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The University of Jordan

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Experiment Number (1)

Vapor-Liquid Equilibrium

Type of the report: short report

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Abstract:

The binary system of n-hexane (1) and toluene (2) will be used in this experiment, however the lab instructor may also assign another system. The activity coefficients are then derived from the reduced equilibrium data. The calculated activity coefficients are fitted to an appropriate model, such as the Margules, Van Laar, NRTL, UNIQUAC, and Wilson equations with two suffixes. The experimental data ~~must be~~ are compared to the UNIFAC method's projected activity coefficients as well as to the documented literature values for the system assigned to the group.

main results

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Results

Table 1: Properties of toluene and hexane

Temperature (°c)	p^{sat} hexane (mmHg)	p^{sat} toluene (mmHg)	ρ Toluene Vapor (Kg/m^3)	ρ Hexane Vapor (Kg/m^3)	ρ Toluene liquid (Kg/m3)	ρ Hexane liquid (Kg/m3)
106.8		681.067	2.643	2.472	785.2	574.9
98.1	1756.16	525.15	2.705	2.530	792.4	583.7
89.4	1392.795	399.03	2.770	2.591	801.1	593.2
83	1164.627	322.764	2.820	2.638	807.5	600
79.2	1043.52	283.34	2.850	2.666	811.3	603.4
70.4	800.49	206.83	2.923	2.734	819.8	613
67.7	735.59	187.06	2.946	2.756	822.4	615.7
64.5	664.1	165.65	2.974	2.782	825.5	619
61.6	594.23	145.15	3.000	2.806	828.2	621.9
57.4	524.92		3.038	2.842	832.2	627.9

Table 2: Vapor phase properties of hexane and toluene

Temperature (°c)	RI, Vapor	Volume-Hexane %	Ø Hexane vapor	Ø toluene vapor	Mole fraction of toluene (Y_T)	Mole fraction of hexane (Y_H)
106.8			34.862	34.859	1	0.0000
98.1	1.4912	0.0450	34.063	34.062	0.9550	0.0450
89.4	1.4745	0.1840	33.261	33.264	0.8160	0.1840
83	1.4271	0.5792	32.675	32.674	0.4208	0.5792
79.2	1.4249	0.5975	32.326	32.330	0.4025	0.5975
70.4	1.433	0.5300	31.519	31.522	0.4700	0.5300
67.7	1.4175	0.6590	31.271	31.272	0.3410	0.6590
64.5	1.403	0.7800	30.978	30.982	0.2200	0.7800
61.6	1.409	0.7300	30.712	30.713	0.2700	0.7300
57.4			30.327	30.327	0.0000	1.0000

Table 2: Liquid phase properties of hexane and toluene

Temperature (°c)	RI, liquid	Volume-Hexane %	Ø Hexane liquid	Ø toluene liquid	Mole fraction of toluene (X_T)	Mole fraction of hexane (X_H)
106.8			0.1499	0.1173	1.0000	0.0000
98.1	1.4951	0.0125	0.1476	0.1163	0.9901	0.0099
89.4	1.4875	0.0758	0.1453	0.1150	0.9390	0.0610
83	1.482	0.1216	0.1436	0.1141	0.9009	0.0991
79.2	1.468	0.2383	0.1428	0.1136	0.8008	0.1992
70.4	1.47	0.2216	0.1406	0.1124	0.8146	0.1854
67.7	1.4312	0.5383	0.1400	0.1120	0.5173	0.4827
64.5	1.4179	0.656	0.1392	0.1116	0.3954	0.6046
61.6	1.3922	0.87	0.1386	0.1113	0.1569	0.8431
57.4			0.1373	0.1107	0.0000	1.0000

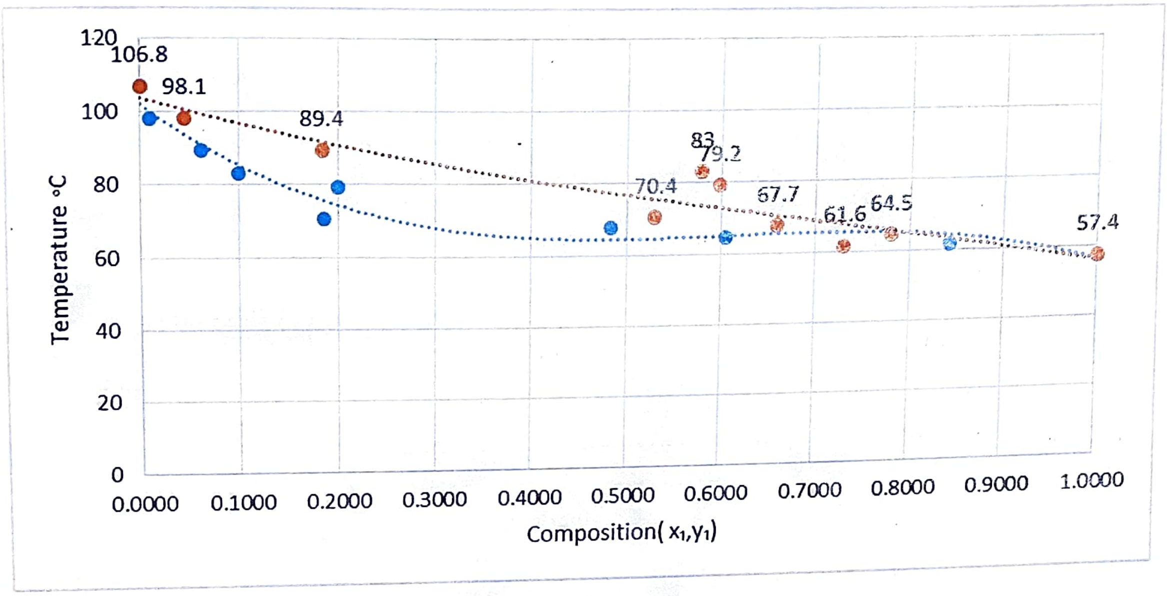


Figure 1: T-XY diagram

Table 4: Activity coefficient using modified Raoul's law

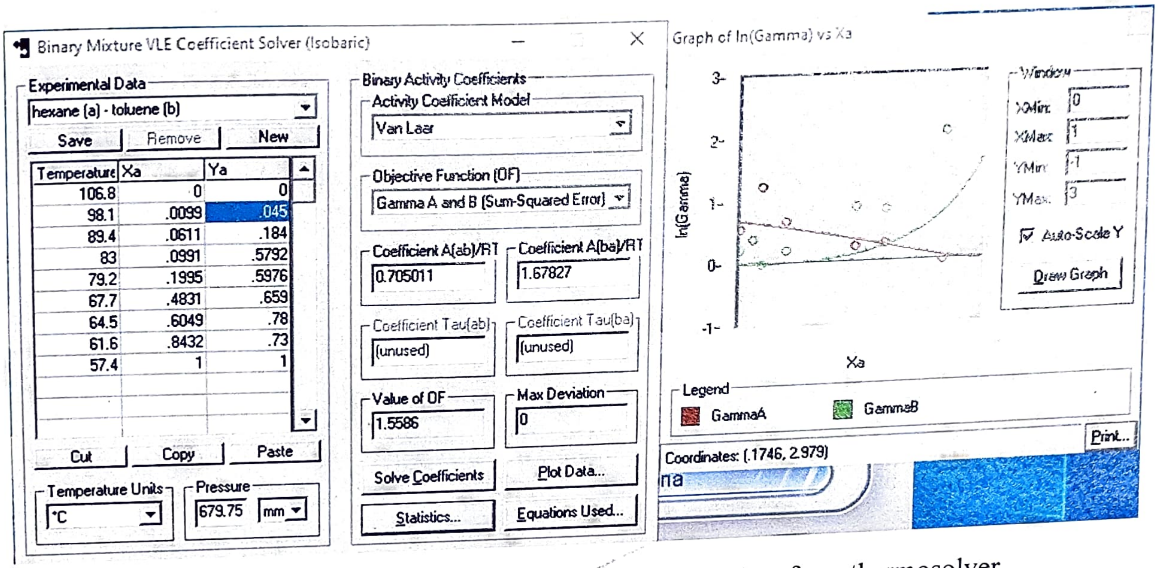
γ1	γ2
	0.9981
1.7645	1.2485
1.4729	1.4803
3.4120	0.9837
1.9538	1.2057
2.4276	1.8961
1.2615	2.3955
1.3206	2.2827
0.9905	8.0577
1.2950	

Table 5: Activity coefficients using van laar modeling

lnγ1	lnγ2	ln (γ1/γ2)	γ1	γ2
7.050E-01			2.0239	1.0000
6.991E-01	2.919E-05	0.1502	2.0120	1.0000
6.681E-01	1.183E-03	-0.0022	1.9505	1.0012
6.441E-01	3.273E-03	0.5401	1.9043	1.0033
5.779E-01	1.502E-02	0.2096	1.7823	1.0151
5.873E-01	1.278E-02	0.1073	1.7992	1.0129
3.638E-01	1.331E-01	-0.2785	1.4388	1.1424
2.614E-01	2.567E-01	-0.2377	1.2988	1.2926
6.646E-02	8.059E-01	-0.9104	1.0687	2.2388
	1.678E+00		1.0000	5.3563

Table 6: Activity coefficients using Two-suffix Margules Equation

lnγ1	lnγ2	γ1	γ2
0.7517	0.0000	2.1207	1.0000
0.7370	0.0001	2.0896	1.0001
0.6629	0.0028	1.9404	1.0028
0.6102	0.0074	1.8407	1.0074
0.4821	0.0298	1.6194	1.0303
0.4988	0.0258	1.6468	1.0262
0.2011	0.1752	1.2228	1.1915
0.1176	0.2748	1.1247	1.3162
0.0185	0.5343	1.0187	1.7063
0.0000	0.7517	1.0000	2.1207



Experimental Data: hexane (a) - toluene (b)

Temperature	Xa	Ya
106.8	0	0
98.1	.0099	.045
89.4	.0611	.184
83	.0991	.5792
79.2	.1995	.5976
67.7	.4831	.659
64.5	.6049	.78
61.6	.8432	.73
57.4	1	1

Temperature Units: °C

Pressure: 679.75 mm

Binary Activity Coefficients

Activity Coefficient Model: Van Laar

Objective Function (OF): Gamma A and B (Sum-Squared Error)

Coefficient A(ab)/RT: 0.705011

Coefficient A(ba)/RT: 1.67827

Coefficient Tau(ab): (unused)

Coefficient Tau(ba): (unused)

Value of OF: 1.5586

Max Deviation: 0

XMin: 0

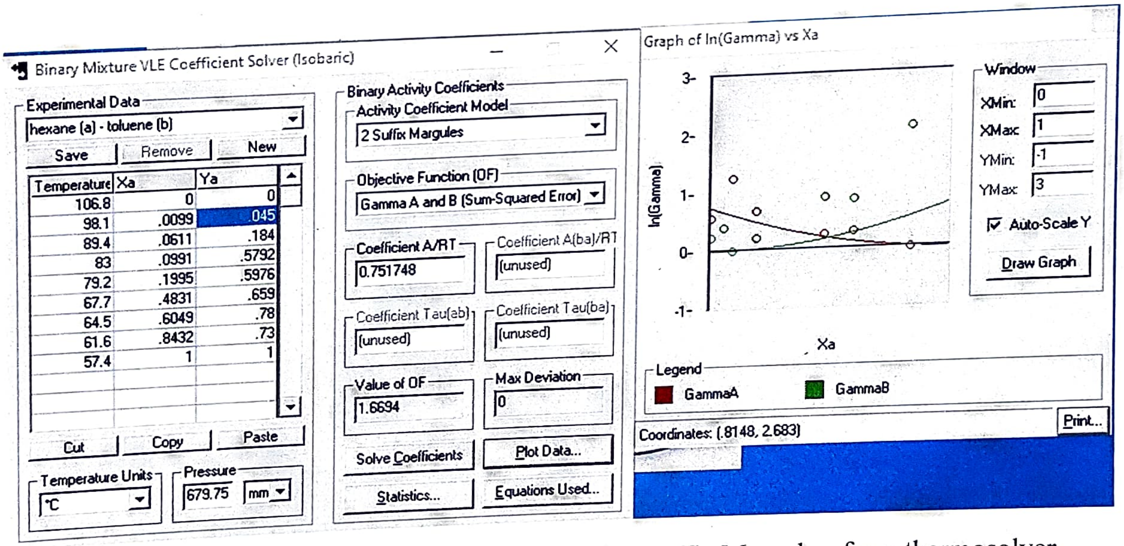
XMax: 1

YMin: -1

YMax: 3

Coordinates: (.1746, 2.979)

Figure 2: ln(gamma) verses X(hexane) in van laar from thermosolver



Experimental Data: hexane (a) - toluene (b)

Temperature	Xa	Ya
106.8	0	0
98.1	.0099	.045
89.4	.0611	.184
83	.0991	.5792
79.2	.1995	.5976
67.7	.4831	.659
64.5	.6049	.78
61.6	.8432	.73
57.4	1	1

Temperature Units: °C

Pressure: 679.75 mm

Binary Activity Coefficients

Activity Coefficient Model: 2 Suffix Margules

Objective Function (OF): Gamma A and B (Sum-Squared Error)

Coefficient A/RT: 0.751748

Coefficient A(ba)/RT: (unused)

Coefficient Tau(ab): (unused)

Coefficient Tau(ba): (unused)

Value of OF: 1.6694

Max Deviation: 0

XMin: 0

XMax: 1

YMin: -1

YMax: 3

Coordinates: (.8148, 2.683)

Figure 3: ln(gamma) verses X(hexane) in Two-suffix Margules from thermosolver

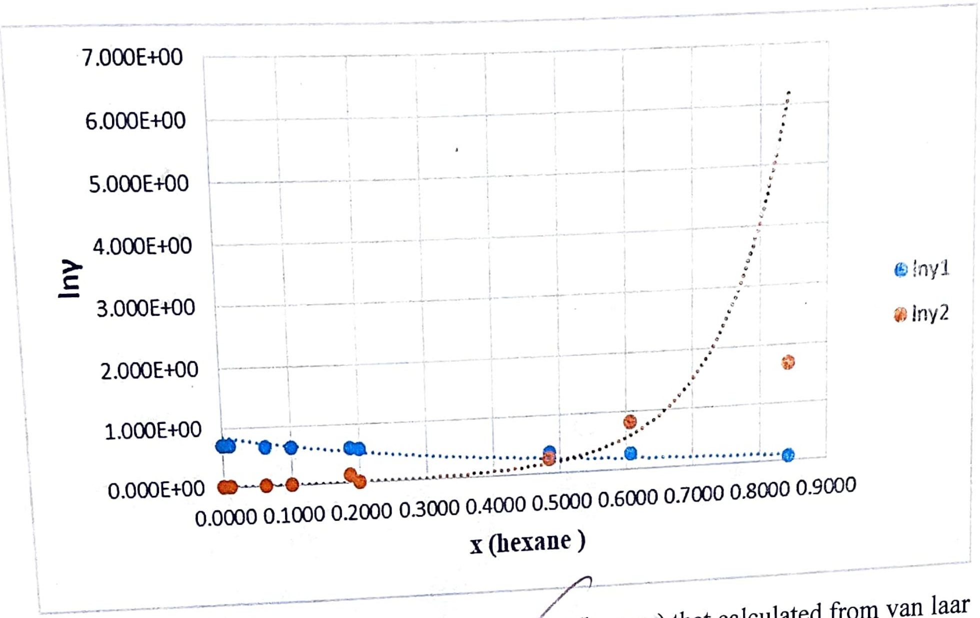


Figure 4: lnγ1(hexane) and lnγ2(toluene) verses X(hexane) that calculated from van laar

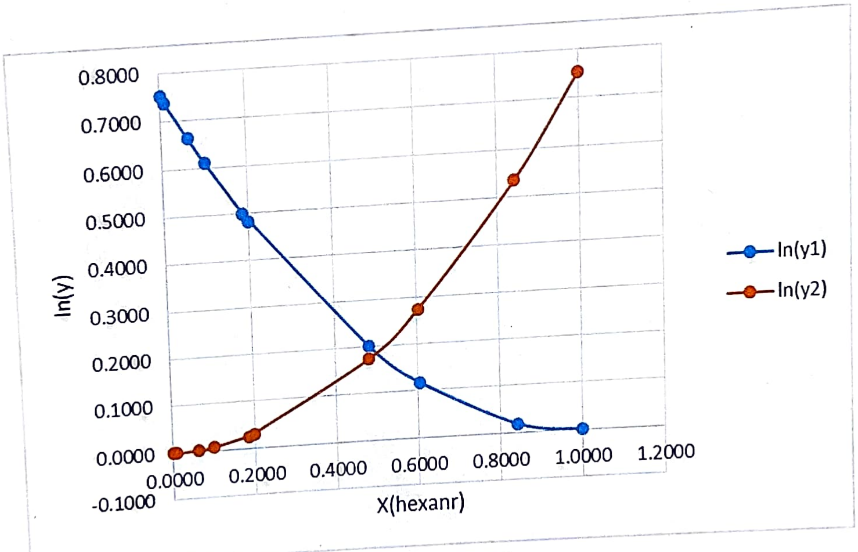


Figure 5: lnγ1(hexane) and lnγ2(toluene) verses X(hexane) that calculated from Two-suffix Margules

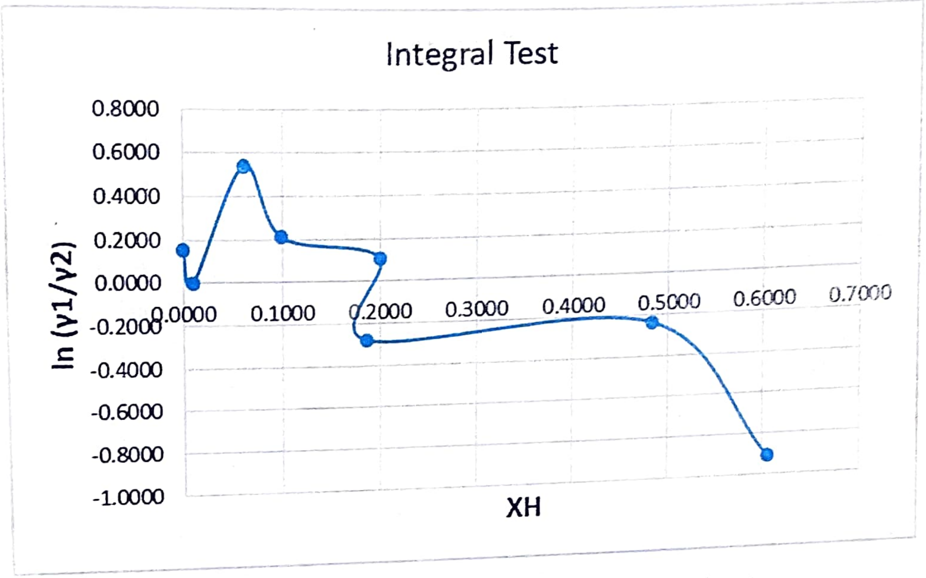


Figure 6: The consistency of data using integral test

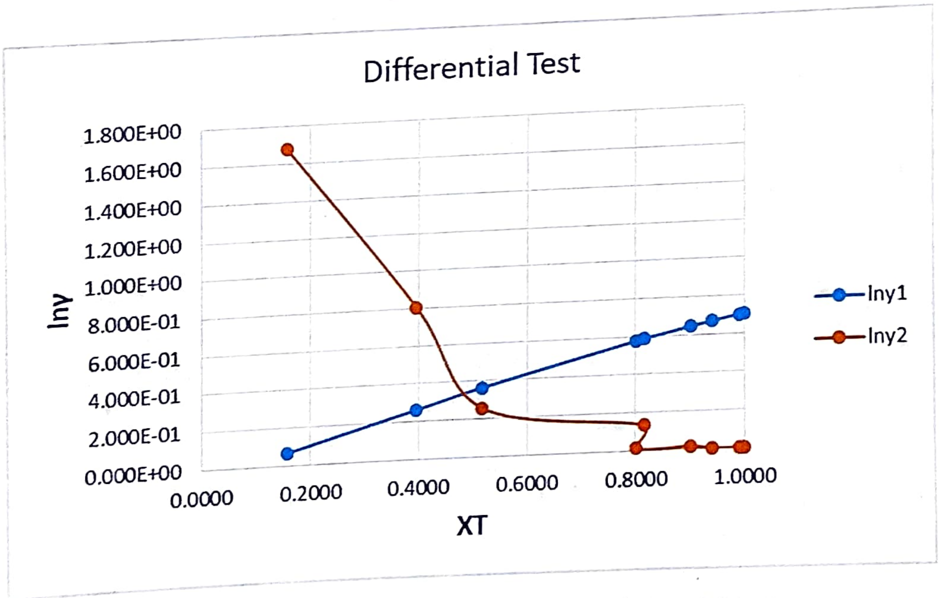


Figure 7: The consistency of data using differential test

Discussion

Vapor-liquid equilibrium, or VLE for short, is the state in which a liquid and its vapor (gas phase) are in equilibrium with one another. In this state, the rate of evaporation (liquid changing into vapor) and the rate of condensation (vapor changing into liquid) are equal on a molecular level, preventing any net (overall) vapor-liquid interconversion. Also, the vapor-liquid equilibrium which is used in thermodynamics and chemical engineering, defines how a chemical species is distributed between a liquid phase and a vapor phase, VLE data can be determined or approximated with the help of certain theories such as Raoult's Law, Dalton's Law, and Henry's Law.

Figure 1 shows the Txy-diagram, which was developed based on experimental equilibrium data for a non-ideal mixture of n-Hexane and Toluene, to illustrate the vapor-liquid equilibrium. The bubble and dew curves of the n-Hexane-toluene system are shown by the T Xy-diagram. The temperature in degrees Celsius is indicated by the Y-axis. Since the bubble curve is above the Raoult's Law line, the system exhibits a positive deviation from that law, as seen in Figure 1: The vapor pressure for the combination is higher than the vapor pressure for each pure component, which causes both components to escape from solution more readily, according to the TXY-diagram, which represents the bubble and Dew curves of the hexane-toluene system.

As it can be noticed in figure 1 there is an error that can be observed in the scattered data, because experimental measurements are inherently imprecise, experimental vapor-liquid equilibrium data always contain random error. The data may potentially include systematic or nonrandom errors brought on by poor experimental design, or it may be a personal error that cause the uncertainty, such as ignoring the bubbles on the in the tube of the device, ? furthermore when taking the samples for the refractive index reading, Part of the system's volume is lost.

According to the data in Table 1: final result of data acquired from the experiment, the boiling temperature of the combination is between the boiling temperatures of pure hexane and toluene, providing an indication of data trustworthiness.

In thermodynamics, an activity coefficient is a factor used to account for departures ? from ideal behavior in a mixture of chemical substances. For this experiment, three models are used to compute the activity coefficient: Modified-Raoult's law, van laar modeling and Two-suffix Margules Equation.

using a table (5) The ascending curve in figure (2), which depicts the activity coefficient for hexane, offers an excellent estimate of gamma I and gamma 2, as can be seen.

The graph demonstrates that when toluene is pure (x = 0), toluene's activity coefficient has the maximum value while hexane's activity coefficient is equal to zero. Hexane's gamma rises as its composition grows, reflecting the efficacy of each component in the combination. As we can see, as the composition of hexane increases, so does the activation of hexane in the solution; conversely, as toluene's activation in the solution decreases.

In order to statistically handle random error and make systematic error easier to identify, a thermodynamic consistency test is proposed.

Data consistency (The thermodynamic consistency test) It is a method of determining if a certain set of experimental VLE data fulfills the basic Gibbs—Duhcm equation.

Figure (6) illustrates the integral test for data consistency, the consistency from the area under the curve is found to be -0.04, which is acceptable.

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Conclusion

- Equilibrium data for the (n-hexane -toluene) binary system has been determined to be used later in any distillation calculation (bubble point, dew point and flash calculation) .
- Since the binary (n-hexane -toluene) system is not ideal due to difference in shape size and molecular interaction, the mixture does not obey Raoul's law and the activity coefficient is far from unity.
- The activity coefficient which is a measure of how much the real mixture differs from ideal mixture has been calculated using different methods (modified Raoul's law, van laar modeling, and Two-suffix Margules Equation)
- The positive deviation from Raoul's law shown in Txy diagram indicates that the vapor pressure for the mixture is higher than the vapor pressure for each component in pure form, which means that the mixture is more volatile that both components in pure form

References

♦The Engineering Toolbox (2022). Water - Specific Heat vs. Temperature. Retrieved November 4,2022, from

https://www.engineeringtoolbox.com/specific-heat-capacity-water-d_660.html

♦The Engineering Toolbox (2022). Water - Heat of Vaporization vs. Temperature. Retrieved November 4,2022, from

https://www.engineeringtoolbox.com/water-properties-d_1573.html

Appendix

Sample of calculation

*The following calculations are for the second row of each table.

1. Vapor phase of hexane and toluene (Table 2):

Let $\varnothing_{i,v} = \frac{\text{molecular wight (MW)}}{\text{density } (\rho_{i,v})}$ be the conversion factor or the vaper phase,

At T= 98.1 C.

Reflective index (RI) =1.4912 Refractive Index

V% of hexane =0.045

V% of toluene= 1- V% of hexane = 1-0.045 = 0.955

Mole fraction of hexane (Y_h) = $\frac{(\rho_{h,v} * V_h\%)/MW_h}{(\rho_{h,v} * V_h\%)/MW_h + (\rho_{t,v} * V_t\%)/MW_t} = \frac{(V_h\%/\varnothing_{h,v})}{(V_h\%/\varnothing_{h,v})+(V_t\%/\varnothing_{t,v})} = \frac{(0.045/34.063)}{(0.045/34.063)+(0.955/34.062)} = 0.0449$

Mole fraction of toluene (Y_t)= 1- Mole fraction of hexane (Y_h) = 0.9550

2. liquid phase properties of hexane and toluene (Table 3):

Let $\varnothing_{i,l} = \frac{\text{molecular wight (MW)}}{\text{density } (\rho_{i,l})}$ be the conversion factor or the liquid phase,

At T= 98.1 C.

Reflective index (RI) =1.4951

V% of hexane =0.0125

V% of toluene= 1- V% of hexane = 1-0.0125 = 0.9875

Mole fraction of hexane (X_h) = $\frac{(\rho_{h,l} * V_h\%)/MW_h}{(\rho_{h,l} * V_h\%)/MW_h + (\rho_{t,l} * V_t\%)/MW_t} = \frac{(V_h\%/\varnothing_{h,l})}{(V_h\%/\varnothing_{h,l})+(V_t\%/\varnothing_{t,l})} = \frac{(0.0125/0.1476)}{(0.0125/0.1476)+(0.9875/0.1163)} = 0.00987$

Mole fraction of toluene (X_t)= 1- Mole fraction of hexane (X_h) = 0.9901

3. Activity coefficient using modified Raoul's law (Table 4):

For hexane: $\gamma_1 = \frac{Y_1 * P_T}{X_1 * P_1^{sat}(T)} = \frac{0.0449*679.75}{0.00987*1756.16} = 1.7608$

For toluene: $\gamma_2 = \frac{Y_2*P_T}{X_2*P_2{}^{sat}(T)} = \frac{0.9550*679.75}{0.9901*525.15} = 1.2485$

*Partial pressure is founded using Antoine equation by thermosolver.

4. Activity coefficients using van laar modeling (Table 5):

*Values of vaan laar coefficients ($A_{12} = 0.705011$) and ($A_{21} = 1.67827$) are taken from Figure (2)

For hexane: $\ln\gamma_1 = \frac{A_{12}}{\left[1+\frac{A_{12}}{A_{21}}*\frac{x_1}{x_2}\right]^2} = \frac{0.705011}{\left[1+\frac{0.705011}{1.67827}*\frac{0.00987}{0.9901}\right]^2} = 0.6991$

$\gamma_1 = e^{0.6991} = 2.0119$

For toluene: $\ln\gamma_2 = \frac{A_{21}}{\left[1+\frac{A_{21}}{A_{12}}*\frac{x_2}{x_1}\right]^2} = \frac{1.67827}{\left[1+\frac{1.67827}{0.705011}*\frac{0.9901}{0.00987}\right]^2} = 2.9186 * 10^{-5}$

$\gamma_2 = e^{2.9186 * 10^{-5}} = 1.00003$

5. Activity coefficients using Two-suffix Margules Equation (Table (6)):

*Values of Two-suffix Margules coefficient (A_{12})=.751748 is taken from Figure (3)

For hexane: $\ln\gamma_1 = A_{12} * X_2^2 = 0.751748 * 0.9901^2 = 0.7369$

$\gamma_1 = e^{0.7369} = 2.0894$

For toluene: $\ln\gamma_2 = A_{12} * X_1^2 = 0.751748 * 0.00987^2 = 0.00007$

$\gamma_2 = e^{0.00007} = 1.00007$

سارة بجى نور ليله تالين.

Liquid-Liquid Equilibrium Data Sheet

Tie-Lines Determination:

Volume of water (ml)	Volume of Toluene (ml)	Volume of Acetone (ml)	RI of water layer	RI of Toluene layer
20	15	15		
① 18	20	13	1.8499	
② 26	17	8	1.3480	
20	25	5	~~1.3~~	
③ 19	29	3	1.3388	

Solubility curve

A. Water rich phase:

Volume of Acetone (ml)	Volume of water (ml)	Volume of Toluene (ml)
5	20	10.7 − 10.0 = 0.7
10	20	11.7 − 10.7 = 1.0
15	20	12.3 − 11.7 = 0.6
10	10	13.7 − 12.3 = 1.4
20	10	32.4 − 31.0 = 1.4
30	10	31.0 − 25.9 = 5.1

B. Organic solvent rich phase:

Volume of Acetone (ml)	Volume of Toluene (ml)	Volume of water (ml)
5	20	20.3 − 20.0 = 0.3
10	20	~~16.0 − 15.5 = 0.5~~ 16.3 − 16 = 0.3
15	20	16.3 − 16.3 = 0.3
10	10	16.6 − 10.3 = 0.2
20	10	17.3 − 16.8 = 0.5
30	10	20.0 − 17.3 = 2.7

20 → 20.3.

Instructor signature:

Date: