| 435.42 | 0.6000 | 0.8565 | 459.10 | 0.6000 | 0.8479 |
| 433.62 | 0.7000 | 0.8858 | 457.05 | 0.7000 | 0.8797 |
| 431.93 | 0.8000 | 0.9179 | 455.14 | 0.8000 | 0.9138 |
| 430.31 | 0.9000 | 0.9550 | 453.32 | 0.9000 | 0.9529 |
| 428.74 | 1.0000 | 1.0000 | 451.58 | 1.0000 | 1.0000 |

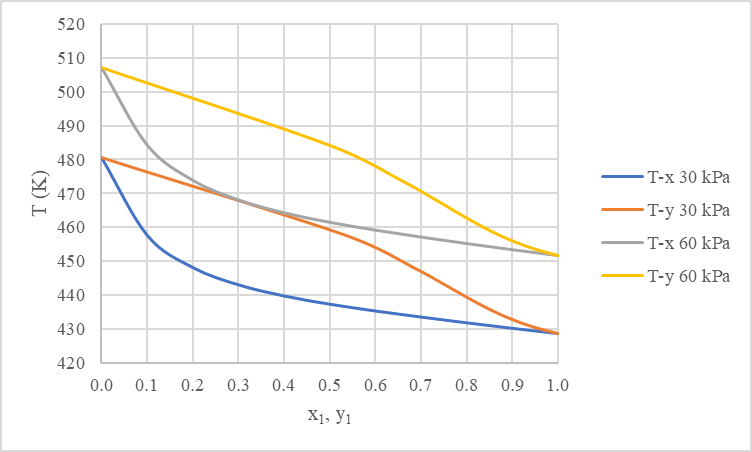
**TABLE 5.** Calculation Results for Vapor-Liquid Equilibrium Predictions for the Eugenol (1) + β-Caryophyllene (2) Binary System at Pressures of 30 and 60 kPa using the UNIFAC Method

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **P = 30 kPa** | | | **P = 60 kPa** | | | |
| **T (K)** | **x1** | **y1** | **T (K)** | **x1** | **y1** |
| 480.68 | 0.0000 | 0.0000 | 507.13 | 0.0000 | 0.0000 |
| 470.16 | 0.1000 | 0.3186 | 496.01 | 0.1000 | 0.3076 |
| 466.85 | 0.2000 | 0.4180 | 492.08 | 0.2000 | 0.4141 |
| 465.66 | 0.3000 | 0.4625 | 490.54 | 0.3000 | 0.4641 |
| 465.24 | 0.4000 | 0.4867 | 489.97 | 0.4000 | 0.4924 |
| 465.14 | 0.5000 | 0.5028 | 489.80 | 0.5000 | 0.5119 |
| 465.23 | 0.6000 | 0.5180 | 489.89 | 0.6000 | 0.5300 |
| 465.58 | 0.7000 | 0.5399 | 490.31 | 0.7000 | 0.5545 |
| 466.66 | 0.8000 | 0.5823 | 491.57 | 0.8000 | 0.5987 |
| 469.79 | 0.9000 | 0.6824 | 495.14 | 0.9000 | 0.6976 |
| 479.68 | 1.0000 | 1.0000 | 506.47 | 1.0000 | 1.0000 |



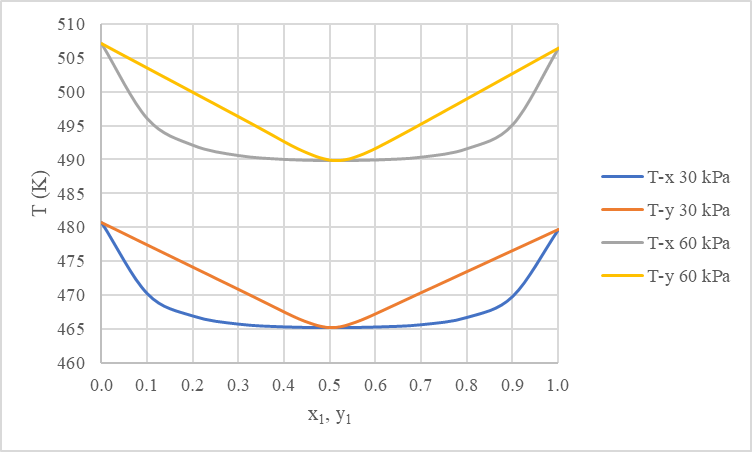


**Figure 1.** T-x-y diagram Prediction of Vapor-Liquid Equilibrium for the Linalool (1) + Eugenol (2) Binary System at Pressures of 30 and 60 kPa using the UNIFAC Method





**Figure 2.** T-x-y diagram Prediction of Vapor-Liquid Equilibrium for the Linalool (1) + β-Caryophyllene (2) Binary System at Pressures of 30 and 60 kPa using the UNIFAC Method





**Figure 3.** T-x-y diagram Prediction of Vapor-Liquid Equilibrium for the Eugenol (1) + β-Caryophyllene (2) Binary System at Pressures of 30 and 60 kPa using the UNIFAC Method

From Table 3 and Figure 1, data on the prediction of the vapor-liquid equilibrium of the linalool + eugenol binary system at pressures of 30 and 60 kPa using the UNIFAC method are obtained. For these two pressures, the lowest T-x-y diagram is at a pressure of 30 kPa, because the lower the pressure, the lower the equilibrium temperature. However, the largest area of the T-x-y diagram is at a pressure of 60 kPa, because the largest difference in boiling points of linalool and eugenol is at a pressure of 60 kPa, namely 54.89 K. This shows that the optimal pressure for the separation process of the linalool + eugenol binary system is 60 kPa. Linalool and eugenol are not isomers and are both different types of compounds, namely terpene alcohol and allylbenzene, so the two compounds are quite easy to separate.

From Table 4 and Figure 2, data on the prediction of the vapor-liquid equilibrium of the linalool + β-caryophyllene binary system at pressures of 30 and 60 kPa using the UNIFAC method are obtained. For these two pressures, the lowest T-x-y diagram is at a pressure of 30 kPa, because the lower the pressure, the lower the equilibrium temperature. However, the largest T-x-y diagram area is at a pressure of 60 kPa, because the largest difference in boiling points of linalool and β-caryophyllene is at a pressure of 60 kPa, namely 55.55 K. This shows that the optimal pressure for the separation process of the linalool + β-caryophyllene binary system is 60 kPa. The area of the T-x-y diagram of the linalool + β-caryophyllene binary system is the largest compared to the other two binary systems, because the difference in boiling points of linalool and β-caryophyllene is the largest compared to the other two binary systems. Linalool and β-caryophyllene are not isomers and are both different types of compounds, namely terpene alcohols and sesquiterpenes, so these two compounds are the easiest to separate.

From Table 5 and Figure 3, data on the prediction of the vapor-liquid equilibrium of the eugenol + β-caryophyllene binary system at pressures of 30 and 60 kPa using the UNIFAC method are obtained. For these two pressures, the lowest T-x-y diagram is at a pressure of 30 kPa, because the lower the pressure, the lower the equilibrium temperature. In the eugenol + β-caryophyllene binary system there is an azeotrope, because the azeotrope is influenced by the activity coefficient through the equation:

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Notes:

α12 = Relative volatility

γ1 = Activity coefficient of component 1

γ2 = Activity coefficient of component 2

P1sat = Saturation vapor pressure of component 1

P2sat = Saturation vapor pressure of component 2

When the value of α12 at x1 = 0 is greater than 1, while the value of α12 at x1 = 1 is smaller than 1 then there is an azeotrope because α12 is a continuous function of x1 and must pass through the value 1 in a certain composition. Even though eugenol and β-caryophyllene are not isomers and they are different types of compounds, namely allylbenzene and sesquiterpenes, the two compounds cannot be separated by simple distillation because there is an azeotrope.

From the three binary systems studied, the lower the pressure, the lower the equilibrium temperature, so the higher the quality of the essential oil. However, the calculation results show that from the three binary systems, the lower the pressure does not necessarily produce the most optimal separation process. Using the UNIFAC method, activity coefficient (γ) values were obtained for the three binary systems. For the linalool + eugenol binary system, the γ value ranges from 0.9195 – 1.3311. For the linalool + β-caryophyllene binary system, the γ value ranges from 1.0000 – 2.6988. For the eugenol + β-caryophyllene binary system, the γ value ranges from 1.0000 – 6.2884. This shows that the three binary systems are non-ideal solutions.

# CONCLUSION

In this study, predicted data for the vapor-liquid equilibrium of the binary systems linalool + eugenol, linalool + β-caryophyllene, and eugenol + β-caryophyllene at pressures of 30 and 60 kPa were obtained using the UNIFAC method. The calculation results show that from the three binary systems, the lower the pressure does not necessarily produce the most optimal separation process. T-x-y diagrams are obtained for the three binary systems studied. Even though the area of the T-x-y diagram of the linalool + eugenol binary system is smaller than the linalool + β-caryophyllene binary system, the two compounds are quite easy to separate. The area of the T-x-y diagram of the linalool + β-caryophyllene binary system is the largest compared to the other two binary systems, so these two compounds are the easiest to separate. In the eugenol + β-caryophyllene binary system there is an azeotrope, so the two compounds cannot be separated by simple distillation. Using the UNIFAC method, the activity coefficient (γ) values for the three binary systems were obtained which shows that the three binary systems are non-ideal solutions.

# ACKNOWLEDGMENTS

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