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FACULTY OF ENGINEERING AND TECHNOLOGY

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Chemical Engineering laboratory 2 (0915461)

Section no. (1)

Experiment Number (1)

Vaper - Liquid equilibrium

Short report

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1. ABSTRACT

In this experiment, obtained the equilibrium data for the binary system: n-hexane and toluene to generate a T- XY diagram and to calculate the activity coefficient. The activity coefficient was calculated by the Van Laar model. If the activity coefficient is far from unity, the mixture is not ideal and not obey the Raoult's low

At 61 C°, The composition of hexane in the liquid phase (vol%) = 0.842, and in the vapor phase (vol%) = 0.72

2. RESULTS

Table 1 : vaper phase properties of hexane and toluene

Run	Temperature	Refractometer,V	V-Hex %	ύ Hex vap m3/mole	ύ tol vap m3/mole	Y T	YH
1	106			33.91	33.80	1	0.00
2	97.4	1.4912	0.0450	33.08	32.96	0.95	0.04
3	88.5	1.4711	0.2130	32.21	32.10	0.78	0.21
4	82.7	1.429	0.5630	31.64	31.54	0.43	0.56
5	78.8	1.4275	0.5760	31.26	31.15	0.42	0.57
6	69.6	1.4727	0.1990	30.36	30.25	0.80	0.19
7	66.8	1.4175	0.6590	30.09	29.98	0.34	0.65
8	63.6	1.403	0.7800	29.76	29.66	0.22	0.77
9	61	1.409	0.7300	29.51	29.40	0.27	0.72
10	55.5			28.97	28.86	0	1.00

Table 2 : liquid phase properties of hexane and toluene

Run	Temperature	Refractometer,L	V-Hex %	ύ Hex liq m3/mole	ύ tol liq m3/mole	XH	XT
1	106			0.149	0.117	0.00	1.000
2	97.4	1.4901	0.054	0.147	0.116	0.043	0.957
3	88.5	1.4782	0.153	0.145	0.114	0.125	0.875
4	82.7	1.475	0.18	0.143	0.113	0.148	0.851
5	78.8	1.4721	0.204	0.142	0.113	0.169	0.830
6	69.6	1.4271	0.579	0.140	0.112	0.523	0.476
7	66.8	1.4185	0.651	0.139	0.111	0.598	0.401
8	63.6	1.4071	0.746	0.139	0.111	0.701	0.298
9	61	1.3922	0.87	0.138	0.110	0.842	0.157
10	55.5			0.137	0.1101	1.000	0.000

Table 3 : properties of toluene and hexane

Run	Temperature	psat(kpa) hexane	psat (kpa) tolune	ρ Tol Vap Kg/m^3	ρ Hex Vap Kg/m^32	ρ Tol liq Kg/m^3	ρ Hex liq Kg/m^3
1	106		88.674	2.726	2.541	785.5	574.9
2	97.4	230	68.496	2.795	2.605	794.3	584.5
3	88.5	181.2	51.644	2.87	2.675	803.3	594.1
4	82.7	153.97	42.581	2.921	2.723	809.1	600.3
5	78.8	137.52	37.241	2.957	2.756	813	604.4
6	69.6	104.09	26.763	3.045	2.838	822	613.8
7	66.8	95.302	23.382	3.073	2.864	824.7	616.6
8	63.6	85.979	21.327	3.106	2.895	827.8	619.9
9	61	78.945	19.271	3.133	2.92	830.4	622.5
10	55.5	65.561		3.192	2.974	835.6	627.9

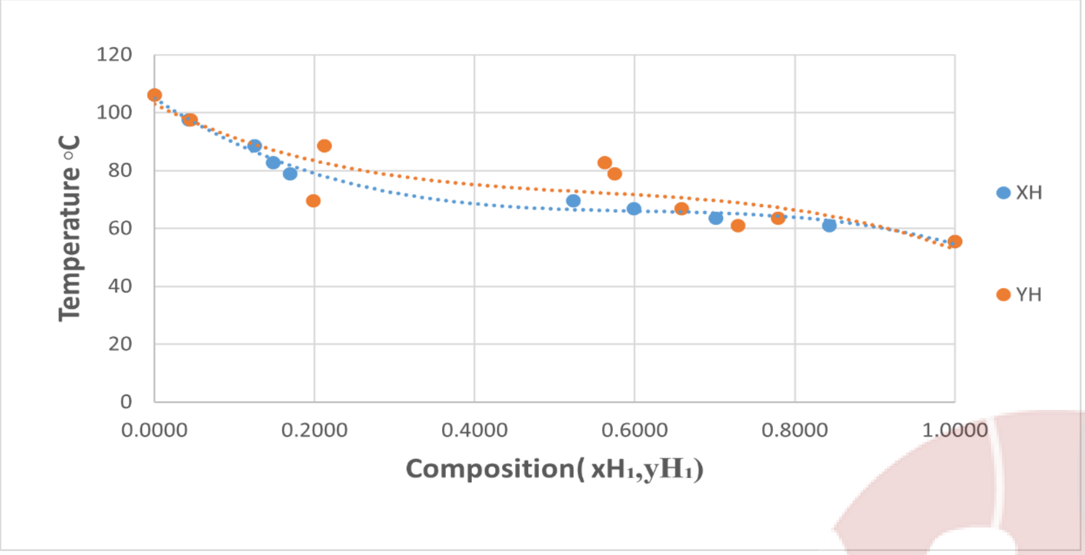
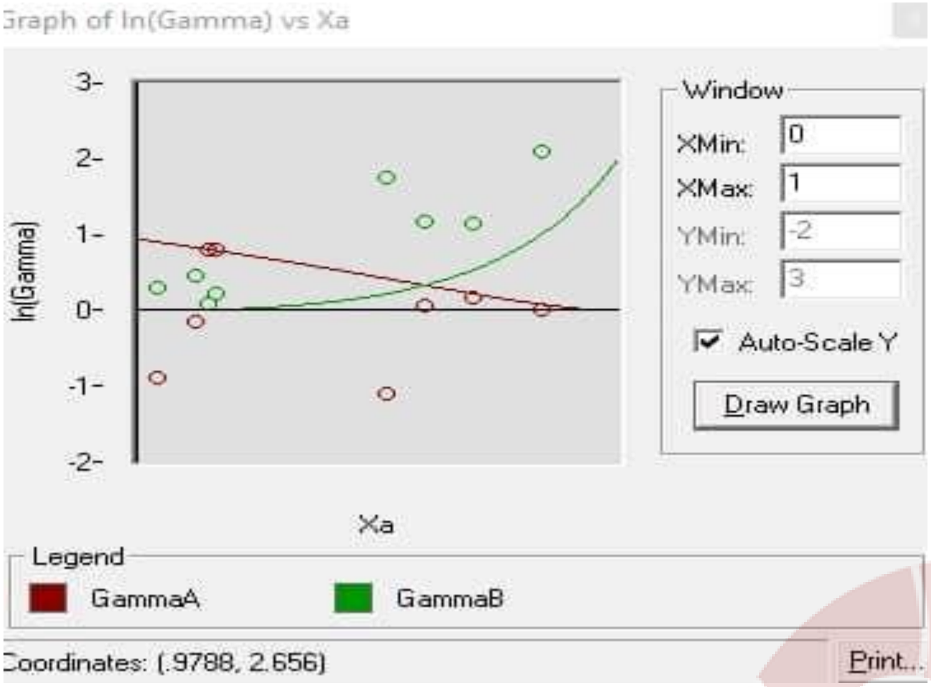


Figure 1 : T-XY DIAGRAM

Table 4 : Activity coefficient using modified raoult's law

Run	**γ1**	**γ2**
1		7.64
2	3.07	9.87
3	6.35	11.81
4	16.69	8.18
5	16.75	9.31
6	2.46	42.60
7	7.82	24.68
8	8.75	23.50
9	7.43	60.60
10	10.34	



XMin: 0

XMax: 1

YMin: -2

YMax: 3

☑ Auto-Scale Y

oordinates: (.9788, 2.656)

Figure 2 : Ln(gamma) vs Xa in van laar from thermosolver

Table 5 : Activity coefficients using van laar modeling

Run	ln γ1	lnγ2	ln (γ1/γ2)	γ1	γ2
1	0.941059			2.562	
2	0.903085419	0.000844823	-0.506730144	2.467	1.0008
3	0.827860684	0.007833377	-0.269081366	2.288	1.0078
4	0.805795817	0.011331328	0.309497994	2.238	1.0113
5	0.785744264	0.015121119	0.255188976	2.194	1.0152
6	0.413429068	0.231092369	-1.236780094	1.511	1.2599
7	0.329156966	0.339294524	-0.499141957	1.389	1.4039
8	0.215542501	0.552496611	-0.428644907	1.240	1.7375
9	0.077477087	1.033075759	-0.911466741	1.080	2.8096
10		2.03111			7.6225

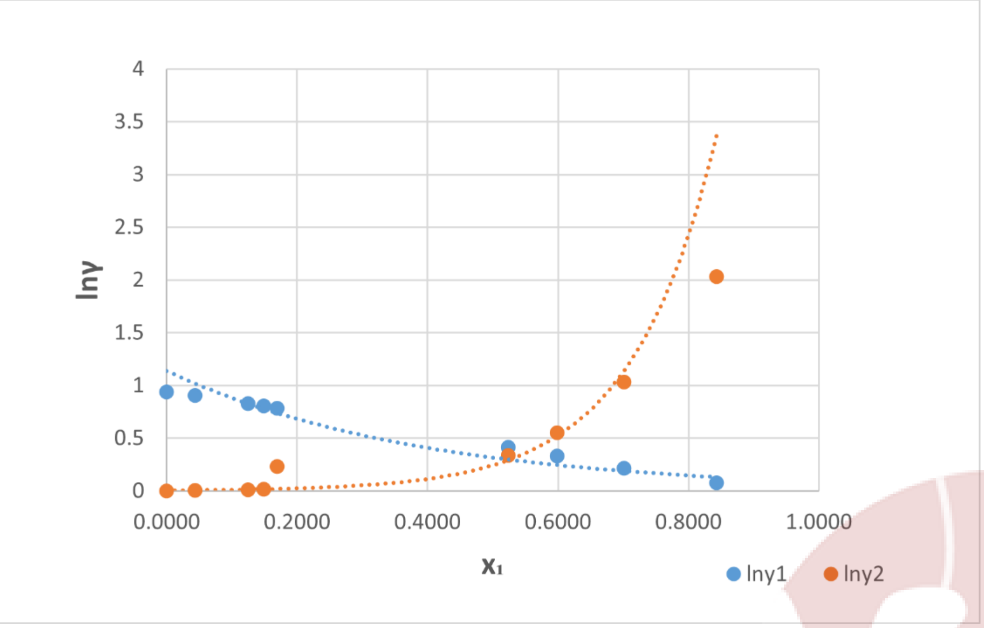


Figure 3 : lnγ1 and lnγ2 vs x1

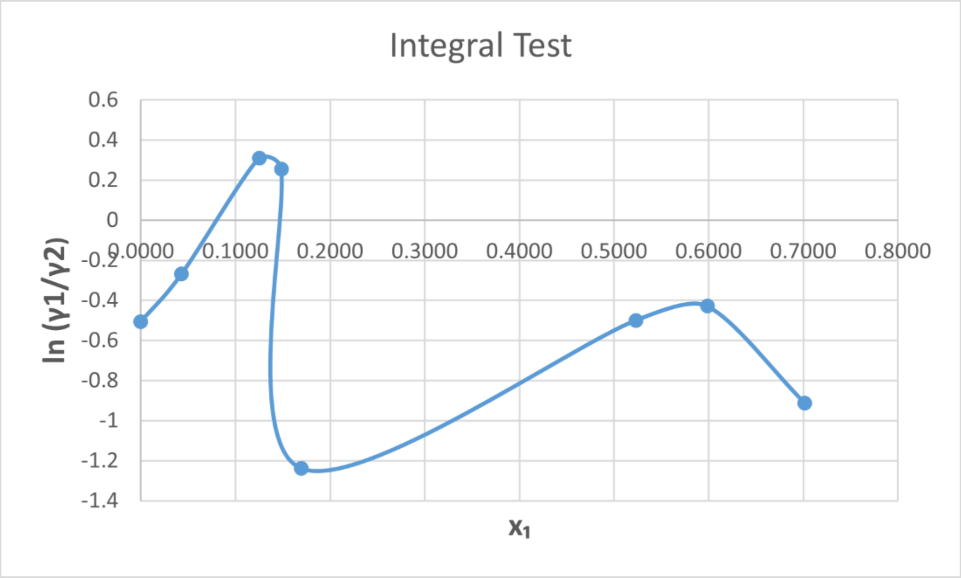


Figure 4 : integral test

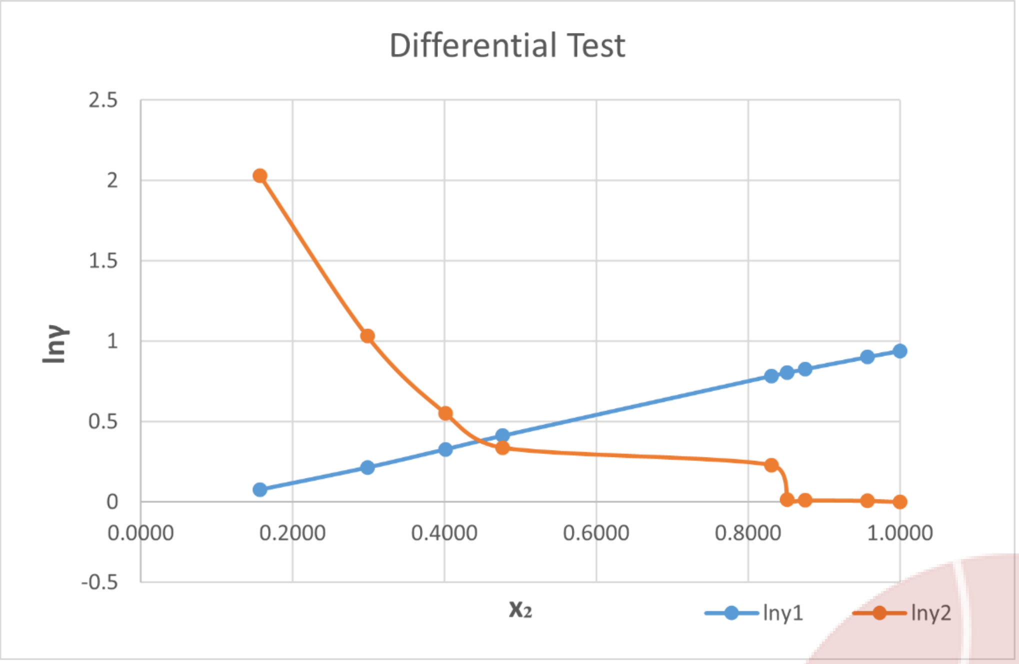


Figure 5 : Differential test

3. DISCUSSION

3.1 T-XY Diagram

Based on table (1) and table (2), this diagram was plotted to represent the vaper liquid equilibrium of mixture of hexane and toluene, at constant pressure.

The mixture is expected to be a non-ideal solution, because of the difference of hexane and toluene structural interaction.

Figure (1) shows the T-xy diagram (referenced to hexane), which consists of two curves, the first one (the upper curve) is a temperature of vaper of the mixture versus the composition of hexane, and it is called Dew curve, while the other is called the bubble curve (the lower curve) and represents the liquid temperature versus composition of hexane.

The region above dew curve is a superheated vaper region, while under the bubble curve is a subcooled liquid region, in between is the saturated vaper liquid region.

X-axis is the composition of component 1 (hexane here), Y-axis is the temperature of the system. Hence, we can also notice at x = 0 (pure toluene) the Temperature of the system is approximately 106 C and at x = 1 (pure hexane), the temperature is approximately 56 C.

3.2 Activity coefficient

In solutions, the activity coefficient is a measure of how much a solution differs from an ideal solution, The activity coefficient can be calculated from different methods, some of which are: The Modified Raoult's Law, Van Laar, and Two Suffix Margules, NRTL,Wilson, and UNIFAC.

Based on table (5) The figure (3) was plotted, as we can see, it gives a good approximation of gamma1 and gamma2, the increasing curve is the curve that represents the activity coefficient for Hexane.

The figure shows when we have a pure toluene (x = 0), the activity coefficient of toluene had the highest value while the activity coefficient of hexane equal zero, and gamma of hexane increases with increasing the composition of Hexane, that's because the effectiveness of the component in the mixture. As we can see if the composition of Hexane increase, the activation of Hexane in the solution will increase, hence, the activation of toluene in the solution will decrease, vice versa too.

3.3 Consistency of data (The thermodynamic consistency test)

It is a way to check whether or not a given set of experimental VLE data satisfies the fundamental Gibbs–Duhem equation.

Figure (4) shows the integral test for consistency of data, by using the area method, we got that the consistency is 0.0205 and this value less than 0.022, hence, our values are acceptable

4. CONCLUSIONS

- Vapor-liquid equilibrium information is useful in designing columns for distillation. distillation is used to separate the component from the liquid mixture by using selective boiling and condensation.

- Txy diagram shows the composition of phase in binary mixture depending on the temperature of the system at constant pressure

- The tie line indicates the equilibrium of liquid and vapor mixture at the same temperature and pressure.

- The activity coefficient function of temperature, pressure,and composition. It's used to account for the deviation from ideality. If it's equal one the mixture obey's raoult's law. if it's greater one implied that molecules have the strong repelling force and positive deviation from raoult's law.

- the integral test use to check the consistency of data, when plotting ln($\gamma1/\gamma2$) versus x1. the area under the curve should be equal zero. From figure (4), the area under the curve cannot be determined, the test is passed.

- It is recommended to take a reading of the boiling temperature directly from a thermocouple when it remains constant, because it is affected by room temperature

5. REFERENCES

1. Balzhiser, R. E.; Samules, M. R.; and Eliassen, J. D., ‘Chemical engineering thermodynamics, Prentice-Hall, Inc. 1972

2. Winnick, chemical engineering thermodynamics, john wiley and sons ny,1997.

3. Atkins and J. de Paula, Physical Chemistry (8th ed., W. H. Freeman 2006)

6. APPENDICES

6.1 Sample of calculation:

For a second run: -

I. For vaper phase

$$R.I_{vap} = 1.4912$$

$$vHex\% = 0.0450$$

$$\text{ύHex}_{\text{vap}} = \frac{MW}{\rho\ Hex\_Vap} = \left(\frac{0.08618}{2.605}\right) = \frac{33.91m^3}{mol}$$

$$\text{ύTol}_{\text{vap}} = \frac{MW}{\rho\ tol_{Vap}} = \left(\frac{0.09214}{2.795}\right) = 32.96\frac{m^3}{mol}$$

$$yH = \frac{\frac{V\_Hex\%}{\text{ύ Hex\_vap}}}{\frac{V\_Hex\%}{\text{ύHex\_vap}} + \frac{1 - V\_Hex\%}{\text{ύTol\_vap}}} = \frac{\frac{0.0450}{33.91\frac{m3}{mole}}}{\frac{0.0450}{33.91\frac{m3}{mole}} + \frac{1-0.045}{32.96\frac{m3}{mole}}} = 0.04$$

$$yT = \frac{\frac{V\_Hex\%}{\text{ύTol\_vap}}}{\frac{V\_Hex\%}{\text{ύHex\_vap}} + \frac{1 - V\_Hex\%}{\text{ύTol\_vap}}} = \frac{\frac{0.0450}{32.96\frac{m3}{mole}}}{\frac{0.0450}{33.91\frac{m3}{mole}} + \frac{1-0.045}{32.96\frac{m3}{mole}}} = 0.95$$

II. For liquid phase

$$R.I_{liq} = 1.4901$$

$$vHex\% = 0.054$$

$$\text{ύHex}_{\text{liq}} = \frac{MW}{\rho\ Hex_{liq}} = \frac{0.08618\frac{kg}{mole}}{584.5\frac{kg}{m3}} = 0.147\frac{m3}{mole}$$

$$\text{ύTol}_{\text{liq}} = \frac{MW}{\rho\ Tol_{liq}} = \frac{0.09214\,\frac{kg}{mole}}{794.3\,\frac{kg}{m3}} = 0.116\,\frac{m3}{mole}$$

$$xH = \frac{\frac{V\_Hex\%}{\text{ύHex\_liq}}}{\frac{V\_Hex\%}{\text{ύHex\_liq}} + \frac{1 - V\_Hex\%}{\text{ύTol\_liq}}} = \frac{\frac{0.054}{0.147\,\frac{m3}{mole}}}{\frac{0.054}{0.147\,\frac{m3}{mole}} + \frac{1 - 0.054}{0.116\,\frac{m3}{mole}}} = 0.043$$

$$xT = \frac{\frac{V\_Hex\%}{\text{ύTol\_liq}}}{\frac{V\_Hex\%}{\text{ύHex\_liq}} + \frac{1 - V\_Hex\%}{\text{ύTol\_liq}}} = \frac{\frac{0.054}{0.116\,\frac{m3}{mole}}}{\frac{0.054}{0.147\,\frac{m3}{mole}} + \frac{1 - 0.054}{0.116\,\frac{m3}{mole}}} = 0.957$$

III. Activity coefficient using modified raoult’s law

$$\gamma_1 = \frac{yH * pT}{xH * pH^{sat}\,(T)} = \frac{0.04 * 678}{0.043 * 230} = 3.075$$

$$\gamma_2 = \frac{yT * pT}{xT * pT^{sat}\,(T)} = \frac{0.95 * 678}{0.957 * 68.496} = 9.87$$

IV. Activity coefficient using van laar model

$$\ln(\gamma_1) = \frac{A}{\left[1+\frac{x1}{x2}*\frac{A}{B}\right]^2} = \frac{0.941059}{[1+\frac{0.941059}{2.0311}*\frac{0.043}{0.957}]} = 0.4105$$

$$\ln(\gamma_2) = \frac{B}{\left[1+\frac{x2}{x1}*\frac{B}{A}\right]^2} = \frac{2.0311}{[1+\frac{2.0311}{0.941059}*\frac{0.957}{0.043}]} = 0.00084$$

$$ln\ (\gamma 1/\gamma 2) = -0.269081366$$