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Measurement of Isobaric Vapor-Liquid Equilibrium for Binary System β- Caryophyllene + Linalool and Eugenol + Linalool at 30 and 60 kPa

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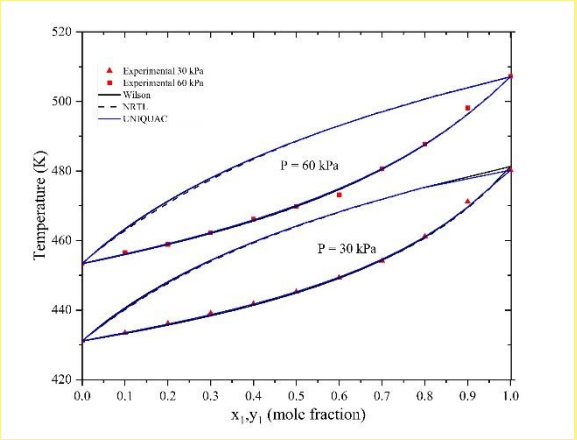
***Abstract*—** The Vapor-Liquid Equilibrium experiment focused on studying thermodynamic behavior of Eugenol, Beta-caryophyllene, and Linalool during their vapor and liquid phases. These compounds were chosen due to their significance in various industries, including pharmaceuticals, cosmetics, and flavorings. Equilibrium data between mixtures is still very limited in various conditions. The experiment tested on Othmer still that has been modified and validated corresponds to the vapor pressure data of each component using the equations of Antoine and Wagner-Ambrose obtained Average Absolute Deviation (AAD) T of 0,424% and 0,246%. This study aimed to obtain vapor-liquid equilibrium data for binary systems, which are Eugenol + Linalool and Beta-Caryophyllene + Linalool at 30 kPa and 60 kPa with a mole composition range (x_1) from 0—1 for each pressure. The equilibrium data were then correlated with Wilson, Non-Random Two-Liquid (NRTL), and Portmanteau of Universal Quasichemical (UNIQUAC) equations to represent all experiment data. The results obtained of this study were the AAD values for each system of β-Caryophyllene + Linalool and Eugenol + Linalool at pressures of 30 and 60 kPa whose values were below 0,5%.



***Keywords*—** Eugenol; Industry; Linalool; Thermodynamic Correlations; Vapor-Liquid Equilibrium; β-Caryophyllene

I. INTRODUCTION

The Covid-19 pandemic that occurred in 2019 had a significant impact on global health and economic problems. The virus has claimed millions of victims and reduced economic activity due to lockdown policies implemented in all countries in the world, including in Indonesia. However, of the many negative impacts due to Covid-19, there are also positive impacts, one of which is the increasingly massive research related to health so that it can assist in treatment [1].

One of the commodities that are exploited for medicinal ingredients, both for pharmaceutical and agricultural purposes, are chemicals derived from plants. Indonesia, which is a tropical country with various types of plants, will certainly benefit from this. One of them is the ylang plant (*Cananga odoratum*) which is widely cultivated in many regions in Indonesia.

TABLE 1.
QUALITY STANDARDS FOR YLANG OIL (SNI 06-3949-1955)

Parameters	Specification
Organoleptic Test	Color: Light—Dark Yellow Odor: Fresh
Specific Gravity at 20°C/20°C	0.906 – 0.9206 g/m/L
Bias Index	1.495 – 1.504
Solubility at Ethanol 95%	1: 0.5
Residual Steam Distillation	Max. 5
Optical Rotation	(-15) – (-30) °C
Ester Number	15 – 30

Part of the ylang plant, especially the ylang flower, is often used for its essential oil and is used as a traditional medicine: sedative, aromatherapy and uplifting the spirit. Furthermore, it can be used to treat marital relationship

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problems. Research conducted by Anggia et al.,2014 stated that ylang flower oil can be used as an antibacterial.

Based on research conducted by Herlina et al., 2020 stated that ylang flower essential oil extract can be formulated as an active ingredient on hand sanitizers because they have antibacterial properties, especially against Staphylococcus aureus and Escherichia coli [2]

The potential for essential oil produced by the flower part of the ylang plant will have high economic value if it is produced on an industrial scale. Based on research by Yulianita, 2009 quoted in Kasem, 2022, the essential oil produced from the flower parts of ylang has a yield of 0.8-1.3% by mass of the whole flower mass, which means that every 1 kg of essential flowers that is distilled has the potential to produce 13 grams of essential oil [3]. Ylang oil in Indonesia itself has quality requirements according to SNI 06-3949-1995 as shown in the Table 1.

The largest chemical composition within essential oils obtained from ylang flowers is β-Caryophyllene of 16.153% then linalool of 6.225%. In addition, it was also found to contain other chemical compounds, one of which is Eugenol [4].

As previously mentioned, the highest content of essential oil in ylang flowers is caryophyllene. This compound is known as a compound that can kill bacteria (anti-microbial) and has other medical benefits such as anti-cancer, antioxidant, and anti-inflammatory [5]. With such content, caryophyllene compounds are generally used in the food industry as anti-microbials because they are also non-toxic for consumption materials.

To be able to isolate the caryophyllene compound from the system contained in ylang oil, further purification of the ylang oil is required. One of the optimal methods of purification is through distillation or distillation which uses the principle of different boiling points, with the lower boiling point of the compound going to the top product while the compound having a higher boiling point will be the bottom product. To obtain data on optimal operating conditions in isolating a compound, vapor-liquid equilibrium (VLE) measurement data will help in this regard because it can determine the vapor and liquid fractions of each essential oil component from the reed flower to determine the level of purity at temperature and pressure.

Furthermore, the implementation of the VLE data will be used to determine the number of stages, the number of trays, and the height of the distillation column so that with this data it will make it easier to escalate production from the lab scale to the industrial scale. The optimal value of the interaction of the binary parameters of the thermodynamic model, such as the equation of state or the activity coefficient model, must be carried out by correlating the experimental VLE data with the selected thermodynamic model.

Hence this study aimed to obtain vapor-liquid equilibrium data for binary systems, which are Eugenol + Linalool and Beta-Caryophyllene + Linalool at 30 and 60 kPa with a mole composition range (x_1) from 0—1 for each pressure.

A. Preceding Research

This research was conducted based on a literature review of previous journals that discussed vapor-liquid equilibrium for the related compound systems which are β-Caryophyllene, eugenol, and linalool. But there was no research that provide vapor liquid equilibrium data for mixture of related components. Here preceding research are presented that involving the related compound systems.

Rodrigues et al., (2022) conducted research on the vapor-liquid equilibrium of eugenol/β-Caryophyllene under isobaric conditions at pressures of 5, 10, and 20 kPa. The results obtained are in the form of experimental regression data which is then modelled with binary interaction parameters from the correlation of the NRTL, Wilson, and UNIQUAC equations. This research draws conclusions with the mean absolute deviation from temperature, which is <0.22 K and the molar fraction in the vapor phase, which is 0.0119 [6].

Kuswandi et al. (2019) conducted a study to obtain experimental liquid-liquid equilibrium data from the mixture of β – caryophyllene + 1 - propanol + water [7].

Hidayatullah et al. (2019) conducted a study on measuring the vapor-liquid equilibrium of the binary system Ethanol (1) + Eugenol (2) at a pressure of 400 mmHg and 600 mmHg. Experimental data correlated with the NRTL and UNIQUAC models with maximum Absolute Average Relative Deviation (AARD) at T and y_1 of 7.525% and 2.69%, respectively. The prediction of the vapor-liquid equilibrium of the binary ethanol (1) + eugenol (2) system was also carried out using UNIFAC which produced maximum AARD at T and y_1 of 9.261% and 1.742%, respectively [8].

Hapsari et al., (2018) conducted a study to obtain vapor-liquid equilibrium data for ethanol(1) + eugenol(2) at a pressure of 600 mmHg, and predict vapor-liquid equilibrium data for a binary system ethanol(1) + eugenol(2) and 1-propanol(1) + eugenol(2) at various pressures. The prediction of vapor-liquid equilibrium data was carried out 300 mmHg, 600 mmHg, and 760 mmHg.) [9].

Nehemia & Wiyasa (2018) conducted a study to obtain liquid-liquid equilibrium data for the ternary system Eugenol + β-caryophyllene + NaOH solution measured at 303.15 K. The data obtained from each system is correlated with the NRTL and UNIQUAC equations which give the RMSD of the equilibrium composition of 4.27% and 7.09%, respectively [10].

Abarrio et al. (2013) isobaric vapor + liquid equilibrium data at 26.66, 40.00, and 53.33 kPa for mixtures of linalool (1) + ethanol (2) across the composition range. Three activity coefficient models, namely Wilson, NRTL and UNIQUAC were used to correlate experimental data and to check their thermodynamic consistency [11].

B. Vapor-Liquid Equilibrium

Vapor-liquid equilibrium (VLE) is an equilibrium condition between the vapor and liquid phases in a substance in a closed system at certain temperature and

pressure variables. Equilibrium occurs when the rate of evaporation of a substance from the liquid phase is equal to the rate of condensation of a substance from the vapor phase, so that there is no net change in the amount of substance in each phase, which is indicated by the condition that the temperature in the liquid phase and the temperature of the vapor are close to the same or constant [15].

In the distillation process, VLE data can predict the composition of the mole fraction of a substance in the condenser and reboiler. By developing the model will optimize the distillation process. As for the absorption process, VLE data is used to predict the absorption capacity and composition of the gas and liquid phases under certain operating conditions. Similar to the distillation process, the use of VLE data in the extract process is used to predict the mole fraction of the solvent and the mole fraction of the substance in the vapor and liquid phases [16].

The tendency of a substance to change (liquid-gas/gas-liquid) can be measured by a quantity called fugacity. At equilibrium the observed properties do not change with time, so that the intensive properties or thermodynamic potentials (temperature, pressure, chemical potential) are the same in a system. This uniformity affects the absence of heat transfer, mass transfer, and work from inside or outside the system. For each component in the mixture, the equilibrium conditions can be expressed by the equation:

$$\hat{f}_i^L = \hat{f}_i^V \quad (1)$$

II. METHOD

Research was carried out to obtain vapor-liquid equilibrium data under isobaric conditions for the binary system Eugenol + linalool, Eugenol+β-caryophyllene, β-caryophyllene + Linalool at pressures of 30 and 60 kPa.

Prior to data collection, it is necessary to validate the tool by comparing vapor pressure and temperature data between the obtained data with previous experiments data through the Antoine equation. Then the obtained data were correlated through Wilson, NRTL, UNIQUAC correlations. This study used independent variables, including the mole fraction of the solution from each component, then the controlled variable, which are mixture of compounds and the pressure, then the dependent variables, which are the measured temperature and the vapor fraction mixture.

TABLE 2.
MATERIAL PROPERTIES AND INFORMATION.

Properties	Properties and Information		
Component	β-Caryophyllene	Eugenol	Linalool
CAS Num	87-44-5	97-53-0	78-70-6
Formula	$C_{15}H_{24}$	$C_{10}H_{12}O_2$	$C_{10}H_{18}O$
MW	204.35	164.2	154,25
Melt Point	-7. °C	-7.5 °C	-10 °C
Boil Point	116 °C	253.2 °C	196.3 °C
Density	0.901 g/cm^3 at 25°C	1.065 g/cm^3 at 25°C	0.86 g/cm^3 at 293.15°C
Purity	≥98%	≥ 99%	99%
Sources	PT. Indesso Aroma	PT. Indesso Aroma	Xi'an International Healthcare Factory Co., Ltd
Analysis	GLC	GLC	GC

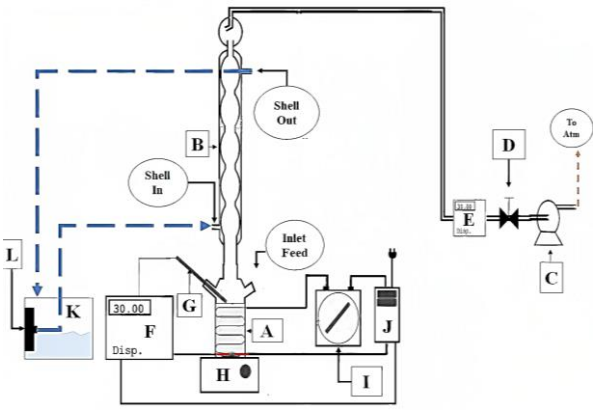

Figure 1. Apparatus used for experiment.

TABLE 3.
DETAILED EQUIPMENT

Notation	Equipment Name
A	Ebulliometer Cell
B	Condenser
C	Vacuum Pump VE 115 ¼ HP 2 CFM
D	Valve
E	Pressure Indicator
F	Temperature Indicator (TC4NS-24R)
G	Thermocouple
H	Magnetic Stirrer
I	Heating System Controller TDGC
J	Relay
K	Water Bath
L	Water Pump

Eugenol ($C_{10}H_{12}O_2$) or a volatile bioactive natural phenolic monoterpenoid [12], belongs to the phenylpropanoid natural product class. For this experiment, Eugenol was provided by PT. Indesso Aroma.

β-Caryophyllene ($C_{15}H_{24}$) or commonly called caryophyllene is a natural sesquiterpene compound and a component of essential oils, especially clove leaf oil, oil from the stems and flowers of *Syzgium aromaticum* (clove) which is a typical flower from the island of Maluku [13]. For this experiment, β-Caryophyllene was provided by PT. Indesso Aroma.

Linalool or 3,7-dimethyl-1,6-octadien-3-ol is a monoterpene acyclic tertiary alcohol which is found in many essential oils in several plant species such as basil (*Ocimum basilicum*) [14]. Materials that were used for the experiment shown at Table 2.

In this research, the apparatus for the experiment was able to gather P, T, and molar liquid fraction (x) experiment data as represented on Figure 1 with the detail of equipment used shown in Table 3. The ebulliometer cell

was the place where vapor-liquid equilibrium was measured. The condenser assembled at the upside of ebulliometer used to change the vapor phase back into liquid when the mixture reaches the equilibrium.

The ebulliometer method has advantages, such as being able to measure at various temperature and pressure variables and does not depend on chemical reactions such as the acid-base method. However, it has drawbacks such as the time required to reach the boiling point of a mixture of substances which is quite long and can be affected by changes in atmospheric pressure during measurement.

The experiment was done as the component was first inserted into the ebulliometer cell according to mass calculation that resulted in the mole fraction of each component. Then, vacuum pump (C) was operated to provide a vacuum condition (30 and 60 kPa) inside the ebulliometer cell. Then the heating system (I) was turned on to increase the temperature of the ebulliometer while the temperature indicator connected with thermo-couple that plugged into the ebulliometer cell to monitor the value of temperature. The temperature then recorded if there is no temperature change for 15 seconds as it can be said that the system has reached the equilibrium conditions at the corresponding pressure.

III. RESULTS AND DISCUSSION

A. *Ebulliometer Validation*

To make sure that the ebulliometer that used for the experiment was able to measure the pressure and temperature accurately, then the first thing that being done was validating the ebulliometer to measure a component vapor pressure (P_{vap}) and the temperature (T). Then, the measured component and temperature were compared with the existing data as the reference.

This validation was carried out by using ethanol as the component that has specification of purity above 99%. The reason why ethanol was being used as the component for the validation of ebulliometer was because ethanol can be considered as general component to be measured in almost every single aspect. This led to an increase in the number of sources of experimental data on ethanol. The more sources that were used for validation, the more valid the ebulliometer used as the experimental tool

Here, two correlations which are Antoine and Wagner Ambrose equations were used to compare the measured vapor pressure and temperature of ethanol. The equation and units of the corresponding correlations are presented in Table 4 and Table 5.

TABLE 4.
ANTOINE PARAMETERS AND EQUATION.

Component	A	B	C
Ethanol	8.1348	1662.48	238.131

$\log_{10} P^{sat}$(mmHg) = $A - B/(T(C) + C)$

TABLE 5.
WAGNER AMBROSE PARAMETERS AND EQUATION.

Component	A	B	C	D	T_c (K)	P_c (bar)
Ethanol	-8.685	1.178	-4.876	1.588	513.92	61.32

$$\ln P^{sat}(bar) = (A\tau + B\tau^{1.5} + C\tau^{2.5} + D\tau^{5})/Tr$$

$$\tau = 1 - \frac{T}{Tc}$$

TABLE 6.
VALIDATION RESULTS.

P (kPa)	T_{exp} (K)	T_{Wagner} (K)	$T_{Antoine}$ (K)	$\%AD_{Wagner}$	$\%AD_{Antoine}$
23.42	319.45	318.45	317.27	0.314	0.682
28.72	322.75	322.60	321.58	0.046	0.363
34.82	326.85	326.64	325.77	0.063	0.330
47.22	334.35	333.29	332.65	0.317	0.509
51.72	336.65	335.34	334.74	0.391	0.566
56.32	338.25	337.29	336.79	0.284	0.432
63.22	341.03	339.96	339.57	0.315	0.429
68.92	342.95	341.97	341.67	0.285	0.372
80.22	346.35	345.64	345.45	0.205	0.260
Absolute Average Deviation				0.246	0.424

TABLE 7.
EXPERIMENTAL RESULTS OF PRESSURE (P) & TEMPERATURE (T) FOR 3 COMPOUNDS.

Eugenol		Linalool		β -Caryophyllene	
P (kPa)	T (K)	P (kPa)	T (K)	P (kPa)	T (K)
8.79	443.45	19.48	418.45	7.79	439.65
10.09	446.75	21.87	422.80	10.29	447.75
11.99	450.65	27.78	428.65	11.00	449.75
13.20	453.85	34.88	435.75	13.00	454.45
14.79	458.15	37.00	438.25	14.59	458.65
17.49	462.75	39.93	440.15	19.09	467.55
20.39	467.15	43.78	442.85	21.49	471.75
22.09	470.05	46.03	444.45	23.99	475.05
25.79	475.95	49.35	446.85	29.99	479.95
30.19	481.15	53.07	449.25	39.19	490.55
35.99	488.15	55.99	451.05	42.29	493.95
40.89	491.55	62.09	454.65	47.09	497.25
45.99	495.45	67.67	457.65	50.99	500.00
50.79	497.15	76.83	461.75	55.49	504.05
55.99	502.45			57.89	505.25
60.01	505.15			60.09	507.00

TABLE 8.
ANTOINE PARAMETERS FITTING RESULT*.

Component	A	B	C
β -Caryophyllene	12.134	2643.781	-178.447
Eugenol	10.188	1598.410	-244.161
Linalool	11.527	1936.592	-192.878

$\ln_{10} P^{sat}$(kPa) = $A - B/(T(K) + C)$
*Validated at least within pressure range of 10 – 70 kPa.

The comparison that carried out the experiment and existing data were represented by Absolute Average Deviation (AAD) of the temperature between the correlations and the experiment. The AAD equation follows equation (2):

$$\frac{1}{n}\sum_{i=1}^{n}|x_i - m_i| \qquad (2)$$

With x_i is the measured temperature, m_i is the correlation result, and n is total data that is being measured.

TABLE 9.
EQUILIBRIUM TEMPERATURE OF B-CARYOPHYLLENE (1) + LINALOOL (2) SYSTEM.

Mole fraction. x_1	T (K)	
	30 kPa	60 kPa
0.00	431.15	453.45
0.10	433.45	456.55
0.20	436.15	458.95
0.30	439.15	462.25
0.40	441.85	466.15
0.50	445.25	469.85
0.60	449.35	473.15
0.70	454.15	480.65
0.80	461.15	487.75
0.90	471.15	498.15
1.00	481.15	507.25

The results of validation that has been done are presented in Table 6 and on Figure 2. Based on those data, the results of the validation experiment using ethanol compounds and using the Antoine equation method and the Wagner Ambrose equation, it was found that the AAD T for all components was less than 0.5%. The AAD T value of validating the pure ethanol component based on the Antoine and Wagner Ambrose equations was 0.424% and 0.246%, respectively. As the AAD T value results in a small deviation, the ebulliometer tool is ready to be used for experiments.

TABLE 10.
EQUILIBRIUM TEMPERATURE OF EUGENOL (1) + LINALOOL (2) SYSTEM.

Mole fraction. x_1	T (K)	
	30 kPa	60 kPa
0.00	431.15	453.45
0.10	432.15	454.25
0.20	434.15	457.65
0.30	436.75	460.35
0.40	439.15	464.65
0.50	442.15	467.55
0.60	447.75	473.45
0.70	451.65	479.15
0.80	454.45	482.15
0.90	463.25	491.15
1.00	479.95	505.95

B. Vapor Pressure

The measurement of the equilibrium model used (Wilson, NRTL, and UNIQUAC) depends on the results of the calculation of the saturated condition. In this system, the compounds β-Caryophyllene, Eugenol, and Linalool were analyzed in pure condition to produce Antoine parameter values. This was done because until this research was written, the parameter values for the compounds β-Caryophyllene and Linalool had never been analyzed so the measurement of the Antoine constant through experiments needed to be carried out. The Antoine parameter calculation is based on the linearization of the Antoine equation as in the following equation (3)

$$y = a0 + a1.x1 + a2.x2 \quad (3)$$

Where y = ln(P), x_1 = 1/T, and x2 = ln(P)/T.

So that the experimental data in form of pressure (P) in kPa and temperature (T) in K were linearized and represented in a graph, which then the values of a0, a1, and a2 were processed into values of A, B, and C. The experimental results of pressure and the temperature carried out can be seen in Table 7.

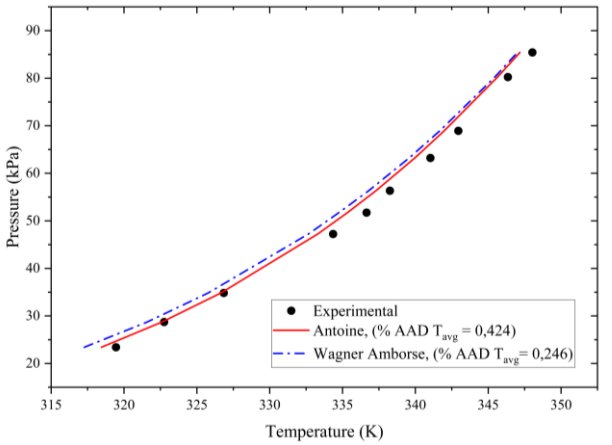

Figure 2. Ethanol validation results representation.

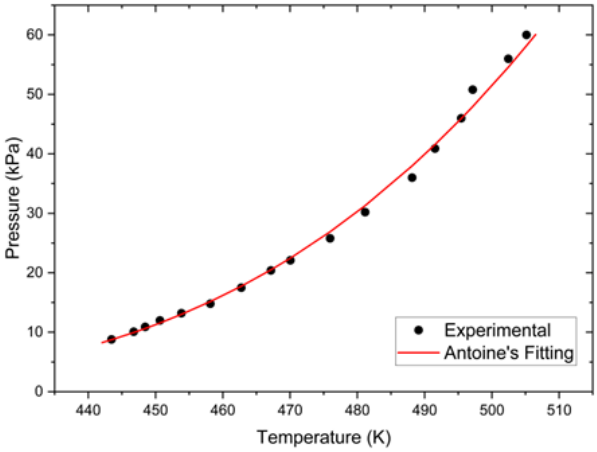

Figure 3. Eugenol fitting results.

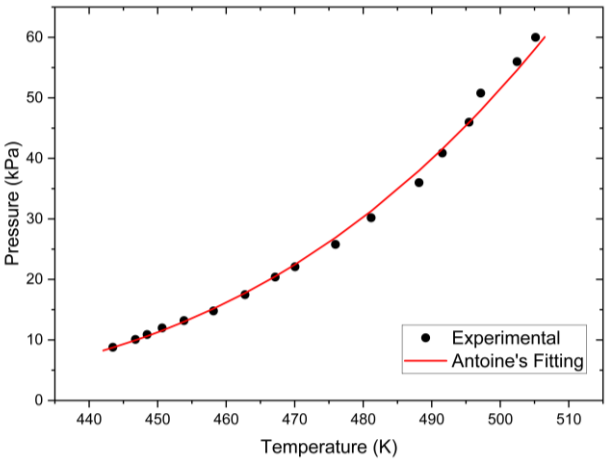

Figure 4. Linalool fitting results.

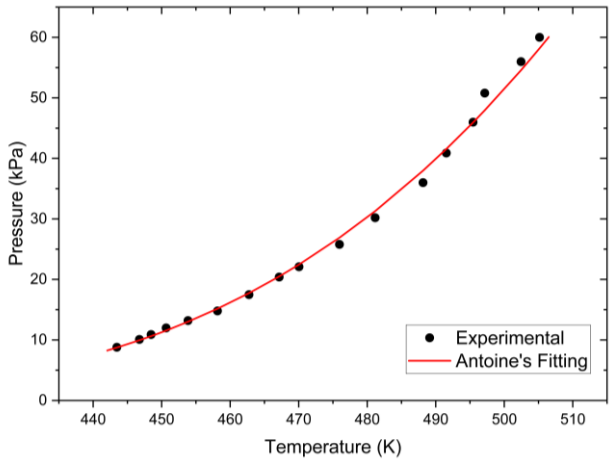

Figure 5. β-Caryophyllene fitting results.

Then the data obtained were processed to obtain the parameters of Antoine: A, B, and C as presented in Table 8. Then it is represented to a graph and being compared with the experimental data as shown in Figure 3 – 5. The figures 3 – 5 showed that there was a little deviation between the experimental recorded vapor pressure of Eugenol, Linalool, and β-Caryophyllene with the resulting Antoine's fitting as the fitting was resulted from the experimental data. These Antoine data obtained were then used for this research to support the correlations calculation.

TABLE 11.
CALCULATION OF THE EQUILIBRIUM PARAMETERS OF THE B-CARYOPHYLLENE (1) + LINALOOL (2) SYSTEM.

Pressure (kPa)	Correlation	Parameter (cal/mol)		AAD T (%)
30	Wilson	a_{12}	6.507	0.087
		a_{21}	17.182	
	NRTL	b_{12}	118.827	0.093
		b_{21}	119.258	
		A	0.47	
	UNIQUAC	u_{12}	18.572	0.066
		u_{21}	4.459	
60	Wilson	a_{12}	-4.787	0.082
		a_{21}	25.476	
	NRTL	b_{12}	513.350	0.081
		b_{21}	-246.739	
		A	0.339	
	UNIQUAC	u_{12}	-50.104	0.102
		u_{21}	65.382	

TABLE 12.
CALCULATION OF THE EQUILIBRIUM PARAMETERS OF THE EUGENOL (1) + LINALOOL (2) SYSTEM.

Pressure (kPa)	Correlation	Parameter (cal/mol)		AAD T (%)
30	Wilson	a_{12}	572.694	0.1589
		a_{21}	-278.182	
	NRTL	b_{12}	272.676	0.1558
		b_{21}	359.052	
		A	0.21	
	UNIQUAC	u_{12}	39.829	0.1678
		u_{21}	45.024	
60	Wilson	a_{12}	698.173	0.1766
		a_{21}	-168.497	
	NRTL	b_{12}	182.195	0.1846
		b_{21}	185.345	
		A	0.21	
	UNIQUAC	u_{12}	492.048	0.1766
		u_{21}	-344.095	

C. Vapor Liquid Equilibrium (VLE) Measurements

Vapor-liquid equilibrium measurement of binary β Caryophyllene + Linalool and Eugenol + Linalool systems using a simple ebulliometer was carried out by heating the mixture and then measuring the temperature when the binary mixture was in a state of equilibrium (equilibrium). Equilibrium is a state in which two processes in opposite directions take place simultaneously and continuously, but there is no macroscopic change to pressure, temperature, and composition. Based on research data on the binary systems β-Caryophyllene + Linalool and Eugenol + Linalool in isobaric condition, the equilibrium temperature for each composition is shown in Table 9 and 10.

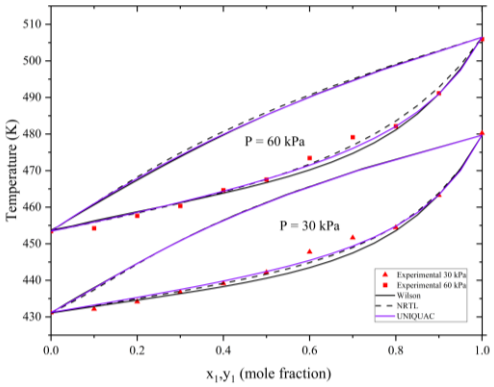

Figure 6. T-x-y Graph of Eugenol (1) + Linalool (2) system.

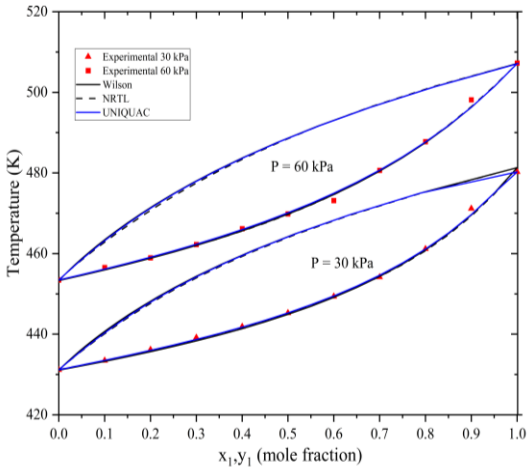

Figure 7. T-x-y Graph of β-Caryophyllene (1) + Linalool (2) system.

D. Isobaric Binary Vapor-Liquid Equilibrium Correlations

The experimental data obtained were correlated with the Wilson, NRTL, and UNIQUAC equations. These models have been widely used to correlate vapor-liquid equilibrium data to obtain optimal parameters. The Wilson correlation model uses two parameters, a12 and a21. The NRTL correlation model uses three parameters, which are b12, b21, and an optimized α value in the range of 0.21 to 0.47 (in the calculation of the NRTL method, the α value solved with the Excel solver method to obtain the minimum temperature AAD) [17]. The UNIQUAC correlation model uses two parameters which are u12 and u21. From the correlation results, the optimal binary parameters were obtained from the data. To obtain optimal binary system parameters for each model by minimizing the AAD value based on the difference in experimental boiling point temperatures for each composition and correlation. The parameter was better if the equilibrium temperature deviation between the experimental data and the resulting model had the minimum possible value. The parameters obtained were used to calculate the T and y_1 correlation results. Parameter fitting results for each system at vacuum pressure (30 and 60 kPa) with Wilson, NRTL, and UNIQUAC modelling can be seen on Table 11 & 12. Thus, a vapor-liquid equilibrium prediction curve can be constructed to be compared with experimental data. The VLE diagrams of each system are represented in Figure 6 for VLE diagram of mixtures between Eugenol (1) and Linalool (2) and system and represented in Figure 7 for VLE diagram of mixtures between β-Caryophyllene (1) + Linalool (2). Both diagrams showed that by qualitative evaluations all of three correlations were having good quality compared to the experimental data (plotted with red dots) as the line represented the experimental data.

From the results of quantitative evaluations represented by the AAD T calculations, both systems produce relatively small values, resulting in <0.2% deviation. Then the resulting equilibrium graph of the systems which are β-Caryophyllene + Linalool and Eugenol + Linalool at 30 and 60 kPa systems have a better profile. Therefore, the experimental results on the 2 systems represent the real value of vapor molar fraction y_1.

The vapor-liquid equilibrium data acquired from the experimental Eugenol + Linalool and β-Caryophyllene + Linalool systems can significantly benefit industries involved in essential oil extraction and purification. These data mark the initial step toward scaling up these processes for industrial use, which could potentially bolster Indonesia's essential oil commodities in the future. Furthermore, by providing a deeper understanding of the thermodynamic behavior of these essential oil mixtures, this research can contribute to the development of more efficient and sustainable extraction techniques. This, in turn, may lead to increased yields and improved quality of essential oils, ultimately benefiting both the industry and consumer.

IV. CONCLUSION

Based on research that had been done regarding the measurement of vapor-liquid equilibrium for binary systems β-Caryophyllene + Linalool and Eugenol + Linalool systems at 30 kPa and 60 kPa, it was concluded that vapor-liquid equilibrium data for binary systems β-Caryophyllene + Linalool and Eugenol + Linalool under vacuum conditions (30 kPa and 60 kPa) in the experimental of P-T-x and y were obtained through a calculation using Wilson, NRTL, and UNIQUAC thermodynamic correlations. The results of the correlation with research data on both binary systems also showed a correlation model that is well represented with the Wilson, NRTL, and UNIQUAC models which are characterized by an Average Absolute Deviation (AAD) value of less than 0.5%.

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REFERENCES

[1] E. Herlina, D. Widiastuti and A. Triadi, "Potensi Minyak Atsiri Bunga Kenanga (Cananga Odorata) Sebagai Antibakteria Dalam Sediaan Hand Sanitizer Gel," Ekologia: Jurnal Ilmiah Ilmu Dasar Dan Lingkungan Hidup, pp. 88-94, 2020.

[2] F. Anggia, Yuharmen and Balatif, "Perbandingan Isolasi Minyak Atsiri dari Bungan Kenangan (Cananga Odorata) Cara Konvensional dan Microwave serta Uji Aktivitas Antibakteri dan Antikosidan," Jurnal Online Mahasiswa Fakultas Matematika Dan Ilmu Pengetahuan Alam Universitas Riau, 2014.
[3] M. Firdaus, "Identifikasi Komponen Minyak Atsiri Bunga Kenangan (Cananga Odorata) dan Uji Efektivitas Aromaterapi Secara In Vivo", Repository Universitas Islam Negeri Ar-Raniry Banda Aceh, 2022.
[4] J. Budi, N. Damayanti, Y. Dhani and N. Dewi, "Ekstraksi dan Karakterisasi Minyak Atsiri Bunga Kenangan (Cananga Odorata) dan Aplikasinya Sebagai Penolak Nyamuk pada Lotion dan Parfum," Jurnal Kimia, 2018.
[5] E. A. Ahmed, H. A. Zahra, R. B. Ammar, M. E. Mohamed and H.-I. M. Ibrahim, "Beta-Caryophyllene Enhances the Anti-Tumor Activity of Cisplatin in Lung Cancer Cell Lines through Regulating Cell Cycle and Apoptosis Signaling Molecules," MDPI, vol. 27, 2022.
[6] V. H. S. Rodrigues, R. N. Almeida, R. M. Vargas and E. Cassel, "Vapor pressure and vapor-liquid equilibrium data for eugenol/caryophyllene binary system at low pressures by experimental and predictive methods," The Journal of Chemical Thermodynamics, vol. 168, 2022.
[7] K. Kuswandi, G. Wibawa, I. Hidayatulloh, C. Mahardhikawati and A. D. Pratiwi, "Ternary liquid-liquid equilibria for β-caryophyllene (1) + 1-propanol (2) + water (3) system at temperatures 303.15, 313.15, and 323.15 K," in IOP Conference Series: Materials Science and Engineering, 2018.
[8] I. Hidayatullah, A. Wiguno and K. Kuswandi, "Isobaric Vapor-Liquid Equilibria for Binary," IPTEK: The Journal of Engineering, vol. 5, 2019.
[9] H. A. Ekasanti, E. P. Hermawati, A. Wiguno and K. Kuswandi, "Prediksi Kesetimbangan Uap-Cair Sistem Biner Etanol + Eugenol dan 1-Propanol + Eugenol pada Berbagai Tekanan," Repository ITS, Surabaya, 2018.
[10] N. Nehemia and L. A. M. Wiyasa, "Kesetimbangan Cair-Cair Sistem Terner Eugenol + β – Caryophyllene + Larutan Naoh pada Temperatur 303,15 K dan pada Tekanan Atmosferik," Repository ITS, Surabaya, 2018.
[11] S. M. García-Abarrio, L. Haya, J. I. Pardo, J. S. Urieta and A. M. Mainar, "Isobaric VLE of the mixture {(±)-linalool + ethanol}: A case study for the distillation of absolute and volatile oils," The Journal of Chemical Thermodynamics, vol. 64, pp. 182-186, 2013.
[12] Lisdiana and Nuraini, "Potensi Eugenol Sebagai Agen Proteksi Kerusakan Struktur Paru Akibat Paparan Asap Rokok," Indonesian Journal of Mathematics and Natural Science, vol. 41, 2018.
[13] C. Ghelardi, N. Galeotti, L. Di Cesare Mannelli, G. Mazzanti and A. Bartolini, "Local anaesthetic activity of b-caryophyllene," Farmaco, 2001.
[14] R. Raguso, "More lessons from linalool: insights gained from a ubiquitous floral volatile," Current Opinion in Plant Biology, vol. 32, pp. 31-36, 2016.
[15] J. M. Smith, H. C. Van Ness, M. M. Abbott and M. T. Swihart, "Introduction to Chemical Engineering Thermodynamics Eighth Edition," 8th ed., New York: McGraw-Hill Education, 2018.
[16] J. R. Elliott and C. T. Lira, "Introductory Chemical Engineering Thermodynamics Second Edition, Prentice Hall," 2012.
[17] R. Wittig, J. Lohmann and J. Gmehling, "Vapor-liquid equilibria by UNIFAC Group Contribution. 6. Revision and Extension," Industrial & Engineering Chemistry Research, pp. 183-188, 2003.