Isobaric VLE Data of Binary System Using Modified UNIFAC Method

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Abstract- *2-Propanol manufacturing, with higher purity (<99%) can be achieved by various pathways. Among which hydrogenation of acetone by strong reducing agent such as (LiAlH4) with a suitable solvent (THF) has been opted for this paper. Eco amicable solvents are the rapidly emerging concept in Green Chemistry. Therefore this conventional solvent (THF) can be replaced by a green solvent (2-MeTHF) due to its better characteristics features than THF. Therefore VLE data of 2-Propanol and 2-MeTHF need to be obtained for the separation of both components. The Modified UNIFAC Dortmund method has been applied, which is one of advance model of group contribution method.*

I. INTRODUCTION

"Eco amicable solvents" are the rapidly emerging concept in Green Chemistry. Scope of 2-MeTHF as a solvent is very broad. As a matter of fact, in this paper 2-MeTHF replaces the conventional solvent in the manufacturing of isopropanol6. To achieve the higher purity of isopropanol as a final product (<99.5%), necessity of separating 2-Propanol and 2-MeTHF arises. Therefore to fulfil this, vapour liquid equilibrium data is generated. Determination of this data is very crucial for designing of any separation processes like distillation, extraction etc. Various thermodynamic methods has been studied and among which one method, Modified UNIFAC Dortmund has been applied for the above cited components constituent.

II. THERMODYNAMIC MODEL

Prediction of VLE data using group contribution method is one of the popular and reliable approaches. Group Contribution methods involves following models11:

(i) ASOG
(ii) UNIFAC
(iii) Modified UNIFAC by (Lyngby)
(iv) Modified UNIFAC by Dortmund
(v) PSRK
(vi) VTPR

Among above cited methods Modified UNIFAC Dortmund has been applied because of its unique characteristics such as:(a) Modified combinatorial (b) More temperature dependent parameter (c) Wide range of applicability (d) Infinite dilute solutions (e) For strongly asymmetric systems10.

III. EXPERIMENTATION

Different groups were identified and data were opted from the literature11. Table No.1 briefs the group identification for modified UNIFAC Dortmund.

The binary interaction parameters were obtained from literature. They are shown in Table No.2. The activity coefficients (γ_1 and γ_2) were calculated at different temperature range. In TableNo.3.The activity coefficient variations with temperature and compositions have been showed.

Table No. 1 Group Identification

Group Identification					
Name	Main No.	Sec. No.	$v_i^{(i)}$	R_i	Q_i
CH_3	1	1	1	0.6325	1.0608
cy-CH_2O	43	27	1	1.7023	1.8784
CH_2	42	78	2	0.7136	0.8635
CH	42	79	1	0.3479	0.1071
CH_3	1	1	2	0.6325	1.0608
CH	1	3	1	0.6325	0.3554
OH	5	81	1	1.063	0.8663

Table No.2 binary interaction parameter for 2-methf and 2-propanol for modified UNIFAC

	a_{nm}	b_{nm}	c_{nm}	
$a_{1,43}$	79.507	0.7089	-0.002098	68.0330667
$a_{43,1}$	186.71	-1.3546	0.002402	7.97355871
$a_{1,42}$	-680.95	4.0194	-0.006878	-119.47285
$a_{42,1}$	1020.8	-6.0746	0.01015	141.652603
$a_{43,42}$	20.834	-0.3472	0	-101.85603
$a_{42,43}$	242.49	- 0.03832	0	228.948866
$a_{1,5}$	2777	-4.674	0.001551	1319.02292
$a_{5,1}$	1606	-4.746	0.000918	43.5498914
$a_{43,5}$	-238.36	5	-0.008186	506.301342
$a_{5,43}$	401.89	-0.4363	-0.002004	-2.5253287
$a_{42,5}$	3246	-4.937	-0.001143	1358.6861
$a_{5,42}$	3856	-17.97	0.02083	106.990981

IV. RESULT AND DISCUSSION

The result were obtained and presented in the form of graphs. The T-x-y data and ln $\gamma_1$and ln γ_2 versus x_1 were shown graphically in Fig No.5 and Fig No.6 respectively.

The predicted data were applied for consistency test. There are various consistency test available in literature among which Herington's Area Test was opted[13], which is tabulated below.

Table No.3 Consistency Test

D	J	D-J	METHOD
20.70	0.87	19.83	MODIFIED UNIFAC

Table No.4 Predicted VLE data

Sr. No	T(K)	$x_{1,mod.\ UNI.\ Dor.}$	$y_{1,\ mod.\ UNI.\ Dor.}$	Υ_1	Υ_2
1	353.37	1.0000	1.0000	1.0000	2.2796
2	352.00	0.9500	0.9092	1.0024	2.0957
3	351.50	0.9000	0.8399	1.0094	1.9289
4	350.06	0.8500	0.7837	1.0210	1.7931
5	349.54	0.8000	0.7371	1.0371	1.6700
6	349.18	0.7500	0.6969	1.0576	1.5635
7	348.95	0.7000	0.6610	1.0826	1.4715
8	348.82	0.6500	0.6279	1.1122	1.3919
9	348.77	0.6000	0.5966	1.1466	1.3230
10	348.79	0.5500	0.5662	1.1862	1.2635
11	348.88	0.5000	0.5359	1.2314	1.2122
12	349.04	0.4500	0.5048	1.2825	1.1680
13	349.27	0.4000	0.4723	1.3401	1.1301
14	349.58	0.3500	0.4374	1.4049	1.0980
15	349.97	0.3000	0.3992	1.4776	1.0710
16	350.47	0.2500	0.3565	1.5592	1.0487
17	351.09	0.2000	0.3078	1.6505	1.0309
18	351.86	0.1500	0.2510	1.7526	1.0173
19	352.81	0.1000	0.1835	1.8667	1.0076
20	353.98	0.0500	0.1016	1.9938	1.0019
21	355.42	0.0000	0.0000	2.1348	1.0000

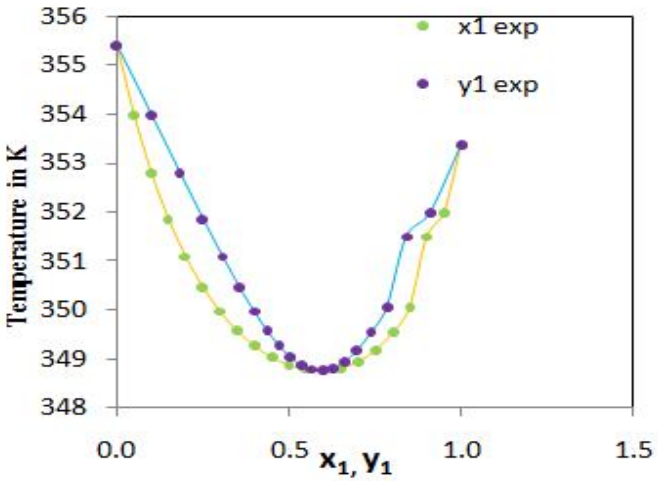

Figure No.5 T-x-y data

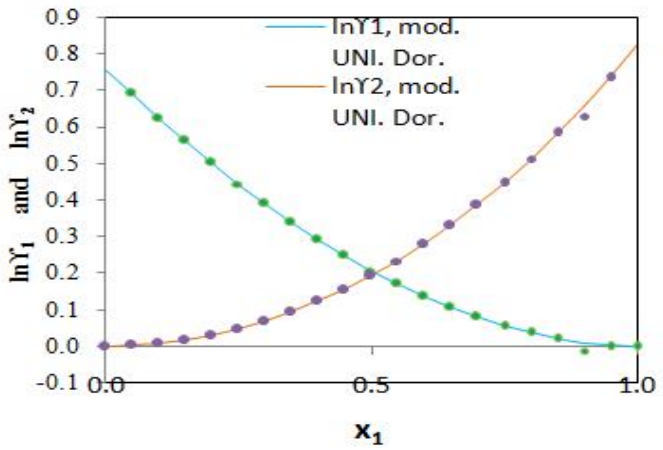

Figure No.6 ln γ_1 and lnγ_2 v/s x_1

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V. CONCLUSION

For the high purity production of isopropanol, hydro genatation of acetone was done accompanied by a green solvent -2 MeTHF. For the separation of final product and solvent distillation or extraction is necessary. Therefore VLE data are generated of binary mixture using Modified UNIFAC method. The predicted data were applied for consistency test. Among various consistency tests Herington's Area Test was opted. The data were found to be not consistent.

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