

Experimental Measurement and Modeling of Liquid–Liquid Equilibria for the Ternary System Water + Propan-1-ol + Ethyl Acetate

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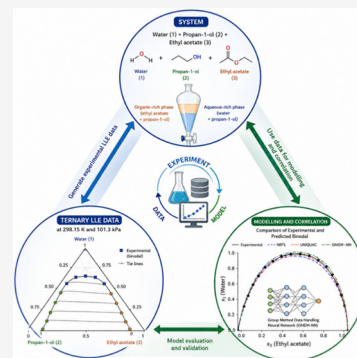
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ABSTRACT: The world's growing energy needs and the depletion of fossil fuels have driven demand for renewable alternatives, such as biofuels. Propan-1-ol is a valuable biofuel component; however, the presence of water during its production remains a significant challenge. A viable solution is liquid–liquid extraction to selectively recover propan-1-ol from a water mixture. Ethyl acetate is considered a promising solvent due to its chemical stability, eco-friendly nature, moderate water immiscibility, and favorable density difference for phase separation in a water–propan-1-ol mixture. In this study, ternary LLE measurements for water (1), propan-1-ol (2), and ethyl acetate (3) were conducted at 298.15, 313.15, and 328.15 K to evaluate ethyl acetate as a solvent for extracting propan-1-ol. The selectivity and capacity of the solvent were calculated. The experimental data were modeled using the NRTL and UNIQUAC activity models, both of which adequately describe the phase behavior, with NRTL slightly better than UNIQUAC. The group method of data handling (GMDH) neural network was also employed to complement the thermodynamic model, accurately predicting phase composition. The findings of this study show that ethyl acetate has excellent potential for selectively extracting propan-1-ol from water, with the extraction efficiency increasing with temperature.



1. INTRODUCTION

At present, approximately 80% of the total global energy resources consist of fossil fuels, which have been significantly depleted due to population growth and industrialization, negatively impacting the environment. These environmental effects include greenhouse gas emissions, ozone layer depletion, and global warming.^{1–3} The quest to reduce and perhaps replace fossil fuels has led to an increased demand for biofuels, which have been shown to be a better alternative. Biofuel has been shown to be a viable component of achieving the sustainable goal of decarbonizing the transport sector to achieve the net-zero carbon target for 2050.⁴ Propan-1-ol, a bioalcohol that has found application as a fuel and a fuel blend, is produced from renewable sources and is economically suitable for internal combustion engines,⁵ and as a component in fuel blends, its presence reduces the amount of soot emission and increases the thermodynamic efficiency of alcohol-based fuel, such as diesel fuel in compression ignition engines.⁶ Propan-1-ol has been used as a solvent for the extraction of natural products, such as fats, polar resins, oils, and others. It is also relevant for the production of other chemicals and intermediates.⁷ Despite the advantages of propan-1-ol as a fuel and fuel additive, its solubility and hygroscopicity in water are major limitations. It is therefore

necessary to extract propan-1-ol from water mixtures. It has been reported that water and propan-1-ol form a minimum boiling point azeotrope,⁸ making its separation challenging because conventional distillation cannot be used for this separation. Other separation methods, such as pressure swing distillation and azeotropic distillation, are energy-intensive. The inclusion of a third component, such as an entrainer or solvent, has the potential of eliminating the azeotrope and thereby making the separation easier and less energy-consuming; however, the choice of a suitable solvent is a fundamental consideration.⁹

The application of LLE for extracting propan-1-ol from a water mixture includes organic liquid solvents and ionic liquids. Phosphonium-based ionic liquids were used to extract propan-1-ol from water by Cumplido et al.⁷ Cyclohexanone was explored as a solvent for the extraction of propan-1-ol from water at 298.15 and 308.15 K.¹⁰ Choline chloride was explored

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Table 1. List of Chemical and Purity Analysis at 298.15 K and 88.21 kPa^a

Chemical	CAS	Supplier	Mass purity (%)	Refractive Index		Density (kg/m ³)	
				Exp	Lit	Exp	Lit
propan-1-ol	71–23–8	Merck	>99.0	1.38309	1.38304 ²⁸	799.644	799.748 ²⁹
ethyl acetate	141–78–6	Merck	>99.5	1.36983	1.36994 ³⁰	894.478	894.33 ³⁰
^b water	7732–18–5			1.33250	1.33250 ³¹	997.064	997.10 ³²

^aStandard uncertainties are $u(T) = 0.14$ K, $u(p) = 0.40$ kPa, $u(n_D) = 0.0001$, and $u(\rho) = 0.050$ kg m⁻³. ^bThe electrical conductivity of distilled water: 0.0085 μ S/cm.

as a potential solvent for the extraction of propan-1-ol from a water solution at different temperatures by Zafarani-Moattar et al.¹¹ Wales et al.¹² investigated the ternary LLE system of water + methoxycyclopentane + propan-1-ol to evaluate the ability of methoxycyclopentane to extract propan-1-ol at 298.15 K. 4-Methyl-2-pentanone was used for extracting propan-1-ol from an aqueous mixture at 283.2 and 323.2 K.¹³ The ternary LLE systems of water + propan-1-ol + ethyl acetate, methyl acetate, and propyl acetate were previously studied by Çehreli et al.¹⁴ at 298.15 K only.

Comprehensive experimental measurements across all possible operating conditions are generally infeasible due to the high cost, extensive time requirements, labor-intensive procedures, and technical constraints associated with experimental measurements.¹⁵ Robust predictive models have proven to be viable alternatives for estimating system behavior beyond the conditions captured experimentally. Artificial neural networks (ANNs) have been applied for modeling and predicting vapor–liquid equilibrium,^{16,17} liquid–liquid equilibrium,¹⁸ thermodynamic and excess properties,^{19,20} and other aspects of phase equilibria. The group method of data handling (GMDH) neural network is a self-organizing neural network that uses a nonlinear polynomial to model the relationship between input variables and predict outputs. GMDH has been applied to predict the solubility of carbon dioxide in ionic liquids,²¹ LLE prediction of ethanol + acetic acid + 2-ethyl-1-hexanol,²² LLE systems of water + propionic acid with different solvents,²³ and other predictions in chemical engineering.

Despite previous work on the extraction of propan-1-ol from water using various solvents, it is essential to consolidate these studies by evaluating the viability of alternative solvents under different conditions.¹⁴ Therefore, the present work presents new LLE ternary experimental data for water (1) + propan-1-ol (2) + ethyl acetate (3) at 298.15, 313.15, and 328.15 K, thereby extending the previous study¹⁴ to 313.15 and 328.15 K, with a view of evaluating the effect of temperature changes on the phase behavior and solubility of the solute in both aqueous and organic phases. A rigorous homotopy-based stability-constrained parameter estimation methodology was also applied to estimate the temperature-dependent and temperature-independent binary interaction parameters for both the NRTL and UNIQUAC activity models. The distribution coefficients and selectivity were calculated and compared to those of different solvents. The group method of data handling (GMDH) neural network model was also used to develop a machine-learning model that adequately predicts the outputs via polynomial equations that capture the nonlinear relationships between inputs.

2. EXPERIMENTAL SECTION

2.1. Materials

The list of chemicals used in the experiment, their suppliers, and the reported purities are presented in Table 1. Both propan-1-ol and ethyl acetate were purchased from Merck, while the distilled water used was obtained from the laboratory in the School of Chemical and Minerals Engineering at the North-West University. Purity checks were further carried out by measuring the refractive index and density of the chemicals with an Atago refractometer model RX-7000i and an Anton Paar densitometer model DSA 5000M, as presented in Table 1. The measured values are very similar to those reported in the literature; therefore, no further purification was carried out.

2.2. Equipment, Apparatus, and Procedure

The direct method of analysis was employed to conduct LLE experiments using a double-walled glass cell, as shown in Figure 1.

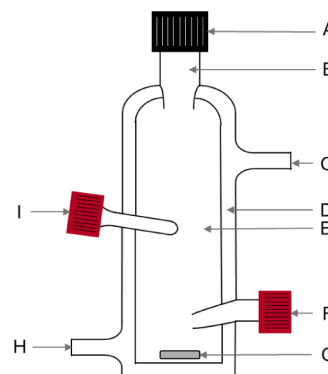


Figure 1. Schematic of double-walled glass cell modified from Venter et al.,²⁵ A: top sampling port cap; B: sampling port of the top phase; C: outlet of hot water from the heating jacket; D: cell wall of the heating jacket; E: inner cell; F: bottom sampling port secured with a chemical-resistant cap; G: magnetic stirrer; H: water inlet for heating; I: thermowell for the temperature probe. Adapted from Venter et al.²⁵ Copyright 2026 American Chemical Society.

The modified glass cell designed by Narasigadu et al.²⁴ was utilized as the base design. Previous modifications included an adjustable thermowell, a magnetic stirrer, and a dedicated sampling port for the denser phase. In a study conducted by Venter et al.,²⁵ the top sampling port was reduced in size (A). This design is further improved by adjusting the position of the bottom sampling port (F) at an angle to minimize LLE formation within the sampling port (F) and minimize disruption of thermodynamic equilibrium during sampling. These improvements provide more accurate temperature measurements and better sampling of the denser phase while causing minimal disturbance to the equilibrium.

The methodology, as outlined by Alders²⁶ was followed. Water and ethyl acetate were added to the glass cell with the resulting liquid–liquid interface positioned above the lowest sampling point. The mixture filled the cell to a level minimizing the vapor space while leaving space for thorough mixing. The water bath was set to the experimental temperature as estimated by the PT-100 temperature sensor, calibrated with a standard Wika CTH 6500 thermometer, with

Table 2. Experimental LLE Data for the Water (1) + Propan-1-ol (2) + Ethyl Acetate (3) system at 88.21 kPa^a

Organic-rich phase			Aqueous Phase			D	S
x_1	x_2	x_3	x_1	x_2	x_3		
298.15 K							
0.1472	0.0000	0.8528	0.9800	0.0000	0.0200	-	-
0.1824	0.0247	0.7930	0.9763	0.0042	0.0196	5.8810	31.4779
0.2341	0.0699	0.6960	0.9672	0.0108	0.0220	6.4722	26.7404
0.2875	0.1080	0.6045	0.9612	0.0164	0.0224	6.5854	22.0169
0.3488	0.1396	0.5116	0.9549	0.0218	0.0233	6.4037	17.5311
0.4024	0.1662	0.4313	0.9518	0.0261	0.0221	6.3678	15.0618
313.15 K							
0.1645	0.0000	0.8355	0.9772	0.0000	0.0228	-	-
0.2088	0.0266	0.7645	0.9754	0.0034	0.0212	7.8235	36.5473
0.2550	0.0694	0.6756	0.9688	0.0089	0.0223	7.7978	29.6253
0.3098	0.1057	0.5845	0.9640	0.0138	0.0222	7.6594	23.8337
0.3586	0.1372	0.5041	0.9570	0.0196	0.0234	7.0000	18.6810
0.4188	0.1635	0.4177	0.9552	0.0235	0.0213	6.9574	15.8686
328.15 K							
0.1723	0.0000	0.8277	0.9777	0.0000	0.0223	-	-
0.2369	0.0251	0.7379	0.9766	0.0027	0.0207	9.2963	38.3232
0.2845	0.0683	0.6472	0.9701	0.0078	0.0221	8.7564	29.8580
0.3347	0.1017	0.5636	0.9647	0.0125	0.0229	8.1360	23.4503
0.4041	0.1295	0.4664	0.9573	0.0184	0.0243	7.0380	16.6729
0.4599	0.1538	0.3864	0.9520	0.0229	0.0252	6.7162	13.9025

^aStandard and expanded uncertainties are $u(T) = 0.22$ K, $u(p) = 0.40$ kPa, $u(x) = 0.0010$.

an uncertainty of 0.22 K ($k = 2$). The water was circulated through the water jacket to ensure a constant temperature throughout the cell. The binary mixture was then stirred for 45 min and allowed to reach equilibrium for 2 h, after which a gas-tight syringe was used to withdraw samples for analysis on the Shimadzu 2030 gas chromatograph (GC) with a thermal conductivity detector (TCD) with a 2 m long Porapak Q packed column with an inner diameter of 2 mm, with helium as the carrier gas. Thermodynamic equilibrium was considered achieved only when the maximum composition error between three consecutive samples was less than 1%, and the average composition was then taken. The area-ratio method, as described by Raal and Mühlbauer,²⁷ was applied to the GC detector calibration using ethanol as the internal standard. The combined uncertainty for GC composition measurements was 0.0034 ($k = 2$). Details of the methodology used in this work can be found in our previous publication.²⁵

2.3. Uncertainty Analysis

The uncertainties in this study were evaluated following the Guide to the Expression of Uncertainty in Measurement (GUM)³³ and the equations are presented below.

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i \quad (1)$$

$$s(x_i) = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n - 1}} \quad (2)$$

$$u = \frac{s(x_i)}{\sqrt{n}} \quad (3)$$

Where x_i is an experimental measurement of a given quantity, while $\bar{x}$ and $s(x_i)$ are the average and standard deviation of n numbers of x_i , respectively, and u is the standard uncertainty. The method used for calculating propagated uncertainty is reported by Farrance and Frenkel.³⁴

2.4. Group Method of Data Handling

The group method of data handling (GMDH) algorithm is a self-organizing algorithm that uses the feedforward network to model data

and develop a hidden pattern that serves as a function relating the inputs to the outputs. These functions obtained via GMDH are often in the form of a polynomial, referred to as the Kolmogorov–Gabor polynomial.³⁵ In GMDH, the input function via the input layer is linked to the hidden-layer neurons by selecting different pairs using a quadratic function. This pattern of connections is transferred from one layer to the next until it gets to the output layers. It is often necessary to determine the coefficients of a quadratic function using regression to obtain the best coefficients that minimize the error between the experimental data and the GMDH predictions.^{22,36,37} The function f combines the n number of inputs ($x_{i1}, x_{i2}, x_{i3}, \dots, x_{in}$) of i th observation in a nonlinear relation to the outputs y_i and uses the same set of inputs to predict the outputs for K number of observations, as shown in eq 4. The difference between the observed and predicted outputs, given in eq 5, is minimized by fitting the GMDH polynomial coefficients.

$$y_i = f(x_{i1}, x_{i2}, x_{i3}, \dots, x_{in}) \quad (4)$$

$$\text{Objective function} = \sum_i^K (\hat{y}_i - y_i)^2 \quad (5)$$

The general form for the polynomial for the GMDH that shows the connections between the inputs and the outputs is shown in eq 6, which is a form of the Volterra function series,³⁷ known as Kolmogorov–Gabor polynomial given in eq 6.

$$y = a_0 + \sum_{i=1}^n a_i x_i + \sum_{i=1}^n \sum_{j=1}^n a_{ij} x_i x_j + \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n a_{ijk} x_i x_j x_k + \dots \quad (6)$$

The Kolmogorov–Gabor polynomial in eq 6 can be presented in a more simplified quadratic form as given in eq 7.

$$\hat{y} = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + a_4 x_4^2 + a_5 x_5^2 \dots \quad (7)$$

a_i denotes the quadratic coefficients that are obtained by the regression techniques.

The suitability and the performance of the GMDH modeling were evaluated using the absolute fraction of variance R^2 , root-mean-square

error (RMSE), and mean absolute error (MAE) in eqs 8, 9, and 10, respectively.

$$R^2 = 1 - \left[\frac{\sum_{i=1}^K (\hat{y}_i - y_i)^2}{\sum_{i=1}^K (y_i)^2} \right] \quad (8)$$

$$\text{RMSE} = \left[\frac{\sum_{i=1}^K (\hat{y}_i - y_i)^2}{K} \right]^{1/2} \quad (9)$$

$$\text{MAE} = \frac{\sum_{i=1}^K |\hat{y}_i - y_i|}{K} \quad (10)$$

3. RESULTS AND DISCUSSION

3.1. Experimental Results

LLE data for the water (1) + propan-1-ol (2) + ethyl acetate (3) system were measured at three different temperatures: 298.15, 313.15, and 328.15 K. The experimental data and the calculated distribution coefficients and selectivity are presented in Table 2. The ternary liquid–liquid equilibrium plots are presented in Figure 2a, b and c for measurements at 298.15, 313.15, and 328.15 K, respectively.

The distribution coefficient and the selectivity are two important parameters for evaluating the effectiveness of a solvent for extracting a solute via a liquid–liquid extraction process. A high distribution coefficient indicates that a large portion of the solute is preferably transferred to the organic phase rather than the aqueous phase. High selectivity indicates that the solvent has a stronger affinity for the solute than water does.

The distribution coefficient (D) and selectivity (S) of the systems were evaluated using eqs 11 and 12, respectively, where x_2 is the mole fraction of propan-1-ol and x_1 is the mole fraction of water, while the superscripts O and W are organic-rich and aqueous phases, respectively.

$$D_2 = \frac{(x_2)^O}{(x_2)^W} \quad (11)$$

$$S = \frac{(x_2)^O / (x_2)^W}{(x_1)^O / (x_1)^W} \quad (12)$$

The values of D and S presented in Table 2 are greater than 1, which implies that ethyl acetate is a good solvent extractor of propan-1-ol from its aqueous mixtures. The plots of the mole fraction of propan-1-ol in the organic phase against selectivity and distribution coefficient at the indicated temperatures are shown in Figure 3a and b, respectively. The plots show that as the mole fraction of propan-1-ol increases, the selectivity and distribution coefficient decrease. It was also observed that increasing temperature increases selectivity, but at higher mole fractions of propan-1-ol in the organic phase, temperature changes have a negligible effect. The plot in Figure 3b shows that at 298.15 K, the distribution coefficient initially increases with propan-1-ol mole fraction, passes through a maximum value of $x_2 \approx 0.3$, and then decreases as the organic phase approaches saturation with the solute. At 313.15 and 328.15 K, this maximum is not observed, and the distribution coefficient decreases monotonically with increasing x_2 , because the higher temperatures increase the solubility of propan-1-ol in the organic phase.

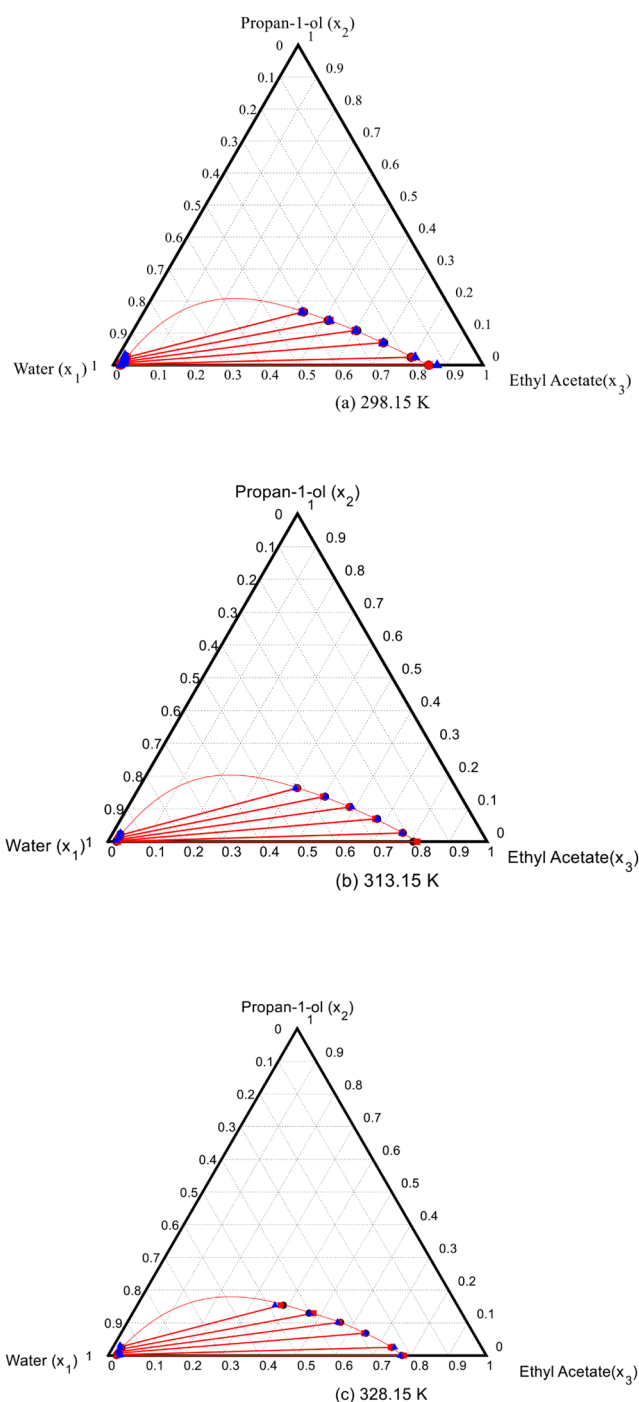


Figure 2. Ternary plot for the water (1) + propan-1-ol (2) + ethyl acetate (3) system at (a) 298.15 K, (b) 308.15 K, and (c) 328.15 K, ●: experimental data, ■: NRTL-fitted data, ▲: UNIQUAC-fitted data.

Generally, as the temperature increases, the selectivity and distribution coefficients increase. This is attributed to the disruption of hydrogen bonds and interactions between the molecules of propan-1-ol and water in the aqueous phase, which lower their mutual affinity and promote the transfer of propan-1-ol to the organic phase, thereby increasing the distribution coefficient and the selectivity.

The comparison of the extraction capacity of ethyl acetate with other solvents is presented in Table 3. Ethyl acetate showed consistently high distribution coefficients (5.8810–

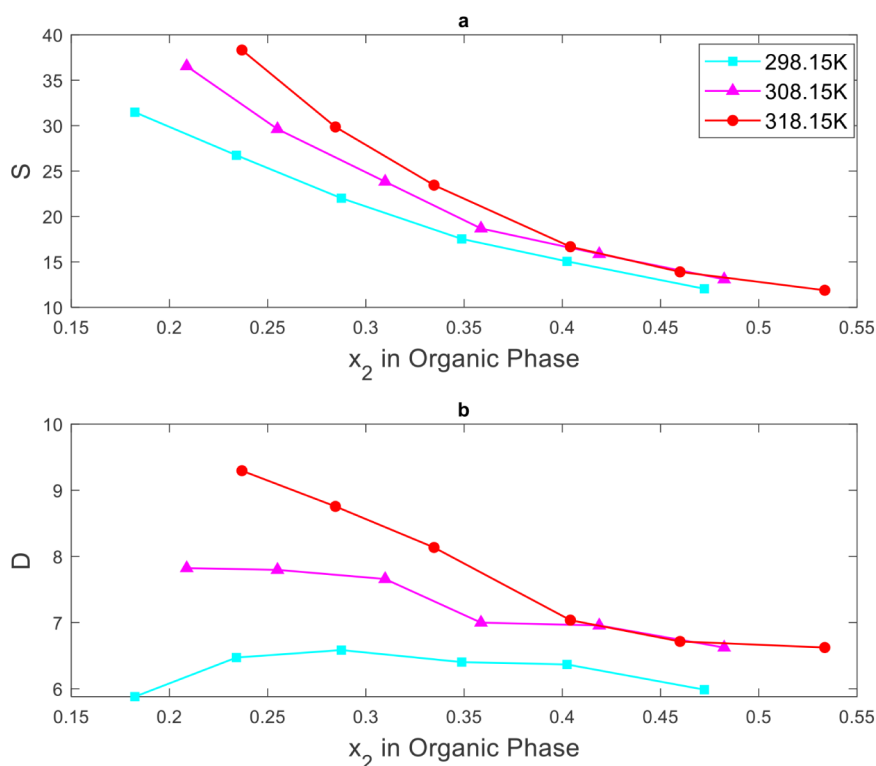


Figure 3. (a) Separation factor and (b) distribution coefficients.

Table 3. Comparison of the Extraction of Propan-1-ol from Aqueous Solution with Different Solvent

Solvent	Temperature (K)	D	S	Reference
Cyclohexanone	298.15	3.27–5.94	4.52–15.43	Wang et al. ¹⁰
Methoxycyclopentane	298.15	5.83–7.64	10.67–40.04	Wales et al. ¹²
methyl acetate	298.15	2.02–2.72	2.61–4.39	Çehreli et al. ¹⁴
Ethyl acetate	298.15	5.88–6.37	15.06–31.48	This work
<i>n</i> -Propyl acetate	298.15	4.46–8.81	6.92–35.57	Çehreli et al. ¹⁴
Cyclohexanone	308.15	3.74–7.27	5.30–18.36	Wang et al. ¹⁰
Ethyl acetate	313.15	6.96–7.82	15.87–36.55	This work
Ethyl acetate	318.15	6.72–9.30	13.90–38.32	This work

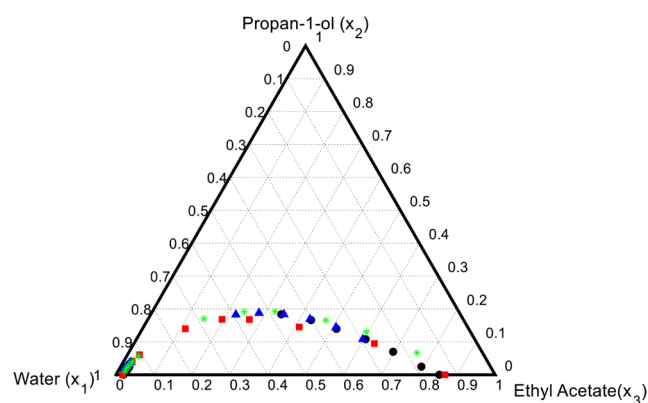


Figure 4. Experimental ternary data of the water (1) + propan-1-ol (2) + ethyl acetate (3) system: black circle, experimental data; red square: Çehreli et al.,¹⁴ blue triangle: Perestrelo et al.,³⁸ and green star: Beech and Glasstone.³⁹

6.3678), comparable to those reported for methoxycyclopentane (5.8301–7.6439) and substantially higher than those of cyclohexanone (3.2654–5.9427). The selectivity of ethyl acetate (15.0618–31.478) as against the previously reported

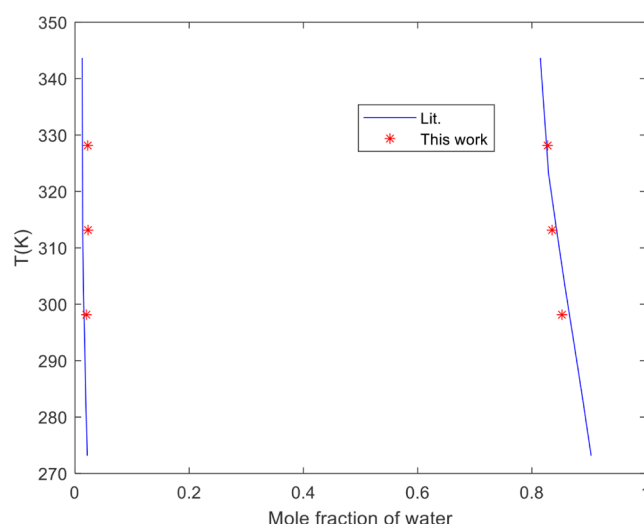


Figure 5. Comparison of mutual solubility of water and ethyl acetate in the study and the literature⁴⁰.

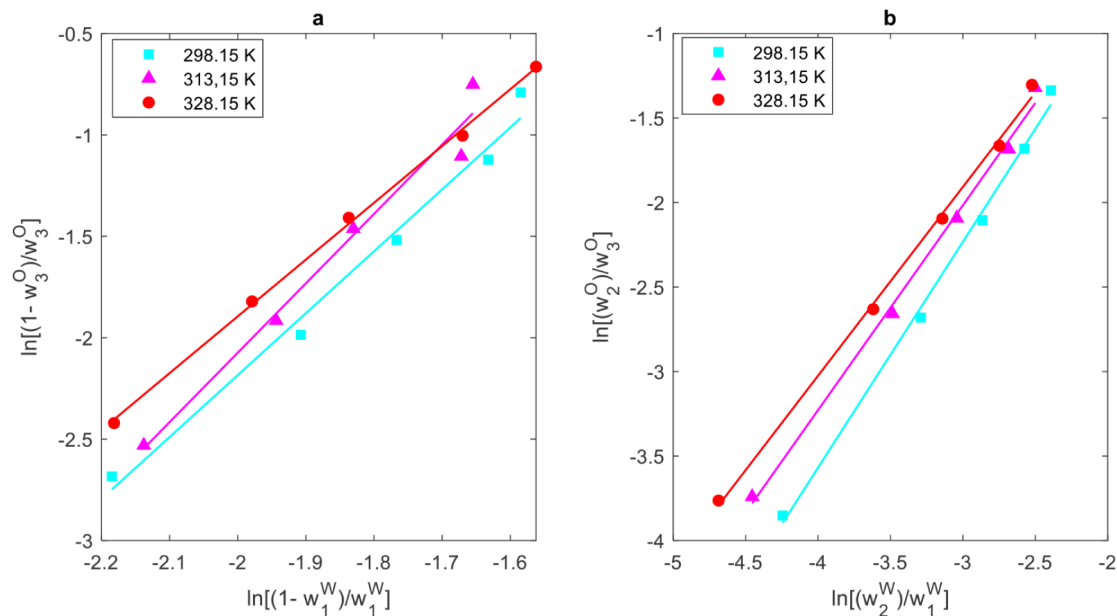


Figure 6. (a) Othmer–Tobias and (b) Hand equation plots for the water (1) + propan-1-ol (2) + ethyl acetate (3) system.

Table 4. Regression Parameters and R^2 Values for Othmer–Tobias and Hand Equations

T (K)	Othmer–Tobias			Hand equation		
	a	b	R^2	a	b	R^2
298.15	3.9217	3.0529	0.9852	1.7769	1.3365	0.9960
313.15	4.7706	3.4222	0.9761	1.6194	1.2120	0.9956
328.15	3.7050	2.7998	0.9987	1.4442	1.1173	0.9975

highest value of 24.9728,¹⁴ the selectivity of ethyl acetate is higher than that of methyl acetate (2.6113–8.2799) and that of cyclohexanone (4.5214–15.4275), which indicates a stronger preference for the extraction of propan-1-ol in water. Although *n*-propyl acetate and methoxycyclopentane have broader selectivity ranges of 6.9160–35.5659 and 10.673–40.043, respectively, ethyl acetate’s performance falls within these ranges, thereby demonstrating that both solvents possess excellent capabilities.

The results of this study were compared with those reported by Çehreli et al.¹⁴ and Perestrelo et al.³⁸ for the comparison of the experimental data measured at 298.15 K and also compared with the data obtained by Beech and Glasstone³⁹ at 293.15 K. The comparison plot in Figure 4 shows that the data reported in this study have a similar trend to those reported by Çehreli et al.¹⁴ The trend and similarity in both data confirm the validity of the measurement carried out in this study. The experimental data reported by Perestrelo et al.³⁸ greatly aligns with those reported in the study and overlap at some data points. The data from Beech and Glasstone³⁹ also follow similar trend with those obtained in this work, but the composition in the ethyl acetate-rich phase were slightly higher, this could be attributed to temperature difference of 5 K. The mutual solubility of the binary system of water + ethyl acetate was compared with data reported by Stephenson and

Table 5. Parameters for the NRTL and UNIQUAC Models

T (K)	$i-j$	NRTL				UNIQUAC		
		a_{ij}	a_{ji}	α_{ij}	RMSD	a_{ij}	a_{ji}	RMSD
298.15	1–2	3.3686	−0.5125	0.3398	0.0019	1.336	−3.7503	0.0035
	1–3	3.3118	1.5885	0.3451		−0.2581	−1.3182	
	2–3	0.8183	0.3185	0.2226		2.6052	−3.3931	
313.15	1–2	3.5135	−1.3188	0.2443	0.0028	1.344	−3.5774	0.008
	1–3	3.3872	0.8158	0.2612		−0.4485	−1.0151	
	2–3	1.3396	−1.5366	0.1838		2.5847	−2.9773	
328.15	1–2	3.5224	−0.5791	0.4360	0.0029	1.6015	−4.3224	0.0042
	1–3	3.3408	1.2311	0.3263		−0.349	−0.9613	
	2–3	1.3245	−0.3550	0.3954		2.6553	−3.3151	
T-dependent	1–2	−0.981766	−0.14932	0.446383	0.0172	1.22751	−3.047345	0.0228
	1–3	4.11162	1.062698	0.35763		−0.348348	−0.97128	
	2–3	−1.43998	−1.74137	0.376563		2.374645	−2.56445	
		b_{ij}	b_{ji}			b_{ij}	b_{ji}	
	1–2	400.9789	−46.42770			42.71053	−195.454	
	1–3	218.938	270.063			−16.3001	−33.79515	
	2–3	398.492	71.95780			73.54484	−141.716	

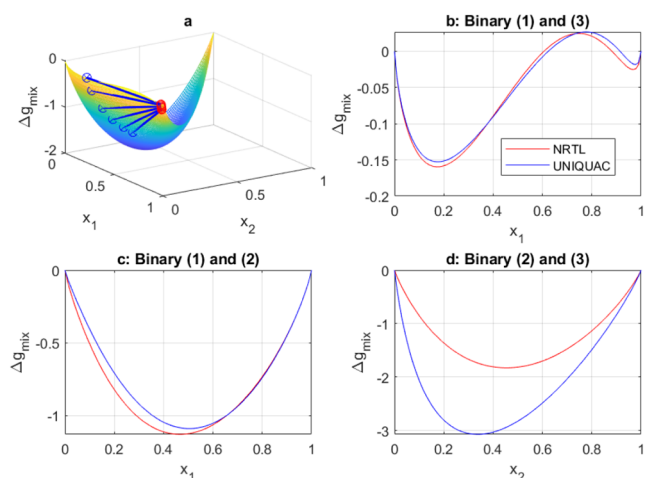


Figure 7. Gibbs excess energy plots: (a) ternary system; (b) water (1) – ethyl acetate (3) binary subsystem; (c) water (1) – propan-1-ol (2) binary subsystem; and (d) propan-1-ol (2) – ethyl acetate (3).

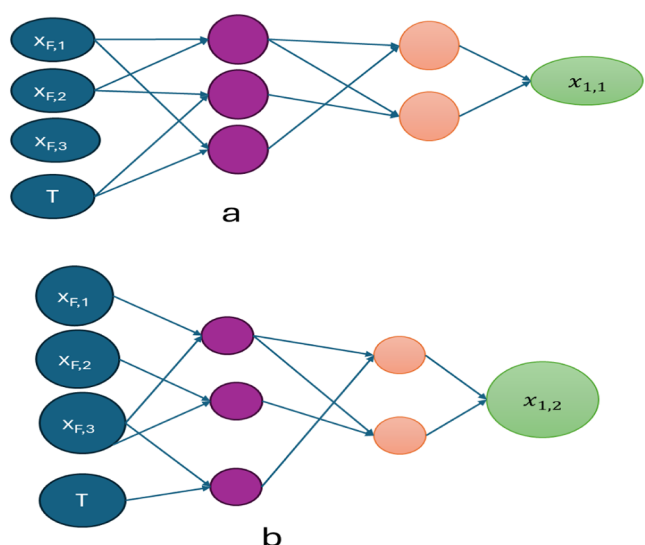


Figure 8. GMDH structure for the organic phase compositions: (a) composition of water and (b) composition of propan-1-ol.

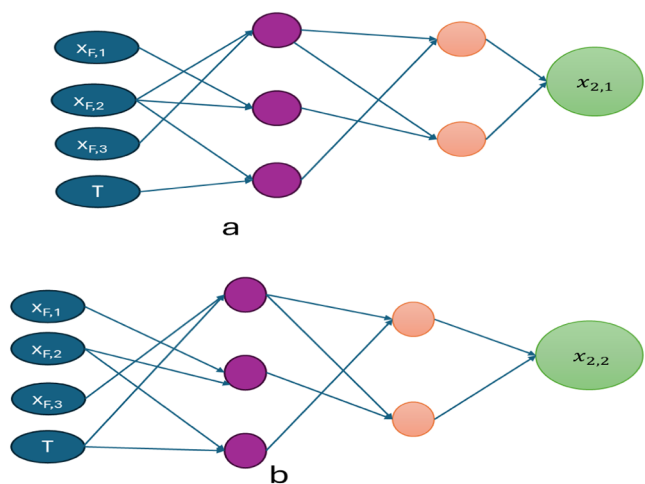


Figure 9. GMDH structure for the aqueous phase compositions: (a) composition of water and (b) composition of propan-1-ol.

Stuart⁴⁰ as presented in Figure 5. The solubility data measured in this study align closely with the literature solubility curve.

3.2. Consistency Evaluation of Experimental Data

The LLE data consistency in this study was checked using the Othmer–Tobias⁴¹ and Hand⁴² equations as presented in eqs 13 and 14, respectively.

$$\ln\left(\frac{1 - w_3^O}{w_3^O}\right) = a + b \times \ln\left(\frac{1 - w_1^W}{w_1^W}\right) \quad (13)$$

$$\ln\left(\frac{w_2^O}{w_3^O}\right) = a + b \times \ln\left(\frac{w_2^W}{w_1^W}\right) \quad (14)$$

Where w_i^O and w_i^W are the weight fractions of component i in the organic and aqueous phases, respectively. And a and b are parameters that are obtained from the linear regression of the experimental data. The Othmer–Tobias and Hand's plots are shown in Figure 6a and b, respectively. The parameters of the equation are presented in Table 4. The R^2 for both equations, at all temperatures, is greater than 0.97, which implies that the experimental data are highly consistent.

3.3. LLE Data Correlation Using Activity Models

The experimental LLE data were correlated using the Gibbs excess-activity NRTL and UNIQUAC models to account for nonideality. The binary interaction parameters for the NRTL and UNIQUAC activity models were evaluated using the parameter problem formulation developed by Bamikole et al.,¹⁵ in which the homotopy continuation method was applied to track the tie-lines and ensure that the experimental tie-lines lie below the Gibbs excess energy surface plot and thus satisfy the stability criteria. Details of this formulation can be found in Bamikole et al.¹⁵ The Pelican–Gorilla hybrid stochastic algorithms developed by Bamikole and Narasigadu⁴³ were used to solve the parameter estimation problem. The binary interaction format used in this study is presented in eqs 15 and 16 for the NRTL and UNIQUAC models, respectively, where a_{ij} and b_{ij} are, respectively, the temperature-independent and temperature-dependent components of the binary interaction parameters obtained during the optimization process. The objective function of the optimization problem is given in eq 17. The objective function ensures that the set of obtained parameters minimizes the discrepancies between the experimental composition $x_{i,j,k}^{\text{exp}}$ and the predicted composition $x_{i,j,k}^{\text{cal}}$ of component i , phase j , and tie-line k , and nt is the number of tie-lines. Aside from the objective function value in eq 17, the fitness of the model parameters was evaluated using root-mean-square deviation (RMSD) in eq 18.

$$\tau_{i,j} = a_{i,j} + \frac{b_{i,j}}{T} \quad (15)$$

$$\tau_{i,j} = \exp\left(a_{i,j} + \frac{b_{i,j}}{T}\right) \quad (16)$$

$$\text{objective function} = \sum_k^{nt} \sum_j^2 \sum_i^3 \left(x_{i,j,k}^{\text{cal}} - x_{i,j,k}^{\text{exp}}\right)^2 \quad (17)$$

$$\text{RMSD} = \left[\sum_k^{nt} \sum_j^2 \sum_i^3 \frac{\left(x_{i,j,k}^{\text{cal}} - x_{i,j,k}^{\text{exp}}\right)^2}{6nt} \right]^{0.5} \quad (18)$$

Table 6. Quadratic Equation for the GMDH Model for the LLE Systems

The mole fraction of water in the organic phase ($x_{1,1}$)
$y_1 = 0.23156 - 0.64662x_{F1} + 0.16850x_{F2} + 0.67037x_{F1}^2 - 0.02573x_{F2}^2$ $+ 1.82379x_{F1}x_{F2}$
$y_2 = 0.04274 + 1.58508x_{F2} + 0.18642T - 0.85476x_{F2}^2 + 0.02915T^2$ $- 0.15361x_{F2}T$
$y_3 = 0.04274 + 1.58508x_{F1} + 0.18642T - 0.85476x_{F1}^2 + 0.02915T^2$ $- 0.15361x_{F1}T$
$z_1 = -0.15939 + 0.95834y_1 + 0.13700y_3 + 0.07404y_1^2 + 0.54587y_3^2$ $- 0.11874y_1y_3$
$z_2 = -0.06930 + 0.23391y_1 + 0.97124y_2 + 1.00668y_1^2 - 0.22972y_2^2$ $- 0.93515y_1y_2$
$x_{1,1} = -0.002698 + 1.339267z_1 - 0.271212z_2 - 2.573104z_1^2 - 0.689347z_2^2$ $+ 3.185967z_1z_2$
The mole fraction of propan-1-ol in the organic phase ($x_{1,2}$)
$y_1 = -11.34636 + 34.73340x_{F1} + 27.74696x_{F3} - 22.75339x_{F1}^2$ $- 16.29423x_{F3}^2 - 40.18608x_{F1}x_{F3}$
$y_2 = 0.23556 + 2.67643x_{F2} - 1.05707x_{F3} - 1.07519x_{F2}^2 + 0.92673x_{F3}^2$ $- 1.48769x_{F2}x_{F3}$
$y_3 = 0.62661 + 0.28595x_{F3} - 0.08760T - 0.99023x_{F3}^2 - 0.00254T^2$ $+ 0.03002x_{F3}T$
$z_1 = -0.04731 + 0.68062y_1 + 0.69216y_3 - 0.18829y_1^2 - 1.19325y_3^2$ $+ 0.93377y_1y_3$
$z_2 = -0.04667 + 0.67734y_2 + 0.69093y_3 - 0.18549y_2^2 - 1.19122y_3^2$ $+ 0.93397y_2y_3$
$x_{1,2} = 0.004353 - 35.717539z_1 + 36.692038z_2 + 46.973811z_1^2$ $- 47.187900z_2^2 + 0.236203z_1z_2$
The mole fraction of ethyl acetate in the organic phase ($x_{1,3}$)
$y_1 = 0.77625 + 0.70985x_{F1} - 0.35501x_{F2} - 0.69011x_{F1}^2 + 0.23582x_{F2}^2$ $- 2.04068x_{F1}x_{F2}$
$y_2 = 4.41098 - 17.70176x_{F1} - 8.95378x_{F3} + 13.71221x_{F1}^2 + 5.31877x_{F3}^2$ $+ 20.04002x_{F1}x_{F3}$
$y_3 = 0.94837 - 1.74154x_{F2} - 0.08382T + 0.92952x_{F2}^2 - 0.02352T^2$ $+ 0.06111x_{F2}T$
$y_4 = 0.91501 - 1.41546x_{F1} - 0.09794T + 1.16276x_{F1}^2 + 0.11019T^2$ $- 0.08938x_{F1}T$
$z_1 = 0.04380 + 1.18827y_2 - 0.29392y_3 - 1.00520y_2^2 - 0.29807y_3^2$ $+ 1.39541y_2y_3$
$z_2 = 0.20686 + 0.03439y_1 + 0.24726y_4 - 0.09287y_1^2 - 1.39851y_4^2$ $+ 2.12390y_1y_4$
$x_{1,3} = 0.001771 - 0.096296z_1 + 1.095311z_2 - 1.361276z_1^2 - 2.316356z_2^2$ $+ 3.682367z_1z_2$

Table 6. continued

The mole fraction of water in the organic phase ($x_{1,1}$)
The mole fraction of water in the aqueous phase ($x_{2,1}$)
$y_1 = 7.75950 - 25.37669x_{F1} - 17.12351x_{F3} + 17.99063x_{F1}^2 + 10.20935x_{F3}^2$ $+ 29.36176x_{F1}x_{F3}$
$y_2 = 0.84594 + 0.79861x_{F1} - 0.69564x_{F2} - 0.85260x_{F1}^2 + 0.45308x_{F2}^2$ $- 2.01078x_{F1}x_{F2}$
$y_3 = 0.87581 - 1.66177x_{F1} + 0.14496T + 1.35090x_{F1}^2 + 0.04652T^2$ $- 0.15711x_{F1}T$
$z_1 = 0.30187 + 0.74821y_1 - 0.83349y_3 - 0.05697y_1^2 + 0.34669y_3^2$ $+ 0.64975y_1y_3$
$z_2 = 0.00111 - 10.95616y_1 + 11.93445y_2 + 14.60459y_1^2 - 14.64969y_2^2$ $+ 0.07324y_1y_2$
$x_{2,1} = 0.008395 + 0.895114z_1 + 0.087069z_2 - 12.615953z_1^2 - 12.969272z_2^2$ $+ 25.604759z_1z_2$
The mole fraction of propan-1-ol in the aqueous phase ($x_{2,2}$)
$y_1 = 0.19350 + 2.45547x_{F1} - 0.89662x_{F3} - 0.78072x_{F1}^2 + 0.79839x_{F3}^2$ $- 1.63987x_{F1}x_{F3}$
$y_2 = 0.09521 - 0.67674x_{F1} + 0.66932x_{F2} + 0.74611x_{F1}^2 - 0.40259x_{F2}^2$ $+ 1.90802x_{F1}x_{F2}$
$y_3 = 0.05828 + 2.10216x_{F2} - 0.17437T - 1.19757x_{F2}^2 + 0.11659T^2$ $- 0.18472x_{F2}T$
$z_1 = -0.01438 + 0.91430y_1 + 0.08606y_3 + 0.47618y_1^2 + 0.49847y_3^2$ $- 0.96261y_1y_3$
$z_2 = -0.01437 + 0.91458y_2 + 0.08586y_3 + 0.47484y_2^2 + 0.49779y_3^2$ $- 0.96062y_2y_3$
$x_{2,2} = -0.000245 + 57.088534z_1 - 56.080630z_2 + 59.065202z_1^2$ $- 59.072411z_2^2 - 0.004130z_1z_2$
The mole fraction ethyl acetate in the aqueous phase ($x_{2,3}$)
$y_1 = 0.13220 + 1.10708x_{F2} - 0.30354T - 0.78143x_{F2}^2 + -0.01940T^2$ $- 0.23018x_{F2}T$
$y_2 = -8.01196 + 20.74495x_{F1} + 20.00861x_{F3} - 12.16410x_{F1}^2$ $+ -11.70870x_{F3}^2 - 24.52017x_{F1}x_{F3}$
$y_3 = 0.28776 - 0.47948x_{F1} + 0.71589x_{F2} + 0.59735x_{F1}^2 - 0.51648x_{F2}^2$ $+ 0.39387x_{F1}x_{F2}$
$z_1 = 0.06446 + 1.83240y_1 - 1.41055y_3 - 1.48171y_1^2 + 2.18414y_3^2$ $+ 0.23499y_1y_3$
$z_3 = 0.06104 + 1.83122y_1 - 1.39199y_2 - 1.47442y_1^2 + 2.16819y_2^2$ $+ 0.22320y_1y_2$
$x_{2,3} = -0.177622 + 80.440963z_1 - 78.320761z_3 - 6.851815z_1^2$ $+ 6.355550z_3^2 - 0.947137z_1z_3$

The estimated interaction parameters for the activity model are given in Table 5. The estimated parameters were used to calculate the mole fractions; the predicted mole fractions from

both the NRTL and UNIQUAC models are very similar to the experimental mole fractions, as shown in the ternary plots in Figure 2a, b, and c. The Gibbs excess energy and tie lines are

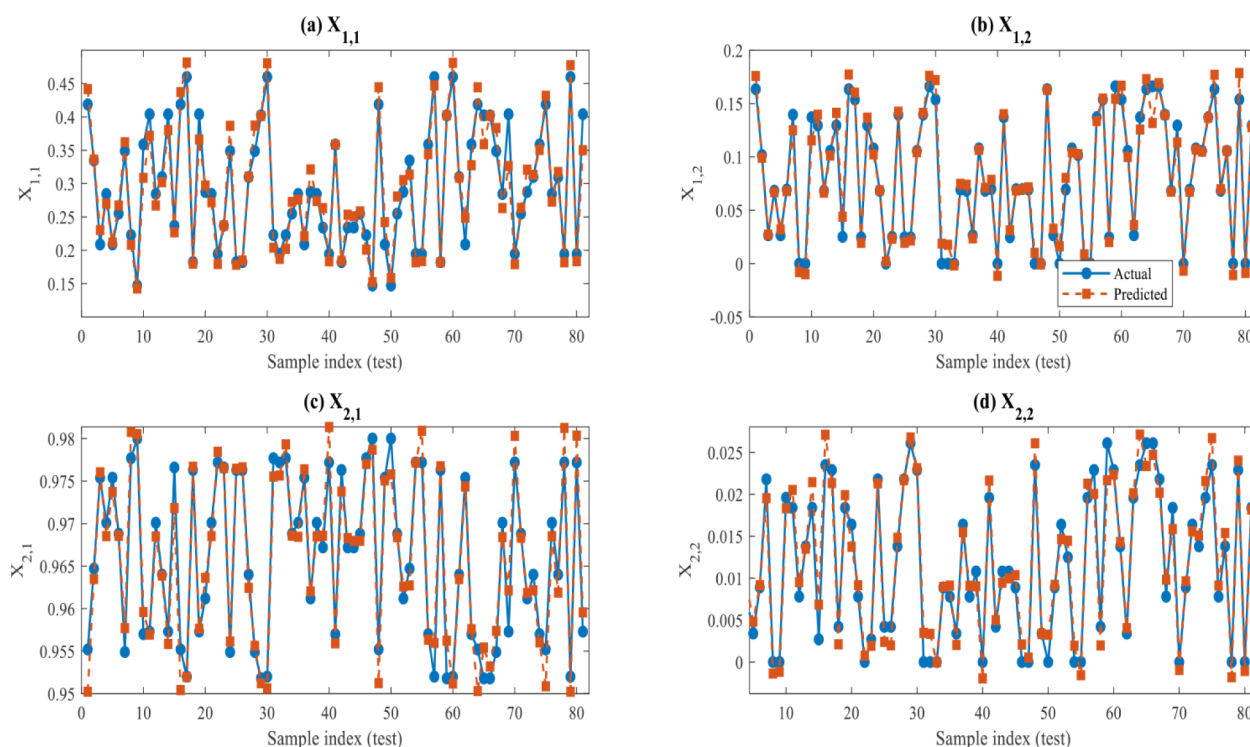


Figure 10. Comparison between the experimental and predicted data using the GMDH model: (a) $x_{1,1}$, (b) $x_{1,2}$, (c) $x_{2,1}$, and (d) $x_{2,2}$.

Table 7. Performance Indices for the GMDH Model for Predicting the LLE System

Output	Training			Testing		
	RMSE	MAE	R^2	RMSE	MAE	R^2
$x_{1,1}$	0.02152	0.01615	0.9382	0.01994	0.01487	0.9529
$x_{1,2}$	0.00706	0.00462	0.9849	0.00851	0.00538	0.9774
$x_{2,1}$	0.00181	0.00143	0.9628	0.00170	0.00130	0.9680
$x_{2,2}$	0.00168	0.00123	0.9620	0.00184	0.00127	0.9554

shown in Figure 7a. As shown in Figure 7a, all tie lines lie below the Gibbs energy surface, indicating that the Gibbs stability criterion is satisfied by the estimated parameters. The studied system is a type I LLE system, as classified by Treybal.⁴⁴ Figure 7b shows the binary plot of the subsystem (1)–(3) exhibits partial miscibility, while subsystems (1)–(2) and (2)–(3) are completely miscible, as shown in Figure 7c and d, which is consistent with the experimental data. The RMSD values in Table 5 indicate that the NRTL model outperformed the UNIQUAC model at all experimental temperatures. The RMSD value in this study for the UNIQUAC model at 298.15 K is 0.0035, which is far lower than 0.0304, the value reported by Çehreli et al.¹⁴

3.4. GMDH LLE Prediction

The GMDH was used to develop a feedforward neural network model to predict the LLE phase characteristics of the water (1) + propan-1-ol (2) + ethyl acetate (3) system. The inputs to the models are the feed compositions of the three components and the temperature, while the outputs are the compositions of the aqueous and organic phases. The GMDH model had four inputs and six outputs. The GMDH model has been shown to be a good optimal model for modeling noisy, inaccurate, and small data sets.²² The robustness of the model was increased by extending the data points with feed set reproduction using the homotopy continuation method.¹⁸

Every experimental data point was extended to 15 different feed compositions, leading to a total of 270 data points for the development of the GMDH models. The data set was randomly split into 70% for training and 30% for testing, using a fixed random seed to ensure reproducibility.

The GMDH developed in this study is shown in Figures 8 and 9. It has two inner layers, labeled y and z for the first and second inner layers, respectively. Figures 8 and 9 show the developed GMDH structure for the outputs. The polynomial equations generated during the modeling, which present the relationship between the input and output variables, are shown in Table 6. The validity, robustness, and prediction ability of the developed GMDH models are demonstrated in Figure 10. The results show that the GMDH model's predicted outputs are in close agreement with the experimental LLE data.

The statistical performance indices presented in Table 7 show that R^2 values are high and RMSE and MAE are quite low; this shows that the developed GMDH model demonstrates a strong capability in predicting the ternary LLE system of water (1) + propan-1-ol (2) + ethyl acetate (3) across the training and test data set.

4. CONCLUSION

The viability of ethyl acetate as a solvent for the selective extraction of propan-1-ol from an aqueous solution via LLE was explored. The findings show that ethyl acetate in the

ternary system exhibits high selectivity and capacity for propan-1-ol, and its solvent extraction ability increases with increasing temperature. This confirms that ethyl acetate has an excellent potential to selectively separate propan-1-ol from water. This system showed type I behavior with an extremely narrow two-phase region at the three temperatures.

The experimental data were modeled using the NRTL and UNIQUAC activity models via the homotopy continuation method. This method estimated the binary interaction parameters that adequately predict the phase behavior, satisfy the Gibbs stability criterion, and yield compositions that are similar to experimentally measured values.

The result also shows that the GMDH model adequately predicts the behavior of the LLE system and captures the nonlinear relationship between the input and output variables. While the activity model will require rigorous regression to estimate the parameters and relate phase compositions only implicitly, the GMDH model provides explicit polynomial expressions linking the feed composition and temperature directly to the equilibrium phase compositions, complementing the thermodynamic models with a fast predictive tool.

The data and estimated activity model parameters can be applied to the design of the solvent extraction of propan-1-ol using ethyl acetate and readily input into process simulation software for design, simulation, optimization, and control of separation processes.

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J.O.B.: Analysis, modeling, manuscript development, reviewing, and editing. C.S.: Conceptualization, formal analysis, investigation, and writing. C.N.: Conceptualization, supervision, resources, methodology, reviewing, and editing.

Notes

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