Influence of salt on tie-line behavior for ternary (water + phenol + 2-butanol) system: experimental data and correlation

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ABSTRACT

Tie-line data for the systems containing phenol, 2-butanol, water and inorganic salts, were determined experimentally at temperature 298.15 K under 101.1 kPa. The addition of sodium chloride (NaCl), potassium chloride (KCl) and lithium chloride (LiCl) to the aqueous phase was tested. The selected salt amounts in initial aqueous solutions were 5% and 10%. Meanwhile, the well-known NRTL and UNIQUAC activity coefficient models were employed to reproduce the measured liquid–liquid equilibrium data and obtaining the binary interaction parameters. The outcomes demonstrate that the salting-out impact of the salts was huge, with the goal that an improvement in the phenol distribution coefficient. In this way, the salting-out impact showed up in the request LiCl > NaCl > KCl under similar conditions, in agreement with the Hofmeister series. Results were interpreted in terms of the salt hydration shells and the ability of the phenol compounds to form hydrogen-bond with water. The Bachman and Hand equations confirmed the consistency of the measured tie-line data.

Keywords: Tie-line data; Experimental; Phenol; Salting-out; Activity coefficient models

1. Introduction

Numerous endeavors have been made for the fluid extraction of phenol from wastewater from coal change, petrochemical, phenol-creation, and phenolic tar enterprises [1]. In this context, solvent extraction process appears to be an operation more friendlily to environmental and economically feasible than distillation process. The proper design of such solvent extraction units needs liquid–liquid equilibrium (LLE) data measurements and knowledge of phase behavior of ternary mixtures with phenol and water. Besides, the addition of inorganic salt to a mixture of solvents can significantly affect the equilibrium behavior of these ternary systems mixtures [2].This phenomenon is often referred to as the salting-out effect, which induces quantitative changes of solute distribution coefficient from aqueous phase in the presence of a salt [3–5]. Up to date, many investigations reported LLE data for water + phenol + solvent [6–19], but only a few studies have been directed for effect of salts on phase behavior in such systems [16–20].

Asrami and Saien [16], for instance, explored the effect of $MgSO_4$, Na_2SO_4, and NaCl on the extraction of phenol

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from water using (propan-2-yl)benzene. It was reported that addition of salts impacted phenol distribution coefficient and separation factor.

In other hand, Na_2SO_4, NaCl, and KCl have been studied by Yun et al. [17] for water + phenol + methyl isobutyl ketone system at temperatures of 333.15 and 343.15 K. It was verified that presence of salts can improve extraction of phenol from water and that coefficients are dependent on salt size in the following order: $Na_2SO_4 >$ NaCl > KCl.

Another work is that of Paulo et al. [18] that have analyzed the impacts of some inorganic salts (Na_2SO_4, KNO_3 and NaCl) for extraction of phenol from fluid stage utilizing Cyanex 923 at 298 K. As indicated by their examination, NaCl has demonstrated more promising results than Na_2SO_4 and KNO_3.

Asrami and Saien [19] studied and compared the effect of Na_2SO_4, NaCl and $MgSO_4$ on the extraction of phenol from water using [Hmim][NTf$_2$]. It was reported that the distribution coefficient of phenol between the ionic liquid and water was increased in the presence of salts due to salting-out effect. This enhancing of the distribution coefficient was in agreement with the Hofmeister series in the order of $MgSO_4 > Na_2SO_4 >$ NaCl.

Xu et al. [20] measured binodal curves and tie lines data for the ternary system containing *n*-ethylpyridinium tetrafluoroborate ([EPy]BF$_4$), 2-chlorophenol, water and salts at 308.15, 318.15, and 328.15 K. It was confirmed that the salts can improve the remove of 2-chlorophenol from aqueous solutions with the following order: $Na_2CO_3 > NaH_2PO_4$.

The effect of NaCl, KCl and LiCl on the solvency temperature for six phenolic mixtures with water has been studied by Noubigh et al. [21]. They have concluded that solubility of phenolic compounds in aqueous chloride solutions increases with increasing temperature. Their investigation revealed salting-out in the order LiCl > NaCl > KCl. Oliveira and Aznar [8] studied the LLE of water + phenol + 2-butanol system at temperatures of 298.15 and 313.15 K for investigating the capability of 2-butanol in extracting phenol from water. It was discovered that 2-butanol, as a mellow dissolvable, shows great effectiveness for the extraction of phenol. However, salt effect on the LLE data for the system (water + phenol + 2-butanol) has not been reported yet.

Therefore, in this work, the effect of some chloride salts (LiCl, KCl, and NaCl), on the removal of phenol molecules from water was explored, which have been used in many separation processes due the stronger affinity with water molecules. The presence of NaCl, KCl or LiCl (5 wt.% and 10% of the total water weight in the system) at temperatures of 298.15 K under 101.1 kPa was investigated in order to

evaluate 2-butanol as solvent to remove phenol from aqueous solutions. NRTL and UNIQUAC models were applied to correlate the experimental tie lines data.

2. Experimental section

2.1. Materials and apparatus

For measuring the LLE, 2-butanol (AR, 99%), phenol (AR, 99%), NaCl (AR, 99%), KCl (AR, 99%) and LiCl (AR, 99%), were of analytical grade, which were purchased from Merck and were utilized without further purification. More information about the compounds are shown in Table 1. Distilled water (conductivity around 1.5 μS cm^{-1}) was set up in our research center and utilized all through.

2.2. Experimental procedure and analysis

Tie lines data for the ternary system water + phenol + 2-butanol + salts were determined experimentally at 298.15 K under 101.1 kPa. Experimental procedure has been reported previously [22–24]. A 50 mL mixture solution of phenol and 2-butanol was added to another 100 mL aqueous solution of an inorganic salt (5 or 10 wt.% of NaCl, KCl or LiCl) in a 200 mL customized glass equilibrium vessel as shown in Fig. 1. The mixture was weighed on an analytical balance (Model Nahita YP402N, precise to ±0.0001 g). The overall mixture was vigorously agitated with a magnetic stirrer for 3 h, in order to allow an intimate contact between both phases, and the equilibrium was achieved by
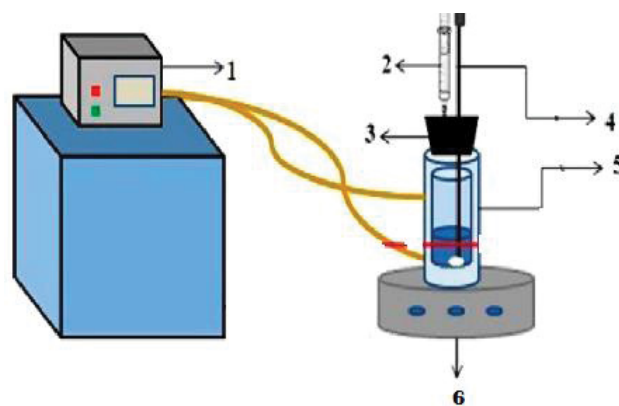

Fig. 1. Schematic diagram for the static apparatus for the LLE measurement: 1, thermostatic water bath; 2, syringe; 3, rubber plug; 4, thermometer; 5, equilibrium cell; 6, magnetic stirring apparatus.

Table 1
The source and purities of the chemicals used

Components	Supplier	Purity (wt.%)	Analysis method	CAS number
2-butanol	Merck	0.99	GC	78-92-2
Phenol	Merck	0.99	GC	108-95-2
NaCl	Merck	0.99	–	7647-14-5
KCl	Merck	0.99	–	7447-40-7
LiCl	Merck	0.99	–	7447-41-8

letting the mixture rest for 12 h. After the above mixture formed two liquid phases, samples of both phases were collected with 5 mL Hamilton syringes and were analyzed by a gas chromatography (GC).

2.3. Analytical methods

Composition of phases in equilibrium were determined with a gas chromatograph (GC-2014 provided by SHIMADZU, Japan) outfitted with a Porapak-Q stuffed section (2 m length, 3 mm measurement) and a thermal conductivity indicator; the hydrogen stream rate was 40 cm^3 min^{-1}. The initial oven temperature of GC was held at 313.15 K for 2 min and then increased to 453.15 K at a ramp rate of 10 K/min. The detector and injector temperatures were held at 523.15 and 533.15 K, respectively. The mass fraction of 2-butanol and phenol in both phases were determined by the internal standard method, where the internal standard of 2-butanol and phenol are 1-pentanol and *n*-Octanol, respectively. The content of water in two phases was determined by mass balance. On the other hand, the gas chromatography technique cannot be used directly to salt containing system, because salt can damage the thermal conductivity detector or the chromatographic column [25]. Thus, it is necessary to eliminate the salt amount in the gas stream. Therefore, an empty column section of 30 cm is placed before the main column [26]. When the organic components were evaporated, the salt was deposited on the inner walls of this empty column section. This empty column section must be cleaned by washing it with distilled water and acetone, and further drying at 393 K. After the salt amount is removed, the mass fraction of the organic components can be determined by GC, while the salt amounts for both phases can be calculated by gravimetric analysis [25]. All measures were performed in triplicate, and then the average value was adopted. It should be noted that the salt amount in the organic phase was found to be negligible after it had been evaporized.

3. Results and discussion

3.1. Experimental tie-line data

The measured LLE data for the water + phenol + 2-butanol system for salt-free and in the presence of used salts at *T* = 298.15 K are presented in Tables 2–4, respectively, where

w_{i1} and w_{i3} are mass fractions of the *i*th (water = 1, phenol = 2 and 2-butanol = 3) constituent in the water rich phase and 2-butanol rich phase, respectively. Meanwhile, the LLE phase diagrams are plotted as illustrated in Figs. 2–4. Mass fractions of salt (w_s) in initial water were 0%, 5% and 10%, respectively.

As indicated by Figs. 2–4, the slope of the tie-lines marginally increments with concentration of phenol, while the tie-line length somewhat increments with an increase in salt mass fraction. The slopes of the tie-lines demonstrate that phenol solubilizes greater in the extract-phase than in the aqueous-phase. The experimental tie-line data without salt was compared with that reported in literature [8] at 298.15 K. The deviation is shown in Fig. 2. The experimental tie lines data in this work agreed well with literature, and this result validated the experiment technique used in this study.

The capability of 2-butanol for the recovery of phenol from aqueous phase was determined by distribution coefficient (*D*) and the separation factor (*S*). The distribution coefficient of phenol between phases (D_2) and the separation factor (*S*) presented in Tables 2–4. These criteria are defined as:

$$D_2 = \frac{w_{23}}{w_{21}} \tag{1}$$

$$S = \frac{w_{23}/w_{21}}{w_{13}/w_{11}} \tag{2}$$

The obtained data of the related distribution coefficient (D_2) and separation factor (*S*) are reported in Tables 2–4. Generally, the distribution coefficient of phenol (D_2) is improved with presence of salts, being stronger under a salt mass fraction of 10% in this work. This can be explained qualitatively using hydration theory. In the presence of salts, water molecules tend to form a hydration shell surrounding the ions, so the concentration of free water molecules will diminish and the solute will transfer into organic phase [16].

The results show that the distribution coefficient of phenol (D_2) varies from 6.04 to 13.31 without salt, from 7.12 to 23.33 with NaCl, from 7.12 to 22.83 for KCl, from 11.75 to 38.89 with LiCl (for all concentration). Meanwhile, the

Table 2
Tie-line data for {water (1) + phenol (2) + 2-butanol (3)} system at *T* = 298.15 K and under ambient pressure[a]

	Aqueous phase			Organic phase			D_2	S
	w_{11}	w_{21}	w_{31}	w_{13}	w_{23}	w_{33}		
	0.8774	0.0092	0.1134	0.2873	0.0556	0.6571	6.0435	18.4565
	0.8869	0.0168	0.0963	0.1765	0.2771	0.5464	6.4940	82.8814
	0.8951	0.0272	0.0777	0.1697	0.3621	0.4682	13.3125	70.2181
0%	0.9000	0.0399	0.0601	0.1599	0.4755	0.3646	11.9173	67.0767
	0.9035	0.0503	0.0462	0.1822	0.5735	0.2443	11.4016	56.5386
	0.9140	0.0607	0.0253	0.2314	0.6715	0.0971	11.0626	43.6958
	0.9141	0.0737	0.0122	0.267	0.6895	0.0435	9.3555	32.0294

[a]Standard average uncertainties are: *u*(*w*) = 0.0004 and *u*(*T*) = 0.1 K.

Table 3
Tie-line data for the {water (1) + phenol (2) + 2-butanol (3)} system with (0.05) NaCl, KCl or LiCl mass fractions in water at $T = 298.15$ K and under ambient pressure[a]

	Aqueous phase			Organic phase				
	w_{11}	w_{21}	w_{31}	w_{13}	w_{23}	w_{33}	D_2	S
	0.8825	0.0088	0.1087	0.2778	0.0627	0.6595	7.1250	22.6343
	0.8887	0.0154	0.0959	0.1686	0.2883	0.5431	18.7208	98.6783
	0.8982	0.026	0.0758	0.1601	0.3724	0.4675	14.3231	80.3560
NaCl	0.9017	0.0411	0.0572	0.1528	0.4841	0.3631	11.7786	69.5075
	0.9091	0.0453	0.0456	0.1729	0.5895	0.2376	13.0132	68.4230
	0.9175	0.0583	0.0242	0.2235	0.6821	0.0944	11.6998	48.0295
	0.9202	0.0713	0.0085	0.2595	0.6993	0.0412	9.8079	34.7791
	0.8789	0.0088	0.1123	0.2814	0.0627	0.6559	7.1250	22.2536
	0.8856	0.0174	0.097	0.1724	0.2883	0.5393	16.5690	85.1130
	0.8962	0.026	0.0778	0.1613	0.3701	0.4686	14.2346	79.0890
KCl	0.9003	0.0367	0.063	0.1559	0.482	0.3621	13.1335	75.8442
	0.9063	0.0432	0.0505	0.1732	0.5853	0.2415	13.5486	70.8955
	0.9136	0.0583	0.0281	0.2237	0.6777	0.0986	11.6244	47.4744
	0.9145	0.0713	0.0142	0.2617	0.6949	0.0434	9.7461	34.0575
	0.8930	0.0068	0.1002	0.2505	0.0799	0.6696	11.7500	41.8872
	0.8963	0.0109	0.0928	0.1433	0.3055	0.5512	28.0275	175.3040
	0.9061	0.0174	0.0765	0.1364	0.3937	0.4699	22.6264	150.3066
LiCl	0.9070	0.0305	0.0625	0.1313	0.5122	0.3565	16.7934	116.0065
	0.9179	0.0390	0.0431	0.1588	0.6176	0.2236	15.8359	91.5351
	0.9253	0.0497	0.0250	0.2139	0.7014	0.0847	14.1127	61.0494
	0.9295	0.0604	0.0101	0.2448	0.7251	0.0301	12.0050	45.5826

[a]Standard average uncertainties are: $u(w) = 0.0004$ and $u(T) = 0.1$ K.

separation factor(S) from 18.45 to 82.88 without salt, from 22.63 to 132.73 with NaCl, from 22.25 to 124.43 for KCl, from 41.88 to 301.73 with LiCl (for all concentration).

Also, higher separation factor (S) represents the lower stage number in the design of the solvent extraction column and higher distribution coefficients (D) correspond to smaller amounts of solvents [27,28]. The salt impact on the distribution of phenol between the 2-butanol rich phase and water rich phase is plotted in Fig. 5. As can be seen in these figures, the salt improves the extraction of phenol from aqueous solutions. As a consequence, at the same salt concentration, the salting-out efficiency for various salts presents the following order: LiCl > NaCl > KCl. This thermodynamic trend can be attributed to the more pronounced solvation degree of Li+ by water molecules as compared to Na+ and K+, which decreases the degrees of freedom of the water molecules and, consequently, leads to a decrease in phenol solubility in the presence of salts as compared to that in pure water [20,29–34]. Furthermore, this phenomenon can be more explained by effect of Gibbs energy of hydration (ΔG_{hyd}) of ions. Accordingly, the hydration Gibbs energies of Li+ is –475 kJ mol⁻¹, which provide more capability to form the hydration shell than Na+ and K+ with –365 and –295 kJ mol⁻¹, respectively [35].

The reliability of experimentally measured tie-line data for every system was evaluated with Bachman [36] and Hand [37] equations, presented as Eqs. (3) and (4), respectively:

$$w_{33} = a_1 + b_1 \left(\frac{w_{33}}{w_{11}} \right) \tag{3}$$

$$\ln \left(\frac{w_{13}}{w_{33}} \right) = a_2 + b_2 \ln \left(\frac{w_{11}}{w_{21}} \right) \tag{4}$$

where a_1, b_1, a_2, and b_2, are the parameters of the Bachman and the Hand equations, respectively. The linearity of the plots demonstrates consistency with experimental data. The estimations of all parameters are recorded in Table 5, together with the determination coefficient (R^2). As the given R^2 values indicate, there is a good agreement between obtained data and Eqs. (3) and (4) (the minimum R^2 is 0.9997 and 0.890 for Bachman and Hand equation, respectively). The comparison of this linearity of the plots shows that the R^2 value for the Hand equation does not fit the results satisfactorily, while for the Bachman equation a good linear fit is achieved. This shows the Bachman condition can be used to correlate the tie-line data of the studied ternary mixtures.

3.2. NRTL and UNIQUAC correlations

Experimental tie-line data obtained in this work for investigated ternary system can be correlated by the classical NRTL [38] and UNIQUAC [39] activity coefficient

Table 4
Tie-line data for the {water (1) + phenol (2) + 2-butanol (3)} system with (0.10) NaCl, KCl or LiCl mass fractions of initial water of at $T = 298.15$ K and under ambient pressure[a]

	Aqueous phase			Organic phase			D_2	S
	w_{11}	w_{21}	w_{31}	w_{13}	w_{23}	w_{33}		
	0.8930	0.0068	0.1002	0.2618	0.0799	0.6583	11.7500	40.0793
	0.8952	0.013	0.0918	0.1574	0.3034	0.5392	23.3385	132.7356
	0.9039	0.0219	0.0741	0.1498	0.3896	0.4606	17.7900	107.3501
NaCl	0.9080	0.0325	0.0595	0.1422	0.5015	0.3563	15.4308	98.5312
	0.913	0.0411	0.0459	0.1654	0.6045	0.2301	14.7080	81.1876
	0.9225	0.0518	0.0257	0.2151	0.6949	0.09	13.4151	57.5332
	0.9245	0.0627	0.0128	0.2481	0.7185	0.0334	11.4593	42.7011
	0.8919	0.0088	0.0993	0.2707	0.0734	0.6559	8.3409	27.4816
	0.8952	0.013	0.0918	0.1643	0.2969	0.5388	22.8385	124.4369
	0.9051	0.0195	0.0754	0.1558	0.381	0.4632	19.5385	113.5062
KCl	0.9082	0.0281	0.0637	0.1526	0.4885	0.3589	17.3843	103.4630
	0.9122	0.039	0.0488	0.1714	0.596	0.2326	15.2821	81.3319
	0.9222	0.0453	0.0325	0.2202	0.6886	0.0912	15.2009	63.6615
	0.9267	0.0583	0.015	0.2542	0.7099	0.0359	12.1767	44.3907
	0.8994	0.0088	0.0918	0.2316	0.0991	0.6693	11.2614	43.7326
	0.9019	0.0109	0.0872	0.1307	0.3271	0.5422	30.0092	207.0794
	0.9132	0.0109	0.0759	0.1177	0.4239	0.4584	38.8899	301.7355
LiCl	0.9141	0.0239	0.062	0.1156	0.54	0.3444	22.5941	178.6618
	0.9247	0.0325	0.0428	0.1411	0.6454	0.2135	19.8585	130.1426
	0.9345	0.039	0.0265	0.201	0.7271	0.0719	18.6436	86.6788
	0.9363	0.0538	0.0099	0.2269	0.7532	0.0199	14.0000	57.7708

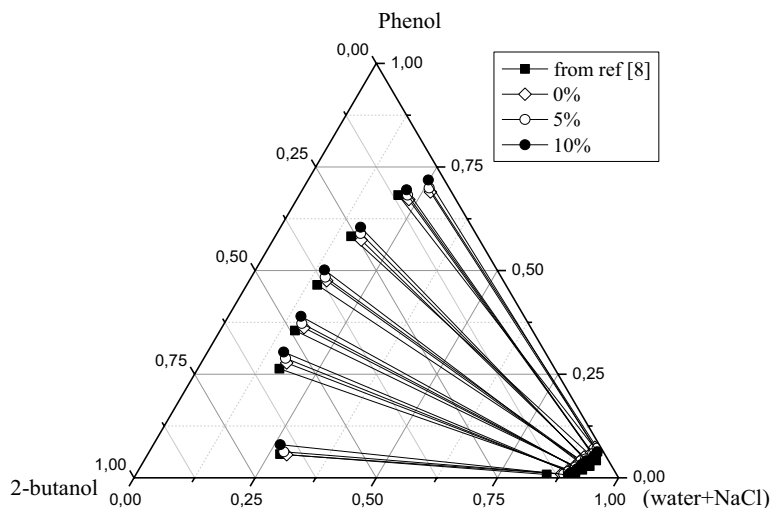[a]Standard average uncertainties are: $u(w) = 0.0004$ and $u(T) = 0.1$ K.

Fig. 2. Ternary diagram for experimental tie-line data of {water (1) + phenol (2) + 2-butanol (3)} at 298.15 K in the presence of NaCl.

models using Aspen Plus (V. 11.0) simulator. The non-randomness parameter (α_{ij}) of NRTL model was fitted with the best values of 0.2 and 0.3.

In both models, all adjustable binary interaction parameters have been determined from the experimental tie lines data as listed in Tables 2–4.

This software employs an objective function, "maximum likelihood" and an algorithm called "Britt-Luecke", to find model parameters by minimizing the differences between the experimental and calculated mass fractions for each of the components over all tie lines, using the root-mean square deviation (RMSD), defined as [22]:
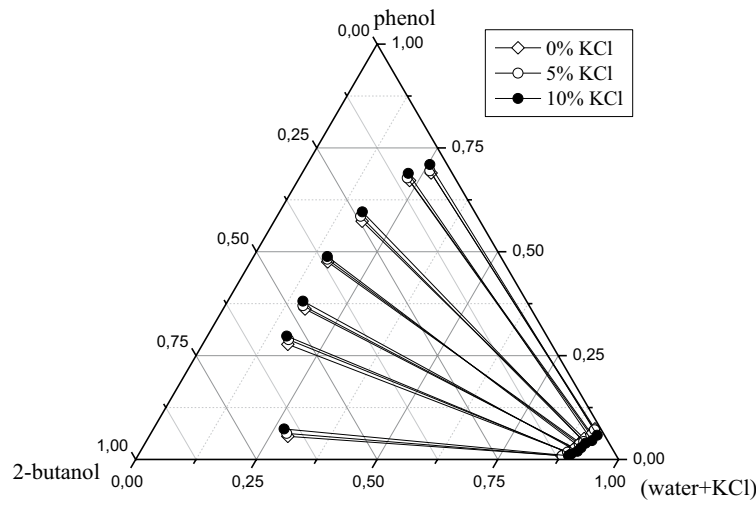
Fig. 3. Ternary diagram for experimental tie-line data of {water (1) + phenol (2) + 2-butanol (3)} at 298.15 K in the presence of KCl.
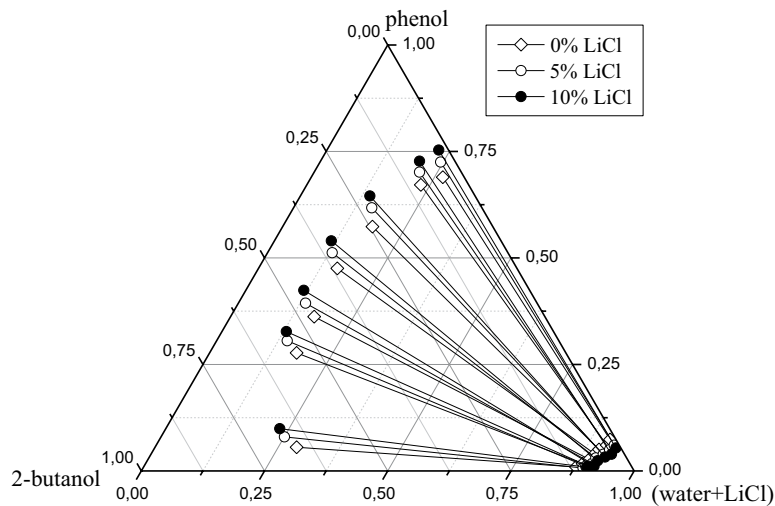

Fig. 4. Ternary diagram for experimental tie-line data of {water (1) + phenol (2) + 2-butanol (3)} at 298.15 K in the presence of LiCl.
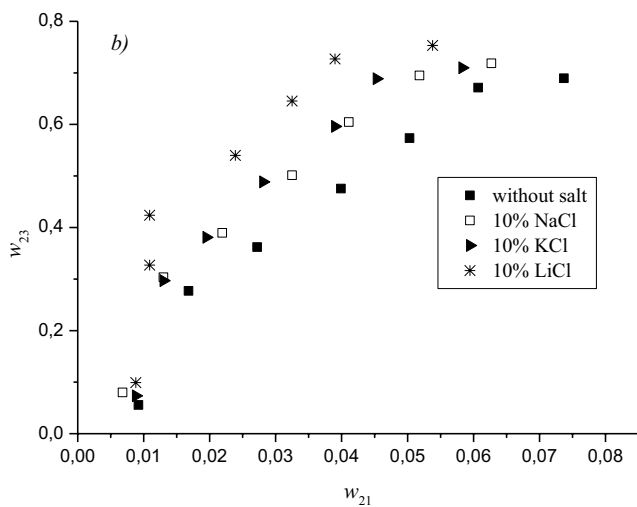

Fig. 5. Distribution of phenol between phases at 298.15 K with (a) 5% and (b) 10% mass fraction of salt.

$$\min F = \sum_{k=1}^{M}\sum_{j=1}^{2}\sum_{i=1}^{3}\left(w_{ijk}^{cal} - w_{ijk}^{exp}\right)^2 \tag{5}$$

The fitting quality is evaluated using two statistics equations; the root-mean square (RMSD) and the absolute average relative deviation (AARD) that were calculated using the following expressions, defined as:

$$\text{RMSD} = \left[\frac{\sum_{k=1}^{M}\sum_{j=1}^{2}\sum_{i=1}^{3}\left(w_{ij}^{exp} - w_{ij}^{calc}\right)^2}{6M}\right]^{0.5} \tag{6}$$

$$\text{AARD} = \frac{1}{6M}\sum_{k=1}^{M}\sum_{j=1}^{2}\sum_{i=1}^{3}\left(\frac{\left|w_{ijk}^{exp} - w_{ijk}^{cal}\right|}{w_{ijk}^{exp}}\right) \tag{7}$$

where, M are the number of tie lines, w^{exp} and w^{cal} indicates the experimental and calculated mass fraction, i and j represent the phases at equilibrium, the constituents and the tie lines, respectively.

Results of interaction parameters identification, together with corresponding RMSD and AARD values, are tabulated in Tables 6. As can be seen in this table, correlation of tie lines data for water + phenol + 2-butanol + salts

(LiCl, NaCl or KCl) mixture utilizing the UNIQUAC model gives RMSD and AARD values between 0.0028 and 0.0056, and 0.0046 and 0.0075, respectively. Additionally, the scopes of RMSD and AARD for this mixture in the presence of salts with NRTL model are between 0.0033 and 0.0068, and 0.0055 and 0.0092, respectively, which indicate that the measured tie lines data can be represented by the UNIQUAC and NRTL models.

In Fig. 6, comparison between measured LLE data of all composition vs. the calculated equilibrium compositions for both phases with NRTL and UNIQUAC are shown. It can be verified that that the experimental LLE compositions for both phases are in great concurrence with the determined ones (almost all data points fall on the diagonal) and, consequently, a good match with the phase diagrams was also obtained for the studied systems.

Therefore, results presented in this work can provide information for water + phenol + solvent systems thermodynamics, which in turn can be use to design solvent extraction processes applied to purified water streams containing phenol.

4. Conclusions

LLE data for the system of (water + phenol + 2-butanol and contained NaCl, or KCl, or LiCl) salts at temperature

Table 5
Parameters of the Bachman and Hand equations for the used system with (0.05 and 0.10) mass fractions of initial water of NaCl, KCl or LiCl and without salt at 298.15 K

State	Bachman correlation			Hand correlation		
	a_1	b_1	R^2	a_2	b_2	R^2
Salt free	0.0050	0.8779	0.9997	3.445	2.285	0.9228
5% NaCl	0.0048	0.8817	0.9998	3.439	2.229	0.9220
10% NaCl	0.0038	0.8914	0.9999	3.443	2.091	0.9166
5% KCl	0.0051	0.8784	0.9998	3.573	2.326	0.9587
10% KCl	0.0039	0.8907	0.9999	4.022	2.453	0.9376
5% LiCl	0.0039	0.8917	0.9999	3.557	2.105	0.9158
10% LiCl	0.0037	0.8984	0.9999	4.364	2.466	0.9000

Table 6
Binary interaction parameters of NRTL and UNIQUAC models for the water (1) + phenol (2) + 2-butanol (3) system with and without salts at temperature of $T = 298.15$ K and under ambient pressure of $p = 101.3$ kPa

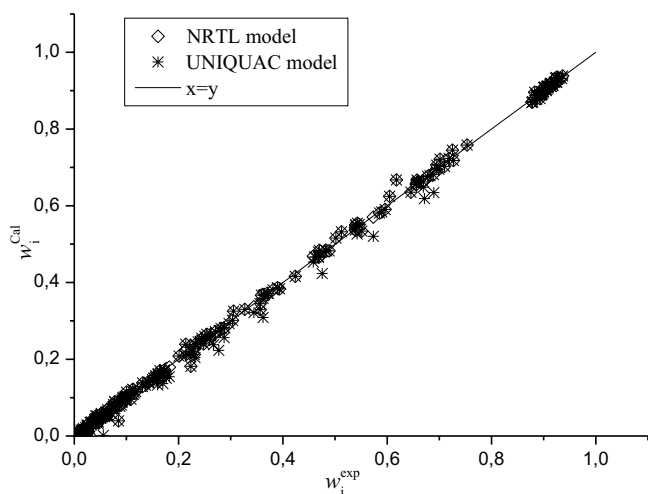| Salt mass %	$i–j$	b_{ij} (K)	NRTL b_{ji} (K)	α_{ij}	RMSD	AARD	UNIQUAC a_{ij} (K)	a_{ji} (K)	RMSD	AARD
	1–2	608.5821	–289.2680	0.2			–230.0483	408.0926		
0%	1–3	252.8368	2,182.1552	0.2	0.0068	0.0092	–44.64914	28.9721	0.0056	0.0075
	2–3	858.2135	1,288.9204	0.2			980.3698	828.2224		
					NaCl					
	1–2	624.6731	–322.5431	0.3			–210.0483	588.0926		
5%	1–3	276.0516	2.190.9947	0.3	0.0062	0.0088	–44.6491	28.9721	0.0049	0.0061
	2–3	851.5794	1.314.2456	0.3			980.3698	828.2224		
	1–2	626.2831	–325.8927	0.2			–203.0248	582.7718		
10%	1–3	272.2560	2,195.1863	0.2	0.0043	0.0060	–48.6076	22.0230	0.0038	0.0051
	2–3	853.1005	1,.322.6571	0.2			984.9393	830.4003		
					KCl					
	1–2	632.7430	–319.3561	0.2			–183.0248	582.7718		
5%	1–3	280.6258	2,198.3952	0.2	0.0052	0.0073	–48.6076	19.0230	0.0041	0.0066
	2–3	858.8462	1,345.8692	0.2			894.9393	760.4004		
	1–2	634.5219	–321.5380	0.3			–230.0483	408.0926		
10%	1–3	281.9621	2,182.1468	0.3	0.0047	0.0066	–44.6491	28.9721	0.0036	0.0057
	2–3	861.5183	1,348.2261	0.3			980.3698	828.2224		
					LiCl					
	1–2	650.3428	–343.1486	0.3			–243.5802	612.1328		
5%	1–3	289.7250	2,194.0537	0.3	0.0033	0.0055	–48.0627	31.5692	0.0028	0.0046
	2–3	883.1672	1,361.0537	0.3			980.3698	932.1580		
	1–2	652.5038	–347.3107	0.3			–245.1325	622.0256		
10%	1–3	288.2136	2,197.8325	0.3	0.0039	0.0059	–52.1538	38.3471	0.0030	0.0050
	2–3	885.5361	1,362.8236	0.3			986.3256	938.8246		

Fig. 6. Comparison of experimental and calculated data at 298.15 K.

of 298.15 K and under the ambient pressure of was determined. The experimental results show that the addition of salts provides a good effect on phenol distribution coefficient and separation factor whose values obtained are in the ranges of 8.34 to 38.89 and 27.48 to 301.73, respectively. Results show that the effect of salt size on ternary binodal curve has the following order: LiCl > NaCl > KCl, under similar conditions. They also agree very well with results predicted by the UNIQUAC and NRTL models.

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