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Vapor-Liquid Equilibrium Data Prediction by Advanced Group Contribution Methods for a Binary System of Cyclopentyl Methyl Ether and Cyclopentanol at Atmospheric Pressure

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Abstract *-- The isobaric vapor-liquid equilibrium data predictions for the binary system of cyclopentyl methyl ether and cyclopentanol were obtained using UNIFAC and modified UNIFAC Dortmund method. Group identification was done by using artist free software with Dortmund Data Bank. The interaction parameters in the UNIFAC and modified UNIFAC Dortmund method, for the ether group (-*CH_3O*) and alcohol (-OH), were used to predict VLE data. Thermodynamic consistency of the predicted VLE data had been checked by the Herington method. The predicted data were correlated with Van Laar, Wilson and NRTL activity coefficient models. The binary interaction parameters of models had been obtained by regression. The predicted VLE data of UNIFAC method were fitted much more accurately than that of modified UNIFAC Dortmund method by these activity coefficient models Van Laar, Wilson and NRTL.*

Keywords *-- vapor-liquid equilibrium, cyclopentyl methyl ether, cyclopentanol, UNIFAC method, modified UNIFAC Dortmund method*

I. INTRODUCTION

Conventional solvents used in industries create many problems related to environment, health and safety. Green solvents provide an attractive alternate to the conventional solvents. Cyclopentyl Methyl Ether (CPME) is one of the green solvents [1] which has high boiling point (379.15 K) and preferable characteristics such as low peroxide formation, high hydrophobicity, relative stability under acidic and basic conditions, high boiling point and low melting point, low heat of vaporization, narrow explosion area and low solubility of salts. Due to such characteristics CPME is preferred as an alternative to other ethereal solvents such as tetrahydrofuran, 2-methyl tetrahydrofuran, dioxane (carcinogenic), and 1,2-dimethoxyethane, which are hazardous to human health and environment [2]. The synthesis of CPME is carried out by methylation process using different methylating agents with four different routes such as methylation of cyclopentene by methanol, methylation of cyclopentanol (CPL) by dimethyl sulphate, methylation of CPL by trimethyl phosphate and methylation of CPL by methyl iodide [3].

In some of these synthesis routes, unreacted CPL may remain present in CPME product at the end of the process. In which case, both compounds have to be separated by distillation. Similar case has been reported in the patent EP1405840B1 [4] where there is a requirement of separation of these two compounds from their mixture. But unfortunately, VLE data for the binary system of CPME and CPL does not exist in the literature. Thus, determination of VLE data of this system becomes necessary. Numerical simulations using group contribution methods provide an alternative to experimental measurement of VLE data. The aim of this paper is to predict VLE data for CPME with CPL at atmospheric pressure.

II. ADVANCED GROUP CONTRIBUTION METHODS

Prediction of thermodynamic properties is important in chemical process and product design. When experimental binary data is available, phase equilibrium behaviour is easily modelled with the help of cubic equation of state (using fugacity coefficient data) and local composition g^E models (using activity coefficient data). When little or no experimental data are available, group contribution (GC) methods can be employed to predict the phase equilibrium under specified conditions of temperature and composition [5, 6].

Various GC methods are available for prediction of VLE data. Some examples of GC methods which have been developed for the estimation of properties of pure compounds include those published by Joback and Reid [7], Lydersen [8], Ambrose [9], Constantinou and Gani [10] and Marrero and Gani [11, 12]. On the other hand, many GC based property models have also been developed to predict properties of mixtures mainly to predict the non-ideality of the liquid phase using activity coefficients which includes ASOG [13, 14], Original UNIFAC [15], Modified UNIFAC (Dortmund) [16] and PSRK [17]. In the present work, well known and established group-contribution methods such as

UNIFAC method and modified UNIFAC Dortmund method are used to predict liquid phase activity coefficients for binary mixtures of CPME and CPL.

2.1. UNIFAC and modified UNIFAC Dortmund methods

The general UNIFAC equation is as follows with the combinatorial and residual contributions:

$$\ln \gamma_i = \ln \gamma_{i(\text{combinatorial})} + \ln \gamma_{i(\text{residual})} \qquad \ldots(1)$$

Where,

$$\ln \gamma_{i(\text{combinatorial})} = 1 - V_i + \ln V_i - 5q_i \left(1 - \frac{V_i}{F_i} + \ln\left(\frac{V_i}{F_i}\right)\right) \qquad \ldots(2)$$

Where, $\nu_k^{(i)}$, always an integer, is the number of groups of type k in molecule i. Group parameters R_k and Q_k are obtained from the van der Waals group volume and surface areas V_{wk} and A_{wk}, given by Bondi (1968). All other parameters are calculated as following:

$$V_i = \frac{r_i}{\sum_j x_j r_j} \qquad \ldots(3)$$

$$r_i = \sum \nu_k^{(i)} R_k \qquad \ldots(4)$$

$$F_i = \frac{q_i}{\sum_j x_j q_j} \qquad \ldots(5)$$

$$q_i = \sum \nu_k^{(i)} Q_k \qquad \ldots(6)$$

In residual part

$$\ln \gamma_{i(\text{residual})} = \sum_k \nu_k^{(i)} \left(\ln \Gamma_k - \ln \Gamma_k^{(i)}\right) \qquad \ldots(7)$$

Where,

$$\ln \Gamma_k = Q_k \left(1 - \ln\left(\sum_m \theta_m \Psi_{mk}\right) - \sum_m \frac{\theta_m \Psi_{km}}{\sum_n \theta_n \Psi_{nm}}\right) \qquad \ldots(8)$$

Where, the group area fraction θ_m and group mole fraction X_m are given by the following equations:

$$\theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n} \qquad \ldots(9)$$

$$X_m = \frac{\sum_j \nu_m^{(j)} x_j}{\sum_j \sum_n \nu_n^{(j)} x_j} \qquad \ldots(10)$$

Where, the group-interaction parameter Ψ_{nm} is given by the following equation:

$$\Psi_{nm} = \exp\left(-\frac{U_{mn} - U_{nn}}{RT}\right) = \exp\left(-\frac{a_{nm}}{T}\right) \qquad \ldots(11)$$

Where, U_{mn} is a measure of the energy of interaction between group m and n. Note that a_{mn} has units of Kelvin and $a_{mn} \neq a_{nm}$. In the Original UNIFAC model, the interaction parameters are considered to be independent of temperature. Therefore, quantitative predictions of excess enthalpies, H^E could not be obtained. In order to improve this and other things, the modified UNIFAC Dortmund was developed. For both models, modifications have been done in the combinatorial and the residual part of UNIFAC. The Dortmund version, Eq. (2) and Eq. (3) are replaced by Eq. (12) and Eq. (13) as described below.

$$\ln \gamma_{i(\text{combinatorial})} = 1 - V_i' + \ln V_i' - 5q_i \left(1 - \frac{V_i}{F_i} + \ln\left(\frac{V_i}{F_i}\right)\right) \qquad \ldots(12)$$

$$V_i' = \frac{r_i^{3/4}}{\sum_j x_j r_j^{3/4}} \quad \ldots(13)$$

$$\Psi_{nm} = \exp\left(- \frac{a_{nm} + b_{nm}T + c_{nm}T^2}{T} \right) \quad \ldots(14)$$

In addition to that, in the residual part, temperature dependent interaction parameters were used where they have a logarithmic and quadratic dependency towards temperature for Dortmund versions. Due to this temperature dependency, the predictions of VLE, H^E and γ_i^∞ have improved especially for the Dortmund version since it is based on more experimental data. These modified UNIFAC models can also extrapolate reliably the predictions of VLE at higher temperatures compared to Original UNIFAC.

2.2. Group identification

Group identification for UNIFAC method and modified UNIFAC Dortmund is done using the data given in Poling BE (2012) [18] and these groups are presented in Table 1 and Table 2 respectively, also compared with Dortmund Data Bank by using artist free software.

Table 1. Group identification for CPME and CPL for UNIFAC method

Molecule (i)	Name	M^*	S^*	$v_k^{(i)}$	R_k	Q_k
CPME (1)	**CH_2**	1	2	4	0.6744	0.5400
	CH	1	3	1	0.4469	0.2280
	CH_3O	13	24	1	1.1450	1.0880
CPL (2)	**CH_2**	1	2	4	0.6744	0.5400
	CH	1	3	1	0.4469	0.2280
	OH	5	14	1	1.0000	1.2000

Table 2. Group identification for CPME and CPL for modified UNIFAC Dortmund method

Molecule (i)	Name	M^*	S^*	$v_k^{(i)}$	R_k	Q_k
CPME (1)	**c-CH_2**	42	78	4	0.7136	0.8635
	c-CH	42	79	1	0.3479	0.1071
	CH_3O	13	24	1	1.1434	1.6022
CPL (2)	**c-CH_2**	42	78	4	0.7136	0.8635
	c-CH	42	79	1	0.3479	0.1071
	OH	5	81	1	1.0630	0.8663

* M=main group number, S=secondary group number

2.3. Binary interaction parameter (BIP)

Binary interaction parameters (a_{mn}) for UNIFAC method are taken from the literature [18] and (a_{mn}, b_{mn}, and c_{mn}) for modified UNIFAC Dortmund method are taken from the literature [19, 20, 21], which are presented in Table 3 and Table 4 respectively.

Table 3. BIPs for CPME and CPL for UNIFAC method

Group	CH_2	CH	OH	CH_3O
CH_2	0.0	0.0	986.5	251.5
CH	0.0	0.0	986.5	251.5
OH	156.4	156.4	0.0	28.06
CH_3O	83.36	83.36	237.7	0.0

Table 4. BIPs for CPME and CPL for modified UNIFAC Dortmund method

Group		n	m	a_{nm}	b_{nm}	c_{nm}
OH	**CH_3O**	5	13	1102	-7.176	0.009698
OH	**c-CH_2** **c-CH**	5	42	3856	-17.97	0.02083

CH_3O	**c-CH_2** **c-CH**	13	42	251.4	-1.021	0.0000

Group		**m**	**n**	**a_{mn}**	**b_{mn}**	**c_{mn}**
CH_3O	**OH**	13	5	1631	-7.362	0.01176
c-CH_2 **c-CH**	**OH**	42	5	3246	-4.937	-0.00114
c-CH_2 **c-CH**	**CH_3O**	42	13	-86.6	0.9724	0.0000

2.4. Calculation of VLE data using group contribution methods

The VLE data for binary system CPME and CPL are calculated through a spread sheet prepared in Microsoft Excel, in which temperature T and x_1 are given as input and γ_1 and γ_2 are calculated using group contribution methods as described in the precious sections. Now using Antoine Eq. (17), p_1^{sat} and p_2^{sat} are calculated. Then total pressure P is found out and correct temperature T is found out by regression using Eq. (18). The generated data are presented in Table 5 and Table 6 for UNIFAC and UNIFAC Dortmund method.

Table 5. VLE data for CPME and CPL binary system at atmospheric pressure by UNIFAC method

T/K	x_1	y_1	γ_1	γ_2
379.15	1.0000	1.0000	1.0000	2.0940
379.87	0.9500	0.9713	1.0020	1.9010
380.62	0.9000	0.9457	1.0090	1.7440
381.41	0.8500	0.9221	1.0200	1.6150
382.22	0.8000	0.8999	1.0350	1.5080
383.07	0.7500	0.8782	1.0530	1.4190
383.97	0.7000	0.8566	1.0740	1.3440
384.93	0.6500	0.8346	1.0990	1.2810
385.96	0.6000	0.8115	1.1260	1.2270
387.07	0.5500	0.7868	1.1570	1.1820
388.30	0.5000	0.7598	1.1910	1.1440
389.65	0.4500	0.7299	1.2270	1.1120
391.15	0.4000	0.6959	1.2670	1.0850
392.83	0.3500	0.6567	1.3090	1.0630
394.73	0.3000	0.6107	1.3540	1.0450
396.89	0.2500	0.5559	1.4020	1.0300
399.34	0.2000	0.4893	1.4530	1.0190
402.16	0.1500	0.4071	1.5060	1.0100
405.41	0.1000	0.3038	1.5610	1.0040
409.15	0.0500	0.1717	1.6190	1.0010
413.49	0.0000	0.0000	1.6780	1.0000

Table 6. VLE data for CPME and CPL binary system at atmospheric pressure by modified UNIFAC Dortmund method

T/K	x_1	y_1	γ_1	γ_2
379.15	1.0000	1.0000	1.0000	2.1650
379.83	0.9500	0.9703	1.0020	1.9710
380.55	0.9000	0.9437	1.0090	1.8110
381.31	0.8500	0.9194	1.0200	1.6780
382.09	0.8000	0.8966	1.0350	1.5660
382.91	0.7500	0.8745	1.0530	1.4720
383.76	0.7000	0.8528	1.0750	1.3910
384.67	0.6500	0.8308	1.1010	1.3220
385.65	0.6000	0.8081	1.1310	1.2640
386.70	0.5500	0.7842	1.1640	1.2140
387.85	0.5000	0.7583	1.2020	1.1710
389.12	0.4500	0.7298	1.2440	1.1340
390.54	0.4000	0.6977	1.2900	1.1030
392.13	0.3500	0.6609	1.3410	1.0770

393.95	0.3000	0.6176	1.3960	1.0550
396.03	0.2500	0.5659	1.4580	1.0380
398.45	0.2000	0.5025	1.5250	1.0240
401.28	0.1500	0.4229	1.5980	1.0130
404.63	0.1000	0.3205	1.6770	1.0060
408.64	0.0500	0.1850	1.7640	1.0010
413.49	0.0000	0.0000	1.8580	1.0000

$$\ln p_i^{sat} = A_i - \frac{B_i}{T + C_i} \qquad \ldots(17)$$

Table 7. Antoine equation parameters

Compound	Antoine constants			Temperature range/K
	A	B	C	
CPME	3.6039	216.7424	-242.925	357 to 378
CPL	2.6168	36.6346	-352.067	390 to 412

Where Pressure is in kPa and Temperature is in K [22]. The Antoine equation parameters A, B, C of CPME and CPL are listed in Table 7.

III. THERMODYNAMIC CONSISTENCY TEST

In this paper, semi-empirical method reported by Herington is employed to examine the thermodynamic consistency of VLE data for the binary system [23]. The criteria of consistency of this method is that the value of D-J can not be larger than 10. D and J are obtained by Eq. (15) and (16) respectively. The values of D-J for the binary system are listed in Table 8.

$$D = 100 \frac{\int_{x_1=0}^{x_1=1} \ln \frac{\gamma_1}{\gamma_2} dx_1}{\int_{x_1=0}^{x_1=1} \ln \left| \frac{\gamma_1}{\gamma_2} \right| dx_1} \qquad \ldots(15)$$

$$J = 150 \frac{T_{max} - T_{min}}{T_{min}} \qquad \ldots(16)$$

Table 8. Thermodynamics consistency check

D	J	D-J	Method
5.77	13.59	7.82	UNIFAC
49.14	13.59	35.56	modified UNIFAC Dortmund

IV. DATA REDUCTION USING g^E MODELS

In this work, the predicted VLE data are correlated by means of Van Laar, Wilson and NRTL models [24, 25]. The saturated vapor pressures of pure component are calculated by Eq. (17). The binary interaction parameters of these models, obtained by minimization of the objective function %AAD $\sum(\delta P)$, are used to minimize error by the regressions procedure. (%AAD = Absolute Average Deviation and n represent the no. of predicted data points). Similarly AAD $\sum(\delta T)$ and AAD $\sum(\delta y)$ are calculated by Eq. (19) and Eq. (20) respectively. The subscript “pre” and “cal” represent the predicted and calculated values respectively.

$$\%AAD \sum(\delta P) = \frac{100}{n} \sum_{i=1}^{n} \frac{\left| P_{i,pre.} - P_{i,cal.} \right|}{P_{i,pre.}} \qquad \ldots(18)$$

$$AAD \sum(\delta T) = \frac{1}{n} \sum_{i=1}^{n} \left| T_{i,pre.} - T_{i,cal.} \right| \qquad \ldots(19)$$

$$\text{AAD}\sum(\delta y) = \frac{1}{n}\sum_{i=1}^{n}\left|y_{i,pre.} - y_{i,cal.}\right| \qquad \ldots(20)$$

The correlated binary interaction parameters from predicted VLE data by UNIFAC method and modified UNIFAC Dortmund are shown in Table 9 and Table 10 respectively. α is the characteristic constant of the non-randomness for the binary system. $\alpha = 0.3$ is recommended for this binary system as it belongs to type I according to the definition in the literature [25]. The comparison of predicted data by UNIFAC and modified UNIFAC methods with calculated data by Van Laar, Wilson, and NRTL models for binary system CPME (1) + CPL (2) at atmospheric pressure T-x_1-y_1 is shown through Figure 1 to 6.

Table 9. Correlated models BIPs from predicted data by UNIFAC model

Model	**Binary Parameter**		**AAD (Δy)**	**AAD (ΔT)**
Van Laar	A_{12}	A_{21}	0.0019	0.0241
	0.5083	0.7004		
Wilson	a_{12}	a_{21}	0.0027	0.0575
	-670.512	2912.545		
NRTL	b_{12}	b_{21}	0.0029	0.0575
	2561.409	-343.437		

Table 10. Correlated models BIPs from predicted data by modified UNIFAC Dortmund model

Model	**Binary Parameter**		**AAD (Δy)**	**AAD (ΔT)**
Van Laar	A_{12}	A_{21}	0.0267	0.3251
	0.5495	0.8533		
Wilson	a_{12}	a_{21}	0.0255	0.3146
	-637.425	3277.347		
NRTL	b_{12}	b_{21}	0.0256	0.3278
	3076.794	-442.811		

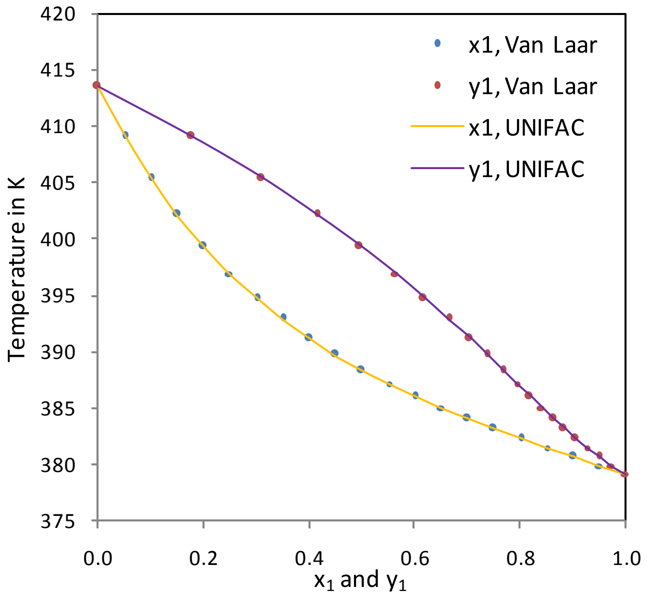

Figure 1. T-x_1-y_1 diagram by Van Laar and UNIFAC models.

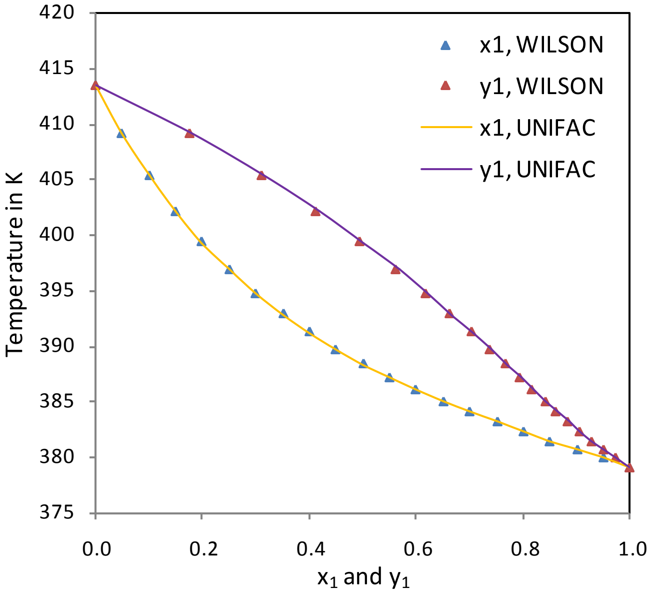

Figure 2. T-x_1-y_1 diagram by Wilson and UNIFAC models.

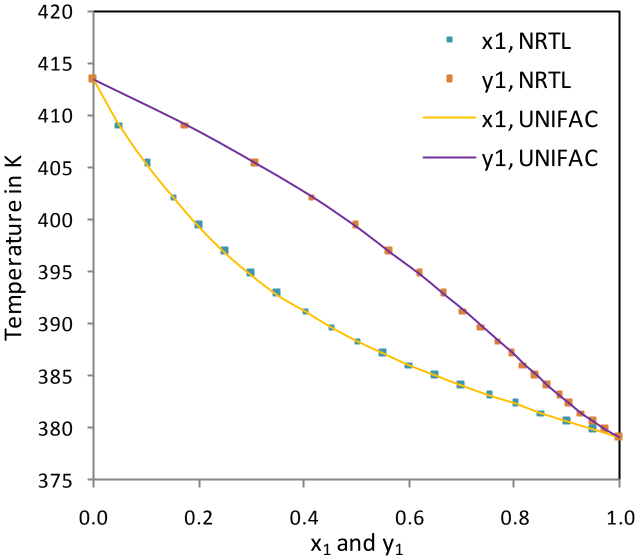

Figure 3. T-x_1-y_1 diagram by NRTL and UNIFAC models.

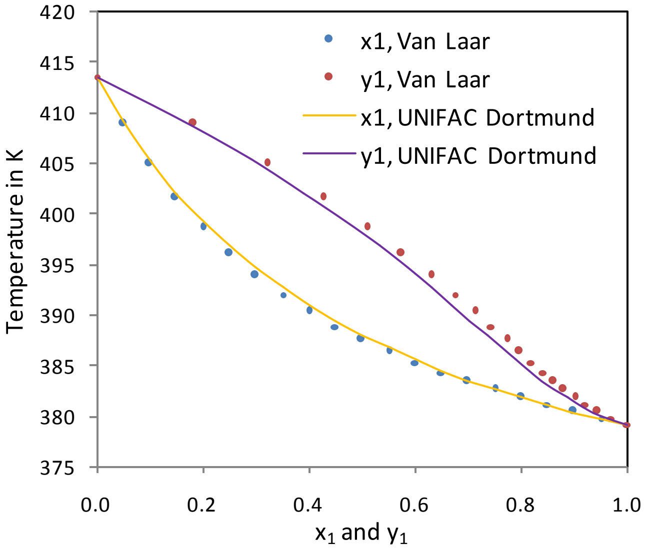

Figure 4. T-x_1-y_1 diagram by Van Laar and modified UNIFAC Dortmund models.

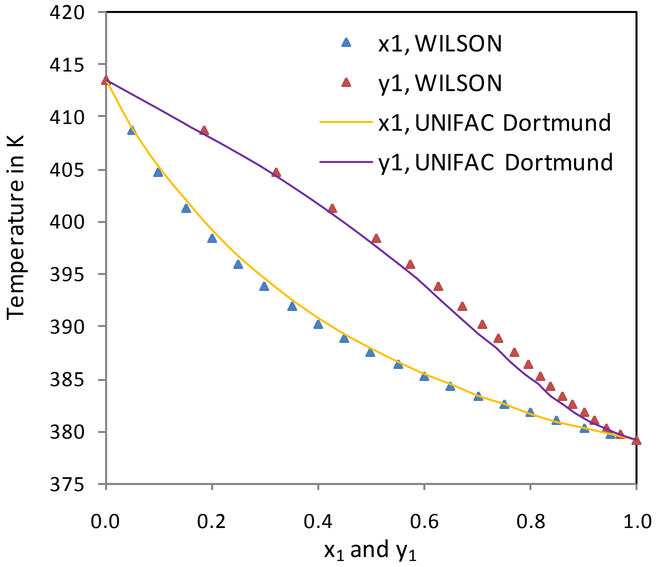

Figure 5. T-x_1-y_1 diagram by Wilson and modified UNIFAC Dortmund models.

From Figures 1, 2 and 3, it can be seen that isobaric VLE data predicted by UNIFAC method is very well represented by Van Laar, Wilson and NRTL models, whereas slight deviation is found in calculated data in case of modified UNIFAC Dortmund method.

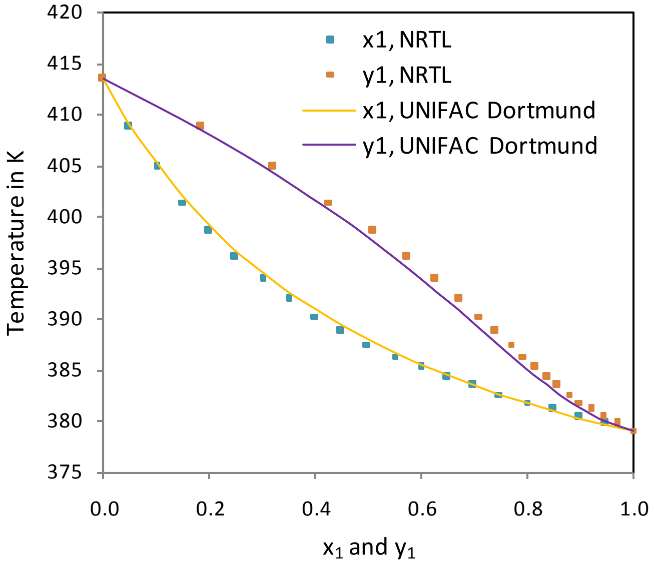

Figure 6. T-x_1-y_1 diagram by NRTL and modified UNIFAC Dortmund models.

V. CONCLUSIONS

The VLE data for the binary system CPME with CPL have been predicted at atmospheric pressure using UNIFAC method and modified UNIFAC Dortmund method. The predicted data by UNIFAC method confirms the thermodynamic consistency by Herington's test but modified UNIFAC Dortmund method fails the consistency test. The activity coefficient models Van Laar, Wilson and NRTL were capable accurately fitting these predicted data by UNIFAC method than the data predicted by modified UNIFAC Dortmund method. No azeotrope is found for this system.

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NOMENCLATURE

P - Absolute pressure, kPa
T - Absolute temperature, K

F_i - Surface area fraction of compound i in the mixture
q_i - Relative van der Waals surface area of compound i
Q_k - Relative van der Waals surface area of subgroup k
r_i - Relative van der Waals volume of compound i
V_i - Volume/mole fraction of compound i in the mixture
V'_i - Modified volume/mole fraction of compound i in the mixture (modified UNIFAC Dortmund method)
X_m - Mole fraction of subgroup m
ln - Natural logarithm (base e)
log - Logarithm (base 10)
x_i - Liquid phase mole fraction of i^{th} species
y_i - Vapor phase mole fraction of i^{th} species
Γ - Temperature dependant integration constant.
γ_i - Activity coefficient of i^{th} species
H^E - Excess enthalpy
A_{ij} - Adjustable parameter (Van Laar Model)
λ_{ij} - Interaction parameter (Wilson Model)
Λ_{ij} - Adjustable parameter (Wilson Model)
α_{ij} - The non-randomness of the fluid empirical parameter
τ_{ij} - Adjustable parameter (NRTL Model)
A, B, C- Antoine equation constants

SUPERSCRIPTS

E - Excess property
sat - Saturated property value
∞ - Property at infinite dilution concentration

SUBSCRIPTS

1 - Component 1
2 - Component 2
i - Property of i^{th} species

REFERENCES

[1] W. Kiyoshi, “The Toxicological Assessment of Cyclopentyl Methyl Ether (CPME) as a Green Solvent”, Molecules, vol. 18, pp. 3183-3194, 2013.
[2] W. Kiyoshi, Y. Noriyuki and T. Yasuhiro, “Cyclopentyl Methyl Ether as a New and Alternative Process Solvent”, Organic Process Research & Development, vol. 11, pp. 251-258, 2007.
[3] P. D. Shah and J. A. Parekh, “Synthesis & Application of New & Alternative Green Solvent Cyclopentyl Methyl Ether”, Institute of technology, Nirma University, vol. 1, pp 1-5, 2010.
[4] K. Idan, O. Genichi, T. Kazuo and W. Kiyoshi, “Organometallic reaction method”, Applicant Zeon Corporation, Patent EP1405840B1, Aug 20, 2014.
[5] J. Gmehling, “From UNIFAC to Modified UNIFAC to PSRK with the Help of DDB”, Fluid Phase Equilibria, vol. 107, pp. 1-29, 1995.
[6] 3rd International Conference on Medical Sciences and Chemical Engineering (ICMSCE'2013), Bangkok (Thailand), Dec. 25-26, 2013.
[7] K. G. Joback and R. C. Reid, “Estimation of Pure-Component Properties from Group-Contributions”, Chem. Eng. Commun., vol. 57, pp. 233 -243, 1987.
[8] A. L. Lydersen, “Estimation of Critical Properties of Organic Compounds”, College Engineering University Wisconsin, Engineering Experimental Station Report 3, Madison, WI, April 1955.
[9] D. Ambrose, “Correlation and Estimation of Vapor-Liquid Critical Properties. I. Critical Temperatures of Organic Compounds”, National Physical Laboratory, Teddington, UK, NPL Report Chem., 92, September 1978.
[10] R. Gani and L. Constantinou, “Molecular Structure Based Estimation of Properties for Process Design”, Fluid Phase Equilibria, vol. 116, pp. 75- 86, 1996.
[11] J. Marrero and R. Gani, “Group-Contribution Based Estimation of Pure Component Properties”, Fluid Phase Equilibria, vol. 183-184, pp. 183-208, 2001.
[12] A. S. Hukkerikar, B. Sarup, A. T. Kate, J. Abildskov, G. Sin and R. Gani, "Group-Contribution+ (GC+) Based Estimation of Properties of Pure Components: Improved Property Estimation and Uncertainty Analysis”, Fluid Phase Equilibria, vol. 321, pp. 25-43, 2012.

[13] E. L. Derr and C. H. Deal, “Analytical Solutions of Groups: Correlation of Activity Coefficients Through Structural Group Parameters. 1”, Chem. E. Symp., Ser. No. 32, Instn. Chem. Engrs., London, 3, 40, 1969.
[14] M. Ronc and G. A. Ratcliff, “Prediction of Excess Free Energies of Liquid Mixtures by an Analytic Group Solution Model”, Can. J. Chem. Eng., vol. 49, pp. 825-830, 1971.
[15] A. Fredenslund, R. L. Jones and J. M. Prausnitz, “Group Contribution Estimation of Activity Coefficients in Nonideal Liquid Mixtures”, AIChE Journal, vol. 21, pp. 1086-1099, 1975.
[16] U. Weidlich and J. Gmehling, “A Modified UNIFAC Model. 1- Prediction of VLE, h^E, and γ^∞”, Ind. Eng. Chem. Res., vol. 26, pp. 1372-1381, 1987.
[17] T. Holderbaum and J. Gmehling, “PSRK: A Group Contribution Equation of State Based on UNIFAC”, Fluid Phase Equilibria, vol. 70, pp. 251-265, 1991.
[18] B. E. Poling, J. M. Prausnitz and J. P. O'Connell, The Properties of Gases and Liquids, 5th ed., The McGraw-Hill Company limited: New York, 2012, pp 8.23.
[19] J. Gmehling, J. Li and M. Schiller, “A Modified UNIFAC Model. 2. Present Parameter Matrix and Results for Different Thermodynamic Properties”, Ind. Eng. Chem. Res., vol. 32, pp. 178-193, 1993.
[20] J. Lohmann, R. Joh and J. Gmehling, “From UNIFAC to Modified UNIFAC (Dortmund)”, Ind. Eng. Chem. Res., vol. 40, pp. 957-964, 2001.
[21] A. Jakob, H. Grensemann, J. Lohmann and J. Gmehling, “Further Development of Modified UNIFAC (Dortmund): Revision and Extension 5”, Ind. Eng. Chem. Res., vol. 45, pp. 7924-7933, 2006.
[22] J. M. Smith, H. C. VanNess and M. M. Abbott, Introduction to chemical engineering thermodynamics, 7th ed., Tata McGraw Hill Education private limited: New Delhi, 2010.
[23] J. A. Wisniak, “The Herington test for thermodynamic consistency”, Ind. Eng. Chem. Res., vol. 33, pp. 177-180, 1994.
[24] G. M. Wilson, “A New Expression for the Excess Free Energy of Mixing”, J. Amer. Chem. Soc., vol. 86, pp. 127-130, 1964.
[25] H. Renon and J. M. Prausnitz, “Local compositions in thermodynamic excess functions for liquid mixtures”, AIChE J., vol. 14, pp. 135-144, 1968.