Original Article

A Model For Predicting The Behavior Of Acetone-Ethanol-Hexane System Through Group Contribution Methods And VLE Modeling

Aileen Grace M. Fronda[1], Jonathan L. Salvacion[2]

[1] School of Chemical, Biological, and Materials Engineering and Sciences, Mapúa University, Manila, Philippines
[2] School of Graduate Studies, Mapúa University, Manila, Philippines
Email: [1] agmfronda@mymail.mapua.edu.ph, [2] jlsalvacion@mapua.edu.ph

*Corresponding Author: Aileen Grace M. Fronda
School of Chemical, Biological, and Materials Engineering and Sciences, Mapúa University, Manila, Philippines
Email: agmfronda@mymail.mapua.edu.ph
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Abstract

Thermodynamic models have been developed for isobaric and isothermal ternary system acetone-ethanol-hexane vapor liquid equilibria (VLE) data. The boiling point, melting point, and heat capacity of the system were estimated through Group Contribution Methods (GCMs) and the application of summability relations. The Peng-Robinson Equation of State (PREOS), Redlich Kwong (RKEOS), and Soave-Redlich Kwong (SRKEOS) were utilized in the calculations of fugacity and fugacity coefficients of the components in the system. The Non-Random Two-Liquid (NRTL), Wilson, Universal Quasi-Chemical (UNIQUAC), and UNIQUAC Functional-Group Activity Coefficients (UNIFAC) models were used in predicting the activity coefficients and in the determination of the bubble point and dew point pressures and temperatures. All the models used in comparing the experimental and calculated activity coefficients appeared to be satisfactory and in good agreement for all the data but among these models UNIFAC and Wilson models exhibited the best fit for 42 total data points based on the regression analyses used namely R2, adjusted R2, SSE, and RMSE. The UNIFAC model also performed exceptionally well when it comes to calculating bubble point and dew point temperatures and pressures. A modified activity coefficient model (MACM) was also formulated and applied to various ternary systems where the results exhibited comparable results to the existing models.

Keywords: Activity Coefficient, Group Contribution Methods, Ternary System, VLE Modeling

I. INTRODUCTION

In the science and engineering, knowledge of thermodynamic properties, particularly of vapor-liquid equilibria (VLE) has been very significant in solving complex problems [1]. The VLE is a necessary tool for fabricating and developing procedures that employ the partition of components of a given mixture [2] and thermodynamic models serve as aids in understanding system behavior [3]. In design, analysis, and optimization, the majority of researchers are relying on theory and data from experiments. Although experiments can offer reliable results for several mixtures under specific phase conditions, these will not suffice for all the needs of industries for their design and other applications.

The conduct of phase equilibrium experiments for several mixed working fluids is very time-consuming and may demand high costs [4]. When models are simulated with adequate accuracy, these can either replace or minimize testing at full scale, and simulations can be used more reliably to predict unavailable data and for conditions that are not easily obtainable. Therefore, proposals of thermodynamic VLE models through numerical simulation using empirical equations have been introduced to provide predictions for VLE of different mixtures by utilizing limited experimental data and as an alternative to expensive and time-consuming experimentation [5].

Another way of estimating phase equilibrium data of systems is through Group Contribution Methods (GCMs) which require group interaction parameters from an extensive database. When an experimental determination is not possible and data on physico-chemical properties is required, this is a practical and essentially empirical estimating strategy. The method has been applied in determining the properties of individual components of biochemical and safety interest [6], phase behavior of binary and multicomponent systems [7] and estimating physico-chemical properties of organic compounds [8].

There are two main categories used in the correlation of VLE data in studies namely the use of equations of state (EOSs) and the activity coefficient models. Bengesai [9] conducted high-pressure VLE measurements for R116 and ethane with perfluorohexane and perfluorooctane and utilized the Non-Random Two-Liquid (NRTL) model and Peng-Robison equation of state (PREOS) in correlating the data; Vrabec et al. [10] used PREOS in modeling N_2+O_2+CO_2; Huang et al. [11] applied PREOS in correlating the VLE data of 33 ternary systems; Koster et al. [12] also utilized PREOS in modeling ethylene + decafluorobutane; and Soujanya et al. [13] used NRTL, Wilson, Universal quasi-chemical (UNIQUAC), and PREOS and Soave-Redlich-Kwong (SRKEOS) for the system containing methanol, isopropyl alcohol, water, and glycerol.

Several studies on extraction processes involved the utilization of the components of the acetone (1) – ethanol (2) – hexane (3) (AEH) system. Periago et al. [14] used AEH mixture as a solution for extracting lycopene, a major carotenoid from raw tomato, tomato sauce, and tomato paste, to confirm that lycopene extraction rates are influenced by the solvent used during extraction in which they believed that there is a positive synergistic interaction of hexane with ethanol and with acetone. The study of Hepsibah and Jothi [15] utilized the three components in their comparative study on the effect of solvents on the phytochemical profile and biological potential of Ormocarpum conchinchinense auct. non (lour.) Merrill where acetone was able to extract phenolic-rich compounds and ethanol was the best for extracting the antioxidant compounds. Acetone, ethanol, and hexane were also used in the comparative study of Sarkar et al. [16] on carotenoid extraction. In the study conducted by Soares et al. [17] on extraction process improvement for High Commercial Value Pigments from Desmodesmus sp. Microalgae also utilized these components and concluded that hexane-ethanol combination yielded the best results. Apart from extraction processes, the components of the AEH system were known in various solvothermal syntheses. Acetone and ethanol have the capacity to affect the morphological and optical properties of ZnO nanoparticles [18]; hexane and ethanol were used as solvents to observe the effects of solvents on the heterogeneous growth of TiO_2 nanostructure arrays [19]; the three components were utilized in the preparation of silver nanoparticles [20]. These suggest that the mixture of the three components is essential and has the potential in the extraction and solvothermal processes.

There is no study that explains how the AEH system behaves as a mixture solvent among the aforementioned and other published studies. Thus, the objective of this study is to develop models that will explain the behavior of the AEH system as a basis for predicting the system's activity in extraction processes and solvothermal syntheses, and the calculated activity coefficients can be utilized in the design of distillation columns.

II. COMPUTATIONAL METHODS

This study used GCMs to estimate the boiling point, melting point, and heat capacity of the AEH system, EOSs to estimate fugacity and fugacity coefficients, and activity coefficient models to estimate activity coefficients, bubble point and dew point temperatures and pressures, all of which can be used to describe how the AEH system behaves. For numerical simulation of the different models, MATLAB programming software was utilized. Among the physical property estimation methods from Perry's Chemical Engineering Handbook (PCEH) [21], the GCMs were applied in the estimation of the different properties by assuming a summative behavior of the structural groups of the constituent molecules. The boiling point (T_b), melting point (T_m), and heat capacity (c_p) of the individual components of the AEH system were estimated using Nannoolal Method (equation (2)), Method of Constantinou and Gani (equation 1), and Domalski-Hearing Method (equation (3)), respectively. Equation (4) shows how summability relations were used to estimate the same attributes for the ternary system.

The number of first-order (N_i) and second-order (N_j) groups of the components to be employed in the calculation of T_m are listed in PCEH Table 2-158 and Table 2-159 where $t_{m1,i}$ and $t_{m2,j}$ are the first-order and second-order group contributions, respectively. The parameters of the Nannoolal Method include the number of nonhydrogen atoms (n), number of occurrences of group i (n_i), number of groups involved (N), and group contribution (C_i) from PCEH Table 2-155. The heat capacity group contribution values $(c_p)_t$ from Domalski and Hearing's study are used to estimate cp (1993).

Equation 4 is used to calculate the AEH properties as a solution, where $\bar{M}_i$ represents pure estimated property values and x_i represents the mole fraction in general for both liquid and vapor phases.

$$T_m=(102.425)\cdot \ln\left(\sum_i N_i\, t_{m1,i}+\sum_j N_j\, t_{m2,j}\right) \tag{1}$$

$$T_b=\frac{\sum_{i=1}^{N} n_i \cdot C_i}{n^{0.06583}+1.6868}+84.3395 \qquad (2)$$

$$C_p=\sum_{i=1}^{N} n_i \left(C_p\right)_t \qquad (3)$$

$$M=x_i\overline{M}_i \qquad (4)$$

The fugacities and fugacity coefficients of the AEH system's components were evaluated using PREOS, RKEOS, and SRKEOS. The fugacity coefficient was calculated using equations 5 and 6 together with the needed parameters:

$$\ln \Phi_i=\frac{b_i}{b}(Z-1)-\ln(Z-\beta)-\bar{q}_i I \qquad (5)$$

$$Z=1+\beta-q\beta\frac{Z-\beta}{Z(Z+\varepsilon\beta)(Z+\sigma\beta)} \qquad (6)$$

Where, the individual fugacity coefficients of each component are represented by Φ_i; a, b, β, and q are cubic EOS parameters; σ, ε are cubic EOS constants; Z is the compressibility factor; P is the absolute pressure; T is the absolute temperature; R is the universal gas constant; and x_i as a general representation of the mole fraction.

Furthermore, rules of mixing by van der Waals were used to relate mixture parameters to pure-specie parameters in which two parameters are involved – the quadratic mixing rule, a, and the linear mixing rule, b, with a_{ij} as the interaction parameter represented by the following equations.

$$a=\sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j a_{ij} \qquad (7)$$

$$b=\sum_{i=1}^{n} x_i b_i \qquad (8)$$

$$a_{ij}=\left(1-k_{ij}\right)\left(a_i a_j\right)^{\frac{1}{2}} \qquad (9)$$

In the equations, x_i was used as a general representation of the mole fraction. But in actual calculations, x_i is used to represent the molar fraction of component *i* in the liquid phase, whilst x_i is the molar fraction of component *i* in the vapor phase. Pure-species parameters, ai and bi can be calculated using equations 10 and 11, respectively, while the interaction parameter can be further evaluated from the pure-specie parameters by combining rules such as the geometric mean rule as expressed in equation 12 where the k_{ij} was set as zero [22]. The involved parameters $\alpha(T_{ri})$, σ, ε, Ω, and Ψ can be calculated depending on what EOS is being applied in the calculations.

$$a_i=\frac{\Psi\alpha(T_{ri})R^2T_{ci}^2}{P_{ci}} \qquad (10)$$

$$b_i=\Omega\frac{RT_{ci}}{P_{ci}} \qquad (11)$$

$$a_{ij}=(1-k_{ij})\left(a_i a_j\right)^{\frac{1}{2}} \tag{12}$$

The activity coefficient models namely NRTL, Wilson, UNIQUAC, and the UNIFAC methods were used in evaluating the activity coefficients. The equations for these models are listed in Table I as equations 13, 14, 15, 16, 17, 18, 19, and 20, respectively. The parameters such as α, b_{12}, b_{21}, etc. are specific to a particular pair of species and are obtained by regression of the experimental data.

The calculations on bubble point and dew point pressure and temperature were conducted through the application of the same activity coefficient models as were previously discussed. Because of their complexity, all of these calculations will require iteration.

Table I. Activity Coefficients Models' Equation for the Ternary Systems

model	Equation		Reference
NRTL	$\ln\gamma_i=\frac{\sum_{j=1}^{3}\tau_{ji}G_{ji}x_j}{\sum_{l=1}^{3}G_{li}\,x_l}+\sum_{j=1}^{3}\frac{x_j G_{ij}}{\sum_{l=1}^{3}G_{lj}x_j}\cdot\left(\tau_{ij}-\frac{\sum_{r=1}^{3}x_r\tau_{rj}G_{rj}}{\sum_{l=1}^{3}G_{lj}\,x_l}\right)$	(13)	[22]
Wilson	$\ln\gamma_i=1-\ln\left(\sum_{j=1}^{3}x_j\Lambda_{ij}\right)-\sum_{k=1}^{3}\left(\frac{x_k\Lambda_{ki}}{\sum_{j=1}^{3}x_j\Lambda_{kj}}\right)$	(14)	[23]
UNIQUAC	$\ln\gamma_i=\ln\gamma_i^C+\ln\gamma_i^R$	(15)	[20]
	$\ln\gamma_i^C=1-J_i+\ln J_i-5q_i\left(1-\frac{J_i}{L_i}+\ln\frac{J_i}{L_i}\right)$	(16)	[20]
	$\ln\gamma_i^R=q_i\left(1-\ln s_i+\sum_j\theta_j\ln\frac{\tau_{ij}}{s_j}\right)$	(17)	[20]
UNIFAC	$\ln\gamma_i=\ln\gamma_i^C+\ln\gamma_i^R$	(18)	[20]
	$\ln\gamma_i^C=1-J_i+\ln J_i-5q_i\left(1-\frac{J_i}{L_i}+\ln\frac{J_i}{L_i}\right)$	(19)	[20]
	$\gamma_i^R=q_i\left[1-\sum_k\left(\theta_k\frac{\beta_{ik}}{s_k}-e_{ki}\ln\frac{\beta_{ik}}{s_k}\right)\right]$	(20)	[20]

III. RESULTS AND DISCUSSION

Experimental VLE Data of Acetone-Ethanol-Hexane System. This paper considered the study of AEH system wherein the VLE data were retrieved from the Dortmund Data Bank [24] for both its isobaric (101.33 kPa) and isothermal (328.15 K) states. The VLE data are graphically represented in Fig. 1 and Fig. 2.

Physical Properties of AEH System. From the estimated values of the physical properties of each component, equation 4 has been applied to approximate the physical properties of the AEH system as a mixture. The results were tabulated in Table II.

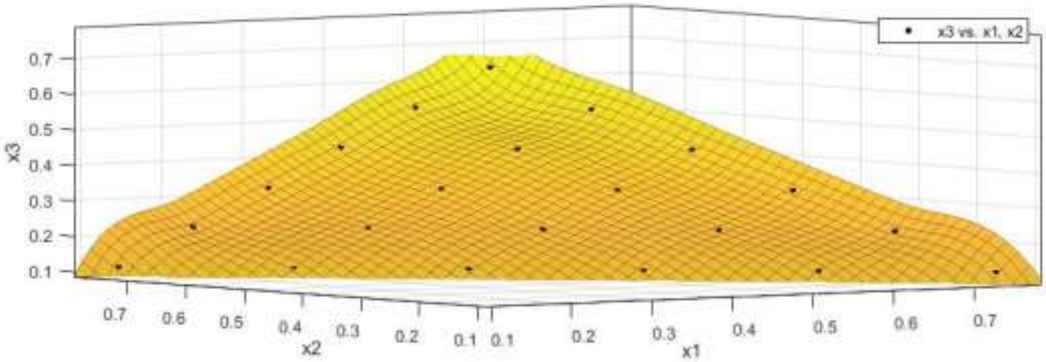

Fig. 1. Experimental VLE data for acetone (1)-ethanol (2)-hexane (3) system at 101.33 kPa.

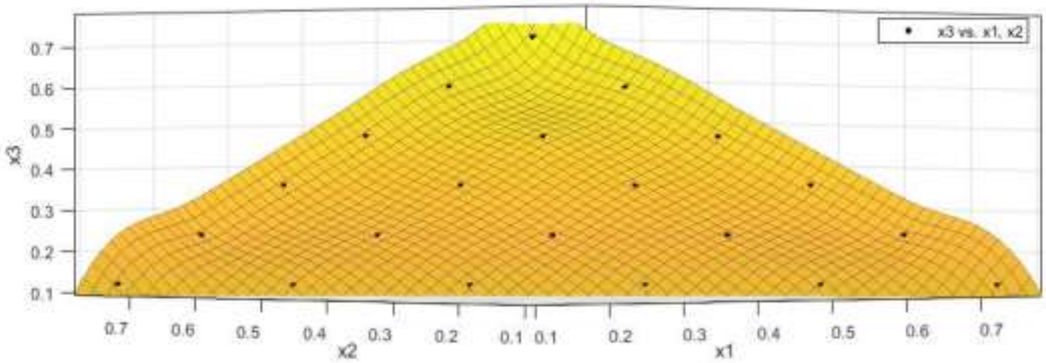

Fig. 2. Experimental VLE data for acetone (1)-ethanol (2)-hexane (3) system at 328.15 K.

Fugacity and fugacity coefficients. The fugacities and fugacity coefficients were correlated with the vapor-phase compositions of the AEH system. These are obtained to explain the behavior of the system most especially vapor phase properties. The PREOS provides results similar to that of SRKEOS compared to the results generated using RKEOS. Fig. 3 and Fig. 4 show the result of the fugacity and fugacity coefficients calculations of each species in the AEH system using RKEOS. The resulting fugacity coefficients using RKEOS presented a positive deviation from ideality as indicated by the values that are greater than 1.0. The correlation of the vapor-phase composition with their respective fugacity coefficients presented low goodness of fit as shown for both figures of the isobaric and isothermal systems.

Activity Coefficients. Based on the VLE data, initial values of activity coefficients were calculated by applying the Modified Raoult's Law (MRL). From the same VLE data, the activity coefficients were also calculated using the different modeling methods – NRTL, Wilson, UNIQUAC, and UNIFAC. The values of the activity coefficients presented positive deviations from ideal activity coefficient values. Fig. 5 and Fig. 6 show the comparisons of the MRL-calculated values and values generated using the activity coefficient models.

Table II. Estimated Physical Properties of the AEH System

T_m(K)		T_b (K)		$c_{p,\,gas}$/J-mol^{-1}-K^{-1}		$c_{p,\,liq}$/J-mol^{-1}-K^{-1}	
Isobaric	isothermal	isobaric	isothermal	isobaric	isothermal	isobaric	isothermal
159.6254	159.6849	346.3516	346.2853	110.6363	110.7619	176.51202	176.14613
161.5106	161.5330	345.5510	345.5208	105.7448	105.7810	167.62609	167.4775
163.3586	163.3734	344.7865	344.7806	102.9506	102.7717	158.95746	158.88875
165.2138	165.2138	344.0404	344.0404	100.3641	100.1598	150.3000	150.3000
167.0836	167.0689	343.2883	343.2942	89.8057	96.7705	141.57383	141.64254
168.9240	168.9093	342.5481	342.5540	89.8057	91.0156	132.98508	133.05379
160.6081	160.6375	343.2456	343.2337	109.5643	109.6283	166.28738	166.14996
162.4856	162.4926	342.4693	342.4876	105.2031	105.1350	157.48133	157.4925
164.3337	164.3330	341.7048	341.7474	102.3958	102.0658	148.8127	148.90375
166.1888	166.1811	340.9586	340.9829	97.5266	97.4223	140.15524	140.23512
168.0369	168.0215	340.1942	340.2427	91.4892	91.7938	131.48661	131.64637
161.5907	161.6048	340.1396	340.1763	108.1393	107.6091	156.06274	156.08508
163.4536	163.4523	339.3692	339.4544	104.0400	104.0187	147.3254	147.5075
165.3087	165.3004	338.6231	338.6899	98.8605	99.2799	138.66794	138.83887
167.1715	167.1408	337.8527	337.9497	93.1359	92.9611	129.9306	130.25012
162.5952	162.5645	337.0460	337.1431	107.5385	107.6707	145.78056	146.10008
164.4209	164.4196	336.3117	336.3970	100.8601	101.5545	137.26052	137.44262
166.2837	166.2677	335.5413	335.6325	93.9584	94.3885	128.52318	128.77399
163.5555	163.5466	333.9702	334.0797	104.9742	105.3067	135.70451	135.96649
165.3959	165.3799	333.2300	333.3212	94.8442	95.7389	127.11576	127.36657
164.5382	164.4992	330.8643	331.0282	98.5323	99.6995	125.47987	125.97032

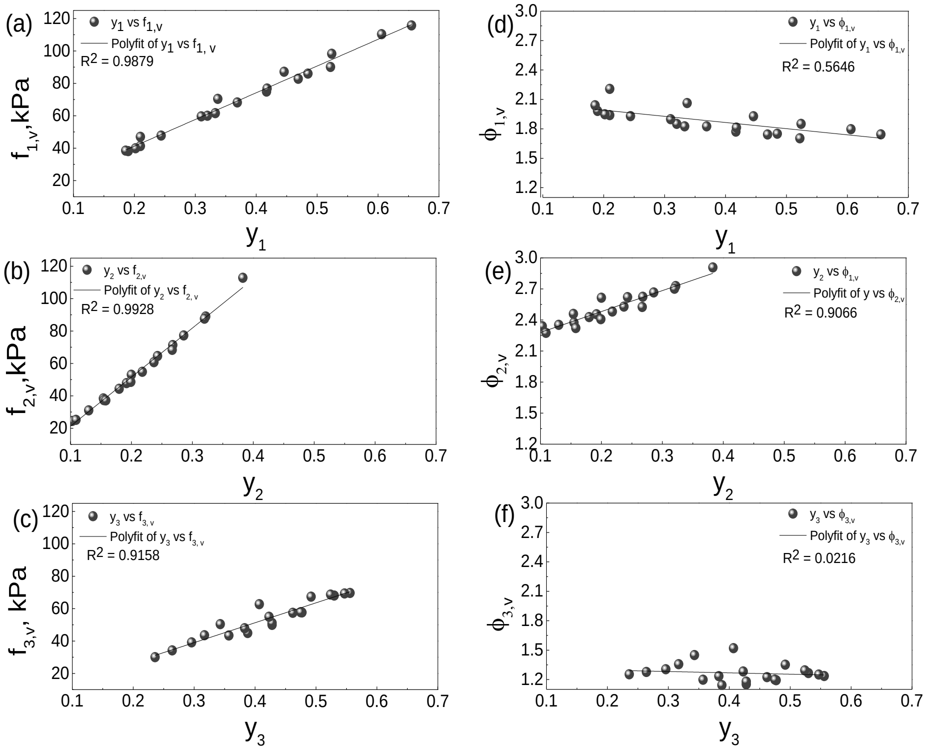

Fig. 3. Correlations of the vapor-phase composition and calculated (a) fugacity of acetone; (b) fugacity of ethanol; (c) fugacity of hexane; (d) fugacity coefficient of acetone; (e) fugacity coefficient of ethanol; (f) fugacity coefficient of hexane for AEH system using RKEOS at 101.33 kPa.

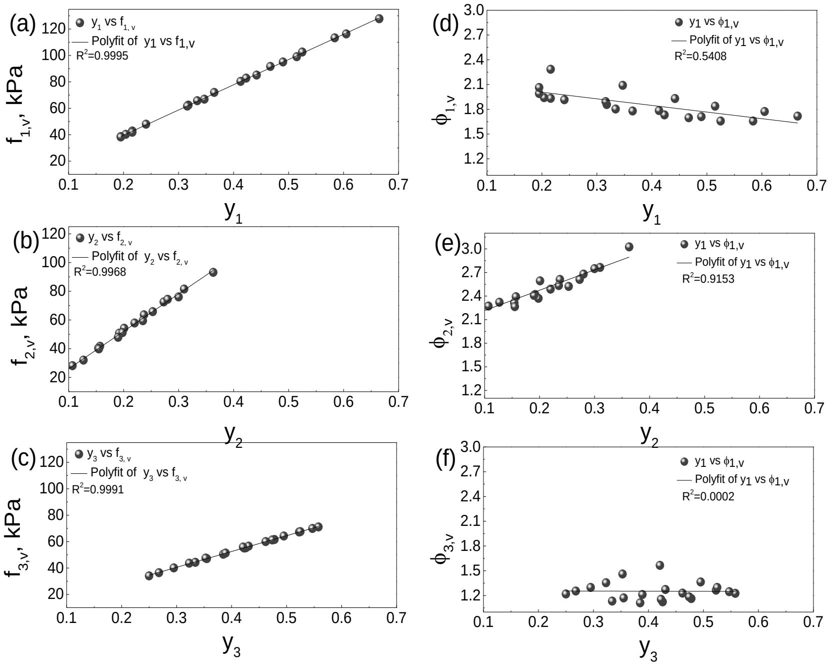

Fig. 4. Correlations of the vapor-phase composition and calculated (a) fugacity of acetone; (b) fugacity of ethanol; (c) fugacity of hexane; (d) fugacity coefficient of acetone; (e) fugacity coefficient of ethanol; (f) fugacity coefficient of hexane for AEH system using RKEOS at 328.15 K.

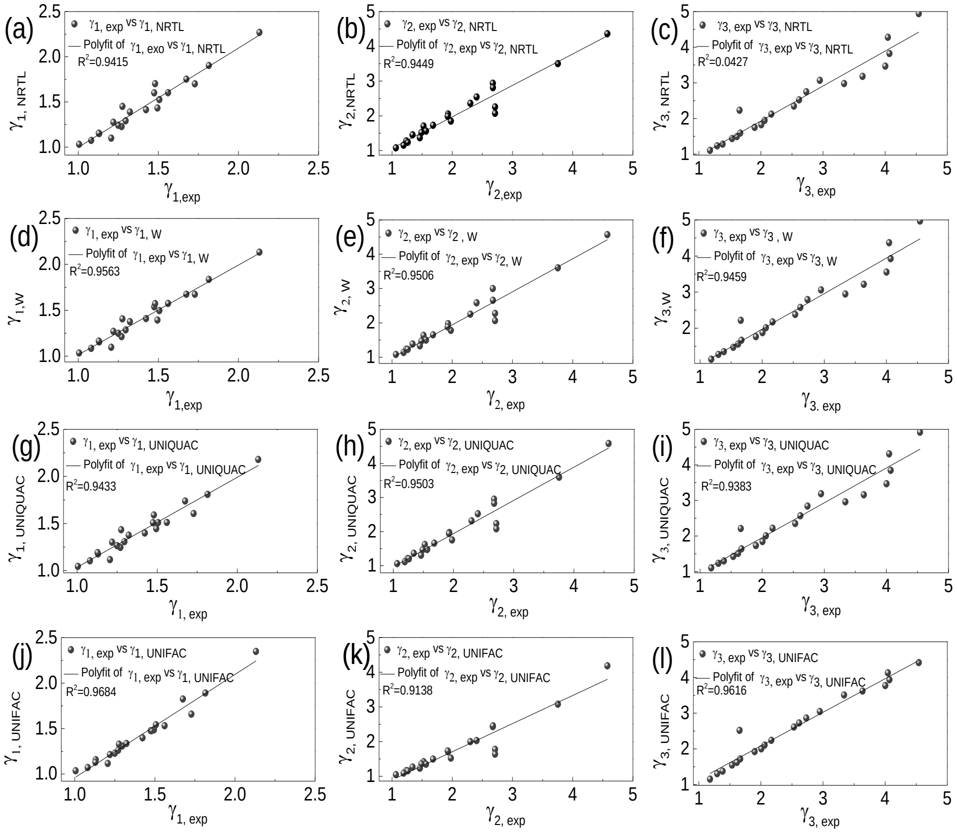

Fig. 5. Comparison of activity coefficients of AEH system at 101.33 kPa. MRL vs. NRTL for (a) acetone, (b) ethanol, and (c) hexane; MRL vs Wilson for (d) acetone, (e) ethanol, and(f) hexane; MRL vs UNIQUAC for (g) acetone, (h) ethanol, and (i) hexane; MRL vs UNIFAC for (j) acetone; (k) ethanol; (l) hexane.

Bubble point and dew point pressures and temperatures. Using the same activity coefficient models and the gamma-phi approach, calculations on bubble point and dew point pressures and temperatures were performed. The list of results of the bubble point and dew point temperatures and pressures are graphically represented in Fig. 7 and Fig. 8.

Fig. 7 and Fig. 8 present the accuracy of the models by relating the calculated bubble point and dew point T based from the VLE data, respectively. In the regression analyses, upon comparing the bubble point and dew point T for the isobaric system, UNIFAC model presented the highest R^2 with a value of 0.901. The bubble point and dew point P for the at 328.15 K, the UNIFAC model still has the highest R^2 with a value of 0.9876.

Modified Activity Coefficient Model. A modified activity coefficient model (MACM) has been formulated to predict the behavior of a system in which the calculation of the activity coefficients of the components will depend on both the molecular structure and VLE experimental data. The process of calculating the activity coefficient is patterned with UNIQUAC but the relative molecular volumes and relative molecular surface area are calculated using equation 21 and equation 24, respectively, where V_k represents the molecular volume, A_k is the molecular surface area, A_{Ctotal} is the total atomic contribution, A_c is the atomic contribution (equation 23), n is the number of repeated atoms, B_c is the bond contribution (equation 22), A_R is the number of aromatic rings, and N_{AR} is the number of non – aromatic rings.

$$\mathrm{V_k}(\mathrm{A}^{\circ 3}/\mathrm{molecule}) = A_{Ctotal} - (5.2549B_c + 17.1802A_R + 16.586N_{AR}) \qquad (21)$$

$$B_c = A - 1 + A_R + N_{AR} \qquad (22)$$

$$A_{Ctotal} = \sum A_C * \mathrm{n} \qquad (23)$$

$$\mathrm{A_k}(\mathrm{A}^{\circ 2}/\mathrm{molecule}) = A_{Ctotal} - (15.5745B_c + 37.1337A_R + 28.9365N_{AR}) \qquad (24)$$

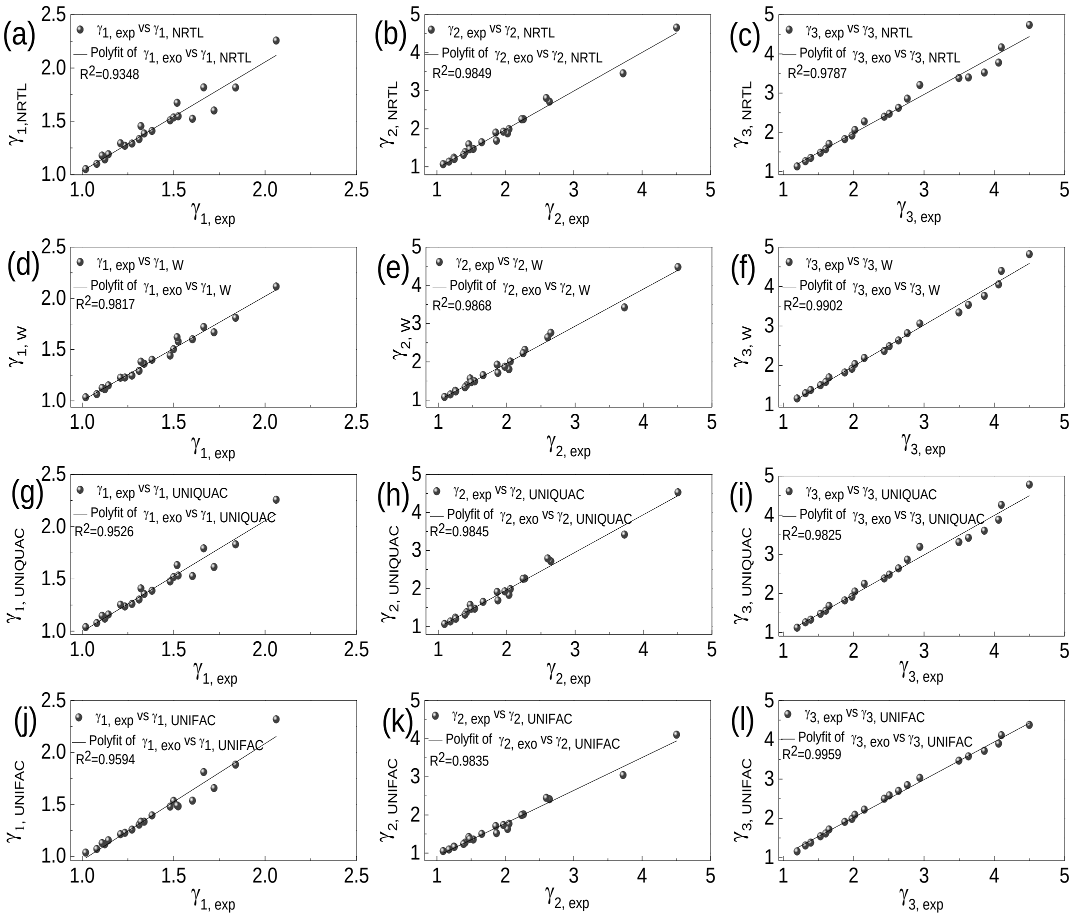

Fig. 6. Comparison of activity coefficients of AEH system at 328.15 K. MRL vs. NRTL for (a) acetone, (b)ethanol, and (c) hexane; MRL vs Wilson for (d) acetone, (e)ethanol, and(f) hexane; MRL vs UNIQUAC for (g) acetone, (h)ethanol, and (i) hexane; MRL vs UNIFAC for (j) acetone; (k)ethanol; (l) hexane.

The modified equation was applied to the AEH system and the results were comparable as presented in Fig. 7 and Fig. 8. The equation also presented good results on the additional ternary systems with the values tabulated in Table III.

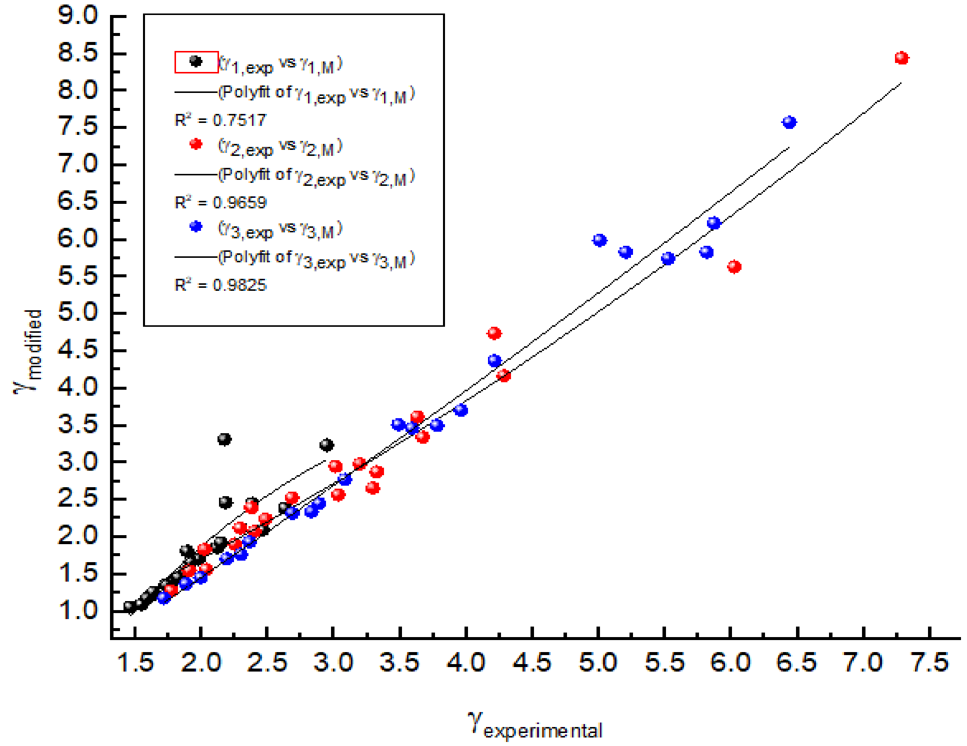

Fig. 7. Comparison of activity coefficients of AEH system at 328.15K. MRL vs. Modified Activity Coefficient Model.

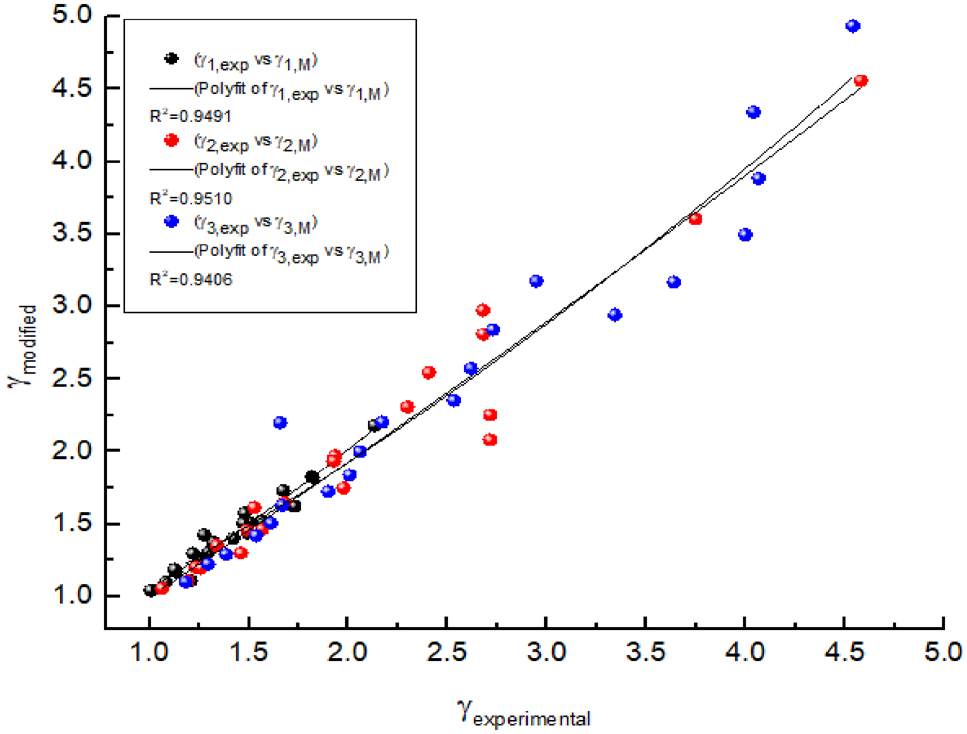

Fig. 8. Comparison of activity coefficients of AEH system at 101.33 kPa. MRL vs. Modified Activity Coefficient Model.

Table III. Comparison of activity coefficients of additional ternary systems using MRL vs. Modified Equation

ternary system	R^2		
	γ_1	γ_2	γ_3
acetone-2-propanol-water	0.8565	0.9812	0.9463
acetone-acetonitrile-water	0.9784	0.9899	0.8818
acetone-benzene-cyclohexane	0.9686	0.5252	0.9785
acetone-benzene-water	0.9972	0.9675	0.9697
acetone-cyclohexane-methanol (1)	0.8405	0.8988	0.949
acetone-cyclohexane-methanol (2)	0.596	0.8882	0.9454
acetone-cyclohexane-methanol (3)	0.2717	0.8974	0.9234
acetone-methanol-2-propanol (1)	0.8998	0.7916	0.5122
acetone-methanol-2-propanol (2)	0.9229	0.8989	0.7
acetone-methanol-benzene	0.9256	0.9766	0.9781
acetonitrile-2-propanol-benzene	0.991	0.9929	0.9923
acetonitrile-methanol-benzene	0.9959	0.9978	0.9992
butanol-acetonitrile-benzene	0.9872	0.9791	0.9824
ethanol-acetonitrile-acetone	0.9939	0.9954	0.9637
ethanol-acetonitrile-benzene	0.9982	0.9987	0.9971
acetone ethanol-hexane (isobaric)	0.9503	0.9509	0.9408
acetone ethanol-hexane (isothermal)	0.7418	0.9686	0.9822

IV. CONCLUSION

GCMs and VLE modeling were used to forecast the behavior of the AEH system at 101.33 kPa and 328.15 K utilizing 21 data points for each system. Constantinou and Gani, Nannoolal, and Domalski and Hearing methods were used to estimate the system's physical parameters such as boiling point, melting point, and heat capacity, respectively. RKEOS had the best fit for all of the relationships reported in the calculation of fugacity and fugacity coefficients as a basis of prediction of the vapor-phase properties, with R^2 up to 0.9995 for fugacity against vapor-phase composition, and ethanol had a linear relationship with its fugacity coefficient based on the outcome of the linear fitting.

The activity coefficient models used to correlate the experimental and calculated data showed good agreement, regression analyses namely goodness of fit (R^2), adjusted R^2, residual sum of squares (SSE), and root mean square error (RMSE) and revealed that the UNIFAC and Wilson models were the best fits. The same models were used to determine the bubble point and dew point temperatures and pressures, with the UNIFAC model providing the best fit among the others.

The Wilson and UNIFAC models were further applied to other ternary systems to validate the result. It was revealed that the Wilson model performs exceptionally well in predicting the behavior of the components of ternary systems, specifically on a wide range of polar organic solvents such as ketones, alcohol, nitriles, and so on; however, the model fails to provide good predictions for immiscible systems such as acetone-cyclohexane-methanol and acetone-benzene-water. Wilson's model should ideally be applied only to completely miscible liquid systems or to those limited regions of partially limited systems where only the liquid phase exists. The UNIFAC model, on the other hand, can accurately predict the interactions between the components of any mixture from a limited set of data, allowing systematic interpolation and extrapolation of VLE data for several chemically related mixtures simultaneously. The UNIFAC model has some limitations, including the inability to distinguish between isomers and the lack of consideration for the physical position of each group in the molecule, and it should not be used with mixtures containing more than ten functional groups.

The modified activity coefficient model presented comparable accuracy with the existing models such as NRTL, Wilson, UNIQUAC, and UNIFAC. The MACM was used to evaluate the activity of the AEH system and other 15 ternary systems, and the results showed that the model can be a viable option to which the molecular structure is taken into account in the calculation of a system's properties. The model can predict the activity of system components based solely on the atomic radii, number of aromatic and non-aromatic rings of the molecules. The calculation does not, however, account for the effect of the molecule's bond length and bond strength on the physical properties accounted for in the calculation.

The AEH physical properties, fugacity and fugacity coefficients, and activity coefficients could be employed to predict the AEH system's behavior for extraction and solvothermal processes. Furthermore, the activity coefficients could be a reference in designing distillation column in separating the components AEH system.

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