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Experimental results for fluid phase equilibria of (n-propanol +water + salt) and comparison with predictions

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ABSTRACT

Salt-containing vapor-liquid equilibrium for the n-propanol + water system was obtained experimentally at atmospheric pressure using a modified Othmer still. The studied salts include lithium chloride (LiCl), sodium chloride (NaCl), potassium chloride (KCl), potassium bromide(KBr) and potassium iodide (KI). The experimental vapor-liquid equilibrium data was compared with that calculated using the LIFAC model. The average relative deviation between experimental data and the correlation are –0.24%, –1.42%, –0.29%, –1.33% and 0.23% for LiCl, NaCl, KCl, KBr and KI, respectively. The corresponding standard deviations are 2.06%, 2.83%, 2.27%, 2.71%, and 2.11%. From these results, it may be seen that the new experimental data for the vapor-liquid equilibrium of the ternary system (n-propanol + water +salt) and the predictive thermodynamic model LIFAC can be used to estimate the influence of the salts on the VLE of the n-propanol + water system. Furthermore, the effect of different salts on relative volatility was studied.

Keywords: Vapor-liquid equilibrium; Thermodynamic predictive model; n-Propanol; Salt

1.Introduction

Distillation is widely used for the separation of a mixture of components based on their different separation factor. For azeotropic systems, however, the separation by conventional distillation is not possible since the liquid and vapor compositions are the same at the azeotropic point. In such a case, special separation techniques such as extractive distillation and liquid-liquid extraction using ionic liquidsare used [1–7]. In the separation process of extractive distillation, a non-volatile extracting agent, called entrainer, is added to alter the separation factor, and subsequently shifts or breaks the azeotropic composition of mixture [3]. Because a salt dissolved in a mixed solvent may affect the equilibrium vapor phase composition (known as the salt effect) [4], phase equilibria of systems that contain electrolytes are of particular interest for the separation of azeotropic systems. A reliable knowledge of electrolyte containing system is essential for the separation of n-propanol + water mixtures.

There are a variety of models developed in the past to describe the phase equilibrium behavior of electrolyte systems [8]. However, only a few models allow a reliable description of the vapor-liquid equilibrium (VLE) up to high salt concentrations [8–13]. Among them, the g^E model LIFAC proposed by Yan et al. is the most promising one. Besides, the correlation and prediction of vapor-liquid equilibrium of electrolyte systems in mixed-solvents has been examined by a number of investigators: Yan et al. [8], Kiepe et al. [9], Held et al. [10], Li et al. [11], Mohs and Gmehling [12], Hector and Gmehling [13], and the calculated results were found to be in good agreement with experimental results. Furthermore, the LIFAC model, which based on the group contribution concept, is much more flexible than the LIQUAC mode published previously. Hence, the LIFAC model becomes the obvious choice to predict phase equilibria for n-propanol + water + salt system in this work.

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N-propanol + water system form a minimum boiling azeotrope at 0.43 mole fraction of n-propanol at a temperature of 360.9 K and 101.3 kPa [14]. The very small difference between the normal boiling temperatures of the two solvent (≈3 K) make it very difficult to move the azeotrope towards larger compositions of n-propanol [14]. To date, there are numerous studies on the effect of various salts over n-propanol + water mixtures [14–17]. The literatures indicate that different inorganic salts give either salting-out or salting-in effects for the binary system. It is very complicated to accurately describe the phase equilibrium behavior for the n-propanol + water + salt mixtures with models. Therefore, the development of reliable model for salt containing mixtures is of particular interest for separation processes of n-propanol + water system when salt is used as an entrainer. In this paper, we will experimentally study the vapor-liquid equilibrium of the ternary system (n-propanol + water + salt). In addition, an attempt is made to apply the LIFAC model to describe the phase equilibrium behavior for the ternary systems.

2. Experimental section

2.1. Chemicals

The n-propanol used in this work was analytical reagent with a minimum purity of 99 wt%. Water was deionized and distilled twice. Salts of lithium chloride, sodium chloride, potassium chloride, potassium bromide and potassium iodide were analytical grade. These chemicals were supplied by Aladdin Industrial Corporation (Shanghai, China) and used without further purification.

2.2. Apparatus and procedure

A modified Othmer still was used in this work for the vapor-liquid equilibrium experiments. The still was used and described in a previous paper [18].Therefore, only an outline is given here. In the side of the still pot, the still has a widened loading port, which facilitates the addition of liquid feed (or salt) and further holding a mercurial thermometer for measurement of the solution temperature. The still pot was heated by a thermostatic oil bath. The vapor jacket was wrapped with an external electrical heating tape to heat the vapor space a few kelvins above the solution boiling point to prevent refluxing. To flexibly control the volume of holdup and sample size, the graduated condensate chamber was fitted with a three-way stock. The holdup may be maintained at any desired level by varying the position of the stopclock. The temperature was measured by mercurial thermometer with an uncertainty of 0.1 K. The pressure control system consisted of a solenoid and throttle valves in series connected with a vacuum pump, a buffer vessel to damp pressure variations, a vacuum measure prove (range 0.35–400 kPa) and an on-off pressure controller actuating the solenoid valve. This control system was able to maintain the system pressure at a given value with an uncertainty of 0.2 kPa.

In each experimental run, an initial n-propanol + water solution of about 150 mL was prepared gravimetrically using a Wante FA-N analytical balance with an accuracy of 0.0001 g to ensure accurate compositions. The initial solution and salt were charged into the still through the loading port. Then, the thermostatic oil bath was turned on to heat the solution in the still, and the temperature and pressure were simultaneously measured. Additionally, constant stir was necessary to ensure a uniform mixing throughout the solution. The heating results in a partial evaporation of the liquid feed, and then the condensate returned to still pot through a capillary tube. After the vapor-liquid equilibrium system was maintained at constant temperature of liquid mixture for 30 min, the liquid temperatures were recorded and the samples were quickly withdrawn into sample vials. When the salt was added for the next run, the experiments were repeated as described above. Samples of the coexisting phases of the ternary system (n-propanol + water +salt) were analyzed using gas chromatography with a thermal conductivity detector (TCD) for n-propanol concentration. Details for the operating conditions were as follows: helium carrier gas flow 25 cm^3 min^{-1}, injector temperature 520 K, oven temperature 460 K, and detector temperature 490 K. The salt content of the sample was gravimetrically determined by solvent evaporation at 398 K of a known mass of sample (about 2 g) [14].

3. Results and discussion

3.1. Experimental results

Vapor-liquid equilibrium data for (n-propanol + water + salt) ternary system were measured using the modified Othmer still. To check the performance of the phase equilibrium apparatus used in the present work, the isobaric vapor−liquid equilibrium in the n-propanol + water binary system and the alcohol + water + salt ternary system were measured for different liquid composition. The experimental results are compared with the literature data for the n-propanol + water system [19,20] in Fig. 1 and for the alcohol + water + $NaNO_3$ system [21] in Table 1, respectively.

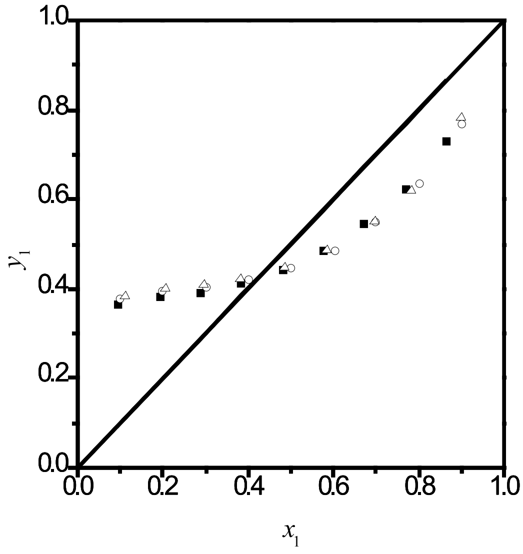

Fig. 1. Comparisons of the experimental results at present work with the literature data for the [n-propanol (1) + water (2)] system: ■, present work; ○, Iliuta and Thyrion [19]; Δ, Vercher et al [20].

Table 1
Comparisons of the experimental results at present work with the literature data for the [alcohol (1) + water (2) + $NaNO_3$ (3)] system [21] at 101.3 kPa[a]

x_1	x_2	x_3	$y_{1,\mathrm{lit}}$ [21]	$y_{1,\mathrm{exp}}$	Δy_1,%
0.099	0.865	0.036	0.527	0.5102	–3.1894
0.200	0.736	0.065	0.656	0.6471	–1.3567
0.303	0.687	0.011	0.603	0.5955	–1.2407
0.402	0.576	0.023	0.657	0.6494	–1.1516
0.500	0.483	0.016	0.685	0.6807	–0.6303
0.610	0.385	0.004	0.712	0.7159	0.5420
0.728	0.268	0.004	0.773	0.7824	1.2105

[a]The combined standard uncertainties u_c is $u_c(x_i) = u_c(y_i) = 0.0028$.

Table 2
Experimental and prediction results for the vapor-liquid equilibrium in the [n-propanol (1) + water (2) + LiCl (3)] system[a]

T/K	x_1	x_3	$y_{1,\mathrm{exp}}$	$y_{1,\mathrm{cal}}$	Δy_1,%
362.1	0.3345	0.0196	0.4165	0.4157	–0.1916
362.4	0.4394	0.0351	0.4453	0.4517	1.4463
362.6	0.4759	0.0479	0.4696	0.4726	0.6356
361.8	0.4453	0.0248	0.4574	0.4457	–2.5551
362.1	0.4950	0.0431	0.4759	0.4760	0.0287
362.9	0.5282	0.0578	0.5081	0.5000	–1.5920
362.7	0.4950	0.0347	0.4950	0.4706	–4.9349
363.9	0.5081	0.0577	0.4982	0.4919	–1.2630
364.9	0.5490	0.0739	0.5181	0.5211	0.5775
366.2	0.6231	0.0463	0.5339	0.5448	2.0374
367.8	0.6077	0.0725	0.5477	0.5544	1.2316
368.7	0.6077	0.0894	0.5567	0.5663	1.7298
					–0.2375
					2.0569

[a]Standard uncertainties u is $u(T)$ = 0.1 K, and the combined standard uncertainties u_c is $u_c(x_i) = u_c(y_i) = 0.0028$.

Table 3
Experimental and prediction results for the vapor-liquid equilibrium in the [n-propanol (1) + water (2) + NaCl (3)] system[a]

T/K	x_1	x_3	$y_{1,\mathrm{exp}}$	$y_{1,\mathrm{cal}}$	Δy_1,%
361.9	0.2948	0.0102	0.3865	0.4014	3.8504
362.1	0.3891	0.0179	0.4365	0.4256	–2.4961
362.1	0.4136	0.0239	0.4453	0.4369	–1.8827
361.4	0.4336	0.0129	0.4423	0.4335	–1.9933
362.3	0.4365	0.0219	0.4513	0.4419	–2.0911
361.4	0.4483	0.0283	0.4573	0.4503	–1.5383
361.4	0.4696	0.0193	0.4727	0.4502	–4.7529
361.5	0.4696	0.0306	0.4727	0.4592	–2.8523
361.5	0.4853	0.0383	0.4696	0.4711	0.3244
362.1	0.5385	0.0245	0.4768	0.4825	1.1986
362.0	0.5282	0.0366	0.4885	0.4873	–0.2554
361.9	0.5080	0.0440	0.5080	0.4847	–4.5786
					–1.4223
					2.8382

[a]Standard uncertainties u is $u(T)$ = 0.1 K, and the combined standard uncertainties u_c is $u_c(x_i) = u_c(y_i) = 0.0028$.

The agreement between the new experimental data and the literature results is considered to be satisfactory.

Therefore, the Othmer still was used to generate the vapor–liquid equilibrium data of the ternary system (n-propanol + water +salt). The studied salts include LiCl, NaCl, KCl, KBr and KI. The results of these vapor-liquid equilibrium measurements are listed in Tables 2 to 6. In these tables, x_i is the mole fraction of component i in the liquid phase, y_i is the mole fraction of component i in the vapor phase and T is the equilibrium temperature. The subscripts (exp and cal) denote experimental and calculated values. The average relative deviation ($\overline{\Delta z}$) and the corresponding standard deviations (σ) are calculated with

$$\overline{\Delta z} = (100/N)\sum_{i=1}^{N}((z_{\mathrm{cal}} - z_{\mathrm{exp}})/z_{\mathrm{exp}})_i \tag{1}$$

$$\sigma = 100(1/(N-1)\sum_{i=1}^{N}((z_{\mathrm{cal}} - z_{\mathrm{exp}})/z_{\mathrm{exp}})_i^2)^{1/2} \tag{2}$$

3.2. Prediction and comparison with experimental data

In this paper, the electrolyte model LIFAC was applied to predict the vapor–liquid equilibrium (VLE) behavior in mixed-solvent electrolyte systems. In the LIFAC model, the activity coefficients are calculated by a long range (LR), middle range (MR) and a short range (SR) term [8]:

$$\ln\gamma_S = \ln\gamma_S^{\mathrm{LR}} + \ln\gamma_S^{\mathrm{MR}} + \ln\gamma_S^{\mathrm{SR}} \tag{3}$$

where S indicates all the solvents. The LR term and MR term can be calculated as shown below [8],

$$\ln\gamma_S^{\mathrm{LR}} = \frac{2AM_S d_{\mathrm{ms}}}{b^3 d_S}\left[1 + bI^{1/2} - (1+bI^{1/2})^{-1} - 2\ln(1+bI^{1/2})\right] \tag{4}$$

$$\ln\gamma_S^{\mathrm{MR}} = \sum_k v_k^{(S)} \ln\gamma_k^{\mathrm{MR}} \tag{5}$$

$$\ln\gamma_k^{\mathrm{MR}} = \sum_l B_{k,l} m_l - \frac{M_k \sum_k \sum_S v_k^{(S)} x'_S}{M_{\mathrm{ms}}} \sum_k \sum_l \left[B_{k,l} + IB'_{k,l}\right] x'_k\, m_l$$
$$- M_k \sum_c \sum_a \left[B_{c,a} + IB'_{c,a}\right] m_c m_a \qquad (l = c \text{ and } a) \tag{6}$$

where

$$A = \frac{1.327757 \times 10^5 d_{\mathrm{ms}}^{1/2}}{(D_{\mathrm{ms}}T)^{3/2}} \tag{7}$$

$$b = \frac{6.359696 d_{\mathrm{ms}}^{1/2}}{(D_{\mathrm{ms}}T)^{1/2}} \tag{8}$$

Table 4
Experimental and prediction results for the vapor-liquid equilibrium in the [n-propanol (1) + water (2) + KCl (3)] system[a]

T/K	x_1	x_3	$y_{1,\mathrm{exp}}$	$y_{1,\mathrm{cal}}$	Δy_1,%
358.6	0.4543	0.0096	0.4172	0.4351	4.2833
361.4	0.4250	0.0168	0.4250	0.4312	1.4581
361.6	0.4109	0.0226	0.4424	0.4309	–2.6008
361.6	0.4394	0.0129	0.4394	0.4335	–1.3358
361.5	0.4394	0.0218	0.4424	0.4388	–0.8090
361.5	0.4424	0.0282	0.4424	0.4439	0.3440
361.3	0.4696	0.0169	0.4665	0.4461	–4.3780
361.4	0.4696	0.0273	0.4635	0.4525	–2.3643
361.8	0.4635	0.0342	0.4543	0.4551	0.1861
362.2	0.5225	0.0221	0.4685	0.4710	0.5379
361.8	0.5214	0.0340	0.4714	0.4779	1.3869
361.8	0.5048	0.0409	0.4765	0.4755	–0.2175
					–0.2924
					2.2733

[a]Standard uncertainties u is $u(T)$ = 0.1 K, and the combined standard uncertainties u_c is $u_c(x_i) = u_c(y_i) = 0.0028$.

Table 5
Experimental and prediction results for the vapor-liquid equilibrium in the [n-propanol (1) + water (2) + KBr (3)] system[a]

T/K	x_1	x_3	$y_{1,\mathrm{exp}}$	$y_{1,\mathrm{cal}}$	Δy_1,%
362.1	0.4081	0.0091	0.4172	0.4262	2.1562
362.1	0.4109	0.0161	0.4222	0.4322	2.3746
362.4	0.4109	0.0217	0.4352	0.4362	0.2373
361.3	0.3098	0.0112	0.4141	0.4060	–1.9613
361.4	0.3119	0.0195	0.4163	0.4127	–0.8606
361.3	0.3098	0.0260	0.4141	0.4169	0.6699
361.3	0.4727	0.0161	0.4665	0.4521	–3.0971
361.5	0.4696	0.0264	0.4696	0.4580	–2.4720
361.5	0.4696	0.0335	0.4796	0.4625	–3.5741
362.6	0.5632	0.0206	0.5025	0.4957	–1.3608
362.3	0.5351	0.0325	0.5051	0.4900	–2.9942
362.1	0.5282	0.0403	0.5181	0.4916	–5.1060
					–1.3323
					2.7093

[a]Standard uncertainties u is $u(T)$ = 0.1 K, and the combined standard uncertainties u_c is $u_c(x_i) = u_c(y_i) = 0.0028$.

$$D_{\mathrm{ms}} = -31.61 + \frac{32733.43}{T} \tag{9}$$

$$d_{\mathrm{ms}} = \sum_{S=1}^{n} v'_S d_S \tag{10}$$

$$v'_S = \frac{x'_S V_S}{\sum_n x'_n V_n} \tag{11}$$

Table 6
Experimental and prediction results for the vapor-liquid equilibrium in the [n-propanol (1) + water (2) + KI (3)] system[a]

T/K	x_1	x_3	$y_{1,\mathrm{exp}}$	$y_{1,\mathrm{cal}}$	Δy_1,%
361.4	0.4351	0.0172	0.4650	0.4602	–1.0317
361.6	0.4209	0.0215	0.4824	0.4620	–4.2192
361.6	0.4444	0.0130	0.4394	0.4567	3.9267
361.5	0.4494	0.0221	0.4824	0.4718	–2.1891
361.5	0.4524	0.0279	0.4724	0.4803	1.6633
361.3	0.4676	0.0175	0.4665	0.4715	1.0713
361.4	0.4689	0.0268	0.4835	0.4848	0.2630
361.8	0.4697	0.0331	0.4943	0.4928	–0.3076
362.2	0.5025	0.0321	0.4985	0.5050	1.3119
361.8	0.5114	0.0332	0.5014	0.5100	1.7132
361.8	0.5148	0.0389	0.5165	0.5181	0.3017
					0.2276
					2.1887

[a]Standard uncertainties u is $u(T)$ = 0.1 K, and the combined standard uncertainties u_c is $u_c(x_i) = u_c(y_i) = 0.0028$.

$$M_{\mathrm{ms}} = \sum_{S=1}^{n} x'_S M_S \tag{12}$$

$$B_{k,l} = b_{k,l} + c_{k,l} \exp\left(-1.2I^{1/2} + 0.250I\right) \tag{13}$$

$$B_{c,a} = b_{c,a} + c_{c,a} \exp\left(-I^{1/2} + 0.125I\right) \tag{14}$$

$$B'_{k,l} = \frac{\partial B_{k,l}}{\partial I} \tag{15}$$

$$B'_{c,a} = \frac{\partial B_{c,a}}{\partial I} \tag{16}$$

The SR term $(ln\gamma_S^S R)$ can be described using the UNIFAC group contribution concept [22].

Assuming ideal vapor phase behavior, vapor–liquid equilibria can be calculated using the simplified equation [9].

$$py_s = p_s^s x_s \gamma_s \tag{17}$$

where y_s is the vapor phase mole fraction of solvent S, x_s is the liquid phase mole fraction of the solvent S based on the assumption of total dissociation of the salt. The saturation vapor pressure of the pure solvent p_s^s was calculated by the Antoine equation, using constants from the literature [23]. For the activity coefficient of the solvent, Eq. (3) was applied. The required parameters are taken directly from literature [8].

The vapor-liquid equilibrium of the ternary system (n-propanol + water + salt) was predicted using the LIFAC model and compared with the experimental results. The prediction results are given in Tables 2–6 together with relative deviations between experimental results and pre-

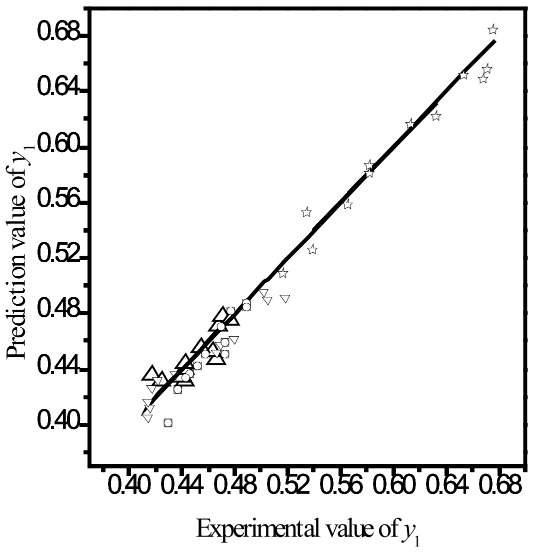

Fig. 2. Comparisons between experimental and prediction values of the vapor-phase mole fraction of n-propanol of the system [n-propanol(1) + H_2O (2) + salt (3)]:—, experimental values; □, prediction values for LiCl; ○, prediction values for NaCl; Δ, prediction values for KCl; ∇, prediction values for KBr; ✰, prediction values for KI.

diction results. In Fig. 2 the calculated and experimental VLE data of the ternary system are compared. As shown in Tables 2–6 and Fig. 2, the agreement between the prediction results and the experimental data is satisfactory, which mean that LIFAC model can give reliable predictions for the vapor-liquid equilibrium of (n-propanol + water + salt) ternary system.

3.3. *Effect of salt on relative volatility*

The relative volatility (α) of n-propanol (1) to water (2) is calculated using the following equation:

$$\alpha_1 = \frac{y_1/x_1}{y_2/x_2} \tag{18}$$

where x_i and y_i are respectively the liquid- and vapor-phase-mole fractions of species *i* at equilibrium. Fig. 3 shows the effect of different salts on relative volatility, which follows the order LiCl > NaCl > KCl > KBr > KI. The salts studied in the present paper are preferentially soluble in water and sparingly in n-propanol. Therefore, the relative volatility of n-propanol to water shifts by adding salt to the binary system. The best entrainer among the various salts is chosen on the basis of relative volatility. The higher the relative volatility, the better is the separation of the azeotrope. The breaking of the azeotrope enhances by increasing the relative volatility and subsequently increasing the concentration of ethyl acetate. Thus LiCl is more effective than NaCl, KCl, K Brand KI to eliminate the azeotrope of the binary system.

When salt concentration increases in then-propanol + water system, the interaction between salt and water becomes much stronger since salts possess greater attraction

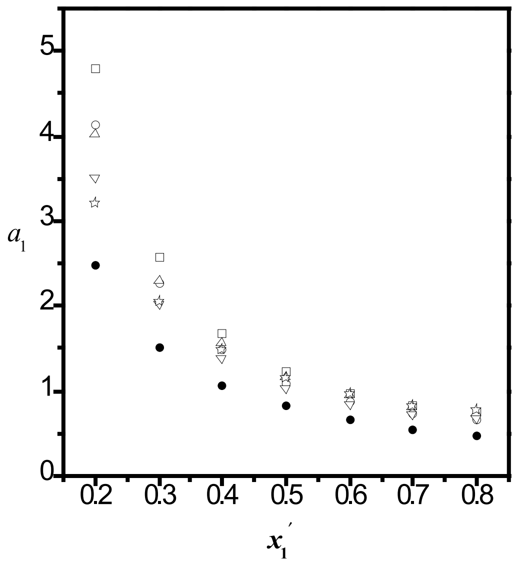

Fig. 3. Relative volatility of n-propanol to water for different salts at $z_3 = 0.04$ (*z* is the salt mole fraction): □, LiCl; ○, NaCl; Δ, KCl; Δ, KBr; ∇, KI; ✰, salt free.

toward water than that with n-propanol. Thus n-proponal concentration moves from azeotropic composition to higher composition. It was further observed that the separation of the azeotrope is better as the salt concentration increases. This observation can be attributed to the combined effect of the cation and anion of the salt.

4. Conclusions

With the vapor-liquid apparatus modified Othmer still, new data for the ternary system (n-propanol-water-salt) were taken at 101.3 kPa. These data extend the liquid phase compositions in the vapor-liquid region. The vapor-liquid equilibrium in the ternary system was also predicted using the LIFAC model. The satisfactory agreement between the experimental data and prediction results show that this model can give a good representation of vapor-liquid equilibrium in ternary system. Thus, LIFAC model can be used to estimate the influence of the salts on the VLE of the n-propanol + water system. It is also found that LiCl has a greater salting-out effect at lower salt concentrations compared to NaCl, KCl, KBrand KI. Therefore, LiCl is the suitable salt for separation of the mixture of n-propanol and water.

Acknowledgements

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Symbols

A — Debye–Hückel parameter
A_j — Constants in Antoine equation for component *j*
b — Debye–Hückel parameter

$b_{c,a}$ — MR interaction parameter between cation and anion

$b_{k,l}$ — MR interaction parameter between solvent group and ion

B — Debye–Hückel parameter

$B_{c,a}$ — Ion–ion interaction parameter

B_j — Constants in Antoine equation for component *j*

$B_{k,l}$ — Solvent group–ion interaction parameter

$c_{c,a}$ — MR interaction parameter between cation and anion

$c_{k,l}$ — MR interaction parameter between solvent group and ion

C_j — Constants in Antoine equation for component *j*

d_{ms} — Mixed-solvent molar density (kmol m^{-3})

d_S — Molar density of the *Sth* solvent

D_{ms} — Mixed-solvent dielectric constant

I — Ionic strength (mol kg^{-1})

m_l — Molality of ion *l* (mol kg^{-1})

M_{ms} — Molar mass of the solvent mixture

M_k — Molar mass of group *k*

M_S — Molar mass of the *Sth* solvent (kg mol^{-1})

p — Pressure

p^{s} — Saturated vapor pressure

T — Absolute temperature

V_n — Molar volumeof the *nth* solvent

V_S — Molar volumeof the *Sth* solvent

x — Liquid phase mole fraction on an ionic basis

x'_n — Salt-free mole fraction of the *nth* solvent

x'_S — Salt-free mole fraction of the *Sth* solvent

y — Mole fraction in vapor phase

$\overline{\Delta z}$ — $\overline{\Delta} z = (100/N)\sum_{i=1}^{N}((z_{\text{cal}} - z_{\text{exp}})/z_{\text{exp}})_i$

σ — $\sigma = 100(1/(N-1)\sum_{i=1}^{N}((z_{\text{cal}} - z_{\text{exp}})/z_{\text{exp}})_i^2)^{1/2}$

γ — Activity coefficient normalized according to Raoult's law

$v_k^{(S)}$ — Number of groups of type *k* in the *Sth* solvent

v'_S — Salt-free volume fraction of the *Sth* solvent in liquid phase

References

[1] X. Xu, T. Zhao, Y. Wang, X. Geng, Y. Wang, Ternary liquid–liquid equilibrium of azeotropes (water + 2-Propanol) with ionic liquids ([Dmim][NTf2]) at different temperatures, J. Chem. Eng. Data, 62(5) (2017) 1667–1672.

[2] L. Xu, D. Xu, P. Shi, K. Zhang, X. Ma, J. Gao, Y. Wang, Salts effect on isobaric vapor–liquid equilibrium for separation of the azeotropic mixture allyl alcohol + water, Fluid Phase Equilibria, 457 (2018) 11–17.

[3] Z. Lei, C. Dai, J. Zhu, B. Chen, Extractive distillation with ionic liquids: A review, AIChE J., 60(9) (2014) 3312–3329.

[4] W. Liu, Z. Zhang, Y. Ri, X. Xu, Y. Wang, Liquid–liquid equilibria for ternary mixtures of water + 2-propanol + 1-alkyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide ionic liquids at 298.15 K, Fluid Phase Equilibria, 412 (2016) 205–210.

[5] Z. Zhu, Y. Liu, Y. Wang, Liquid–liquid equilibrium for the ternary system of 1-butanol + 3-methyl-1-butanol + water at different temperatures, Fluid Phase Equilibria, 335 (2012) 14–19.

[6] P. Shi, Y. Gao, J. Wu, D. Xu, J. Gao, X. Ma, Y. Wang, Separation of azeotrope (2,2,3,3-tetrafluoro-1-propanol + water): Isobaric vapour-liquid phase equilibrium measurements and azeotropic distillation, J. Chem. Thermodynamics, 115 (2017) 19–26.

[7] J. Wu, D. Xu, P. Shi, J. Gao, L. Zhang, Y. Ma, Y. Wang, Separation of azeotrope (allyl alcohol + water): Isobaric vapour-liquid phase equilibrium measurements and extractive distillation, J. Chem. Thermodynamics, 118 (2018) 139–146.

[8] W. Yan, M. Topphoff, C. Rose, Prediction of vapor–liquid equilibria in mixed-solvent electrolyte systems using the group contribution concept, Fluid Phase Equilibria., 162(1) (1999) 97–113.

[9]J Kiepe, O. Noll, J. Gmehling, Modified LIQUAC and modified LIFAC-a further development of electrolyte models for the reliable prediction of phase equilibria with strong electrolytes, Ind. Eng. Chem. Res., 45(7) (2006) 2361–2373.

[10] C. Held, A. Prinz, V. Wallmeyer, G. Sadowski, Measuring and modeling alcohol/salt systems, Chem. Eng. Sci., 68(1) (2012) 328–339.

[11] M.Y. Li, L.S. Wang, J. Gmehling, Thermodynamics of phase equilibria in aqueous strong electrolyte systems, Ind. Eng. Chem. Res., 50(6) (2011) 3621–3631.

[12] A. Mohs, J. Gmehling, A revised LIQUAC and LIFAC model (LIQUAC*/LIFAC*) for the prediction of properties of electrolyte containing solutions, Fluid Phase Equilibria., 337 (2013) 311–322.

[13] T. Hector, J. Gmehling, Present status of the modified UNIFAC model for the prediction of phase equilibria and excess enthalpies for systems with ionic liquids, Fluid Phase Equilibria., 371 (2014) 82–92.

[14] A.V. Orchillés, P.J. Miguel, V. González-Alfaro, Isobaric vapor-liquid equilibria for the 1-propanol + water + 1-ethyl-3-methylimidazolium dicyanamide system at 100 kPa, J. Chem. Thermodynamics, 113 (2017) 116–123.

[15] J. Fu, D. Fu, Salt-containing extractive distillation of 1-propanol/waters 1. Prediction of salt effect on vapor liquid equilibrium, China Petrol. Process. Petrochem. Technol., 14 (2012) 89–96.

[16] A.V. Orchillés, P.J. Miguel, E. Vercher, Isobaric vapor–liquid equilibria for 1-Propanol + Water + 1-Ethyl-3-methylimidazolium Trifluoromethanesulfonate at 100 kPa, J. Chem. Eng. Data, 53 (2008) 2426–2431.

[17] G.Y. Wang, Y.J. Liu, L. Chen, The simulation for separation of n-propanol-iso-propanol-water azeotropic system, J. Jilin Inst. Chem. Technol., 34 (2017) 1–5.

[18] J. Dhanalakshmi, P.S.T. Sai, A.R. Balakrishnan, Effect of inorganic salts on the isobaric vapor-liquid equilibrium of the ethyl acetate-ethanol system, J. Chem. Eng. Data, 58 (2013) 560–569.

[19] M.C. Iliuta, F.C. Thyrion, Effect of calcium chloride on the isobaric vapor-liquid equilibrium of 1-propanol + water, J. Chem. Eng. Data, 41(3) (1996) 402–408.

[20] E. Vercher, F.J. Rojo, A.M. Andreu, Isobaric vapor-liquid equilibria for 1-Propanol + water + calcium nitrate, J. Chem. Eng. Data, 44 (1999) 1216–1221.

[21] M. Pilar Pena, E. Vercher, A. Martinez-Andreu, Isobaric vapor-liquid equilibrium for ethanol + water + sodium nitrate, J. Chem. Eng. Data, 41 (1996) 1097–1100.

[22] A. Fredenslund, R.L. Jones, J.M. Prausnitz, Group-contribution estimation of activity coefficients in nonideal liquid mixtures, AIChE J., 21 (1975) 1086–1099.

[23] J. Gmehling, U. Onken, Vapor-Liquid Equilibrium Data Collection: Chemistry Data Series, DECHEMA, Frankfurt,1977.