Modeling of Liquid-Liquid Equilibria of Aqueous Alcohol + Salt Systems Using a Modified NRTL

M.T. Zafarani-Moattar* and P. Jafari

Department of Physical Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Islamic Republic of Iran
(Received 15 October 2013, Accepted 16 January 2014)

The modified NRTL (m-NRTL) model is used to represent the excess Gibbs free energy of aqueous (alcohol + electrolyte) solutions. In this work, the m-NRTL model, previously developed for representation of vapor-liquid equilibria for (polymer + salt + water) systems, has been extended to represent liquid-liquid equilibria of (alcohol + salt + water) systems. The proposed extension is a modified form/version of the extended NRTL model. The model provides a thermodynamic framework for both correlating and predicting the phase equilibrium of complex systems containing both electrolytes and alcohol. The utility of the model is demonstrated with successful representation of (liquid + liquid) equilibrium of several (alcohol + salt + H₂O) systems at different temperatures. The liquid–liquid equilibria of the ternary systems involved and the mean activity coefficients of the salt + water systems were used simultaneously to obtain the adjustable parameters. For the several aqueous systems containing an alcohol and a salt the performance of this m-NRTL model was examined at the correlation of LLE data. In addition, the results of the suggested model were compared with those obtained using the Setschenow-type equation, extended Wilson (e-Wilson) and extended NRTL (e-NRTL) models.

Keywords: Gibbs energy, Two-phase system, Alcohol + salt, m-NRTL model, e-NRTL model, e-Wilson model

INTRODUCTION

When one alcohol and one organic or inorganic salt such as potassium phosphate are mixed at certain concentrations in an aqueous solution, the solution is separated into two immiscible phases, one rich in alcohol and the other rich in the salt, with water as solvent in both phases. These aqueous two-phase systems can be useful for the recovery and purification of chemical or biological materials [1-3].

Various models with different thermodynamic bases may be used for the correlation of tie-line data for (alcohol + salt + water) systems. The local composition activity coefficient models have been gaining more attention in the correlation of the experimental (vapor +liquid) equilibrium (VLE) and (liquid + liquid) equilibrium (LLE) data due their unique characters, since their advent. These models are comprehensive molecular thermodynamic models for systems with molecular and ionic species, molecules and

___
*Corresponding author. E-mail: zafarani47@yahoo.com

ions with various sizes, and hydrophobic and hydrophilic species. In 2000, van Bochove _et al_.[4] attempted to improve the performance of NRTL model for correlation of tie-line data of mixed solvent electrolyte systems by adding two extra contributions (Born and Born-Guggenheim). This modification has only slightly improved the quality of fitting of LLE data, and introduced extra parameters. These authors have reviewed the performance of previously proposed models [4]. Recently, to represent the excess Gibbs energy of aqueous alcohol + salt systems, Zafarani-Moattar _et al._ [5] and Nemati-Kande _et al_. [6] proposed the generalized NRTL and generalized Wilson local composition models, respectively. However, for LLE of the aqueous alcohol + salt systems, although good results have been achieved using these recent models, there is still possibility for further improvement.

In this work we present m-NRTL model for representing LLE data for (alcohol + salt + water) systems. In this model, the excess Gibbs free energy of an aqueous alcohol + electrolyte solution is represented by the sum of the

contributions of a long-range and short-range interaction terms. This model uses of the Pitzer-Debye-Huckel (PDH) equation for the long-range interactions and m-NRTL model for the short-range interactions. This model is the extension of m-NRTL model presented by Sadeghi [7] for fitting the VLE data of (polymer + salt + water) systems.

The applicability of the developed model is tested using experimental tie-line data of various aqueous (alcohol + salt) systems at different temperatures. Also, the performance of this model at the correlation of LLE data is compared with the previous models such as extended Wilson (e-Wilson) [6] and extended NRTL (e-NRTL) [5] models, and the Setschenow-type equation [8] which usually gives acceptable results in the correlation of these kinds of systems.

MODEL DESCRIPTION

The modified NRTL (m-NRTL) model [7] for the excess Gibbs energy, G^E, is expressed as the sum of two contributions:

$$G^E = G^{E,LR} + G^{E,SR} \tag{1}$$

where, $G^{E,LR}$ is the long-range interaction contribution, and $G^{E,SR}$ is the short-range interaction contribution. The long-range interaction term accounts for the electrostatic interactions between ions and the short-range interaction term considers the non-electrostatic interactions between all species (ion, solvent, and segment). The major difference between this model and that of our previous paper [9] is in their reference Gibbs energies of local composition cells with a central ion. In previous paper [9] the pure completely dissociated electrolyte was used for the reference Gibbs energies of local composition cells with a central ion. However, in this work, a cell with random composition is used.

Accordingly, appropriate derivation of Eq. (1) gives the activity coefficient of component j as follows:

$$\ln \gamma_j = \ln \gamma_j^{m,LR} + \ln \gamma_j^{m,SR} \tag{2}$$

where, j denotes any component (ions, alcohol and water).

For the long-range contribution, the Pitzer-Debye-

Hückel [10] has been used. For the short-range contribution, the m-NRTL model [7] is used.

Long-Range Interaction Contributions to the Excess Gibbs Free Energy

The PDH equation [10] which is generalized to mixed solvents is used for the long-range contribution to the activity coefficients. The PDH equation has the following form:

$$\ln \gamma_M^{LR} = -A_x \left(\frac{2Z_k^2}{\rho} \ln(\frac{1+\rho I_x^{1/2}}{1+\frac{\rho Z_k}{\sqrt{2}}}) + \frac{Z_k^2 I_x^{1/2} - 2I_x^{3/2}}{1+\rho I_x^{1/2}} \right) \tag{3}$$

where, I_x is the ionic strength in mole fraction bases and A_x is the usual Debye-Hückel parameter:

$$I = -0.5\sum_i x_i Z_i^2 \tag{4}$$

$$A_x = -\frac{1}{3}(2\pi N_A d_s)^{1/2} \left(\frac{e^2}{\varepsilon_s KT} \right)^{3/2} \tag{5}$$

In these relations, Z_i is the charge number of the i th ion, and ρ is the closest distance parameter. Also, N_A, k, T and e are Avogadro's number, Boltzmann constant, absolute temperature and the electronic charge, respectively. Moreover, d_s and ε_s are the mixed solvent density and dielectric constant, respectively. In the case of LLE of (organic solvent + salt + water) systems the difference in the dielectric constants and the densities of the solvents will be large, and a physically correct description will require the use of a solvent composition-dependent dielectric constant and density [4]. A possible way to consider the properties of a mixed solvent is taking account the dependency of dielectric constant and density of mixed solvent on the composition of each solvent. In this regard, Chen et al. [11] adopted following equations as the simple composition average mixing rules to calculate the density and dielectric constant of the mixed solvent:

$$\frac{1}{d_s} = \sum_m \frac{x_m}{\sum_m x_{m'}} \frac{1}{d_m} \tag{6}$$

$$\varepsilon_s = \sum_m \frac{x_m M_m}{\sum x_{m'} M_{m'}} \varepsilon_m \tag{7}$$

where, M_m and x_m are the molecular weight and the mole fraction of the solvent m.

Short-Range Interaction Contributions to the Excess Gibbs Free Energy

The model development for the NRTL local interaction contribution has been described in details by Chen *et al.* [12-14]. Here, we only represented general expressions for multi component electrolyte systems. The studied systems in this work have been composed of two molecular species (water, w, and alcohol, m) and one electrolyte, ca. The modified NRTL model presented for the correlation of vapor-liquid equilibria (VLE) for (polymer-salt-water) systems [7] can be extended to (alcohol-salt-water) simply considering alcohol instead of polymer and giving unity for number of segments in the corresponding equation for excess Gibbs energy:

$$\frac{G^{m,SR}}{RT} = n_m \left(\frac{X_m X_w (\tau_{ca,m} G_{ca,m} + X_w \tau_{wm} G_{wm})}{X_m + (X_c + X_a) G_{ca,m} + X_w G_{wm}} \right) + n_w \left(\frac{X_m \tau_{mw} G_{mw} + (X_c + X_a) \tau_{ca,w} G_{ca,w}}{X_m G_{mw} + (X_c + X_a) G_{ca,w} + X_w} \right)$$

$$+ Z_c n_c \left[\left(\frac{X_m X_w (\tau_{m,ca} - \tau_{w,ca})(G_{m,ca} - G_{w,ca}) + X_w X_a \tau_{w,ca}(G_{w,ca} - 1) + X_m X_a \tau_{m,ca}(G_{m,ca} - 1)}{(X_m G_{m,ca} + X_a + X_w G_{w,ca}) A} \right) \right]$$

$$+ Z_a n_a \left[\left(\frac{X_m X_w (\tau_{m,ca} - \tau_{w,ca})(G_{m,ca} - G_{w,ca}) + X_w X_c \tau_{w,ca}(G_{w,ca} - 1) + X_m X_c \tau_{m,ca}(G_{m,ca} - 1)}{(X_m G_{m,ca} + X_c + X_w G_{w,ca}) B} \right) \right]$$

$$(8)$$

$$A = r X_m + X_a + X_w ,$$

G and τ are energy parameters, and are presented as:

$$G_{m,ca} = \exp(-\alpha \tau_{m,ca}), \tau_{m,ca} = \tau_{mc,ac} = \tau_{ma,ca}, \tau_{mk,k'k} = \frac{g_{mk} - g_{kk'}}{RT} = \frac{A_{m,ca}}{RT}$$

$$(9)$$

$$G_{ca,m} = \exp(-\alpha \tau_{ca,m}), \tau_{ca,m} = \tau_{cm} = \tau_{am}, \tau_{km} = \frac{g_{km} - g_{mm}}{RT} = \frac{A_{ca,m}}{RT}$$

$$(10)$$

$$G_{m'm} = \exp(-\alpha \tau_{m'm}), \tau_{m'm} = \frac{g_{m'm} - g_{mm}}{RT} = \frac{A_{m'm}}{RT} \tag{11}$$

In above relations the subscripts w, m, ca, c and a stand for water, alcohol, salt, cation and anion, respectively. α is the non-randomness factor that can be set in a fixed value.

$g_{m'm}$ and g_{mm} are interaction energies between $m'-m$ and $m-m$ species, respectively. The specie m' can be solvent molecules or salt. X_i is the effective local mole fraction based on the number of moles of segments, ions and solvent and is given by:

$$X_i = k_i x_i \qquad (K_i = Z_i \text{ for ions and unity for molecular species}) \tag{12}$$

So, there are six energy parameters ($\tau_{mw}, \tau_{wm}, \tau_{ca,w}, \tau_{w,ca}, \tau_{m,ca}, \tau_{ca,m}$) for aqueous mixed-solvent systems. Interaction parameters for alcohol-water (τ_{mw}), water-alcohol (τ_{wm}), salt-water ($\tau_{ca,w}$) and water-salt ($\tau_{w,ca}$) are obtained using the corresponding VLE data. The remaining interaction parameters corresponding to alcohol and salt ($\tau_{m,ca}, \tau_{ca,m}$) can be calculated from the correlation of LLE data for the investigated aqueous alcohol + salt systems.

From appropriate differentiation of excess Gibbs energy expression (Eq. (8)) the following equations for the activity coefficient of water and salt of the m-NRTL model are obtained:

$$\ln \gamma_{w,NRTL}^{SR} = \frac{X_m G_{wm}}{X_m + (X_a + X_c) G_{ca,m} + X_w G_{wm}} \times (\tau_{wm} - \frac{X_w \tau_{wm} G_{wm} + (X_a + X_c) G_{ca,m} \tau_{ca,m}}{X_m + (X_a + X_c) G_{ca,m} + X_w G_{wm}})$$

$$+ \frac{X_m \tau_{mw} G_{mm} + (X_a + X_c) \tau_{ca,w} G_{ca,w}}{X_m G_{mw} + (X_a + X_c) G_{ca,w} + X_w} \times (1 - \frac{X_w}{X_m G_{mw} + (X_a + X_c) G_{ca,m} + X_w})$$

$$+ X_c \frac{X_m (\tau_{m,ca} - \tau_{w,ca})(G_{m,ca} - G_{w,ca}) + X_a \tau_{w,ca}(G_{w,ca} - 1)}{(X_m G_{m,ca} + X_a + X_w G_{w,ca}) A}$$

$$\times (1 - \frac{X_w G_{w,ca}}{X_m G_{m,ca} + X_a + X_w G_{w,ca}} - \frac{X_w}{A}) - \frac{X_m X_a X_c \tau_{m,ca}(G_{m,ca} - 1)}{(X_m G_{m,ca} + X_a + X_w G_{w,ca}) A}$$

$$\times (\frac{G_{w,ca}}{X_m G_{m,ca} + X_a + X_w G_{w,ca}} - \frac{1}{A}) + X_a \frac{X_m (\tau_{m,ca} - \tau_{w,ca})(G_{m,ca} - G_{w,ca}) + X_c \tau_{w,ca}(G_{w,ca} - 1)}{(X_m G_{m,ca} + X_c + X_w G_{w,ca}) B}$$

$$\times (1 - \frac{X_w G_{w,ca}}{X_m G_{m,ca} + X_c + X_w G_{w,ca}} - \frac{X_w}{B}) - \frac{X_m X_a X_c \tau_{m,ca}(G_{m,ca} - 1)}{(X_m G_{m,ca} + X_c + X_w G_{w,ca}) B}$$

$$\times (\frac{G_{w,ca}}{X_m G_{m,ca} + X_c + X_w G_{w,ca}} + \frac{1}{B})$$

$$(13)$$

$$\frac{1}{Z_c}\ln\gamma_c = -A_x[\frac{2Z_c}{\rho}\ln(1+\rho I_x^{0.5})+\frac{Z_c^2 I_x^{0.5}-2I_x^{1.5}}{Z_c(1+\rho I_x^{0.5})}]+\frac{X_w^2\tau_{ca,w}G_{ca,w}}{(X_c G_{ca,w}+X_a G_{ca,w}+X_w)}$$

$$+\frac{X_a X_w\tau_{w,ca}(G_{w,ca}-1)}{(X_a+X_w G_{w,ca})(X_a+X_w)}+\frac{X_a X_w\tau_{w,ca}(G_{w,ca}-1)(X_w^2 G_{w,ca}-X_c^2)}{(X_c+X_w G_{w,ca})^2(X_c+X_w)^2}-\tau_{ca,w}G_{ca,w}$$

$$(14)$$

and

$$\frac{1}{Z_a}\ln\gamma_a = -A_x[\frac{2Z_a}{\rho}\ln(1+\rho I_x^{0.5})+\frac{Z_a^2 I_x^{0.5}-2I_x^{1.5}}{Z_a(1+\rho I_x^{0.5})}]+\frac{X_w^2\tau_{ca,w}G_{ca,w}}{(X_a G_{ca,w}+X_c G_{ca,w}+X_w)^2}$$

$$+\frac{X_c X_w\tau_{w,ca}(G_{w,ca}-1)}{(X_a+X_w G_{w,ca})(X_c+X_w)}+\frac{X_c X_w\tau_{w,ca}(G_{w,ca}-1)(X_w^2 G_{w,ca}-X_a^2)}{(X_a+X_w G_{w,ca})^2(X_a+X_w)^2}-\tau_{ca,w}G_{ca,w}$$

$$(15)$$

RESULT AND DISCUSSION

The applicability of the proposed model has been tested using experimental LLE data for a variety of (alcohol + salt + water) systems. For the correlation of the tie-line data we used the value of $\rho = 14.9$, that has been frequently used for the aqueous electrolyte solutions [15]. The required densities of water and alcohol were obtained from [16-21] at the studied temperatures and reported in Table 1. Furthermore, the dielectric constants of any alcohol and water at the mentioned temperatures were obtained from [20]. The four interaction parameters ($\tau_{m,ca}$, $\tau_{ca,m}$, $\tau_{w,ca}$, $\tau_{ca,w}$) were calculated from fitting of water activity or osmotic coefficient data for the corresponding binary aqueous salt and alcohol solutions when these data are

available at working temperature, otherwise these interaction parameters can be obtained from the correlation of LLE data. The remaining two alcohol-salt and salt-alcohol parameters were calculated by fitting the LLE data. Each of the three non-randomness factors (α_{wca}, α_{mw} and α_{mca}) is usually set in a fixed value. We examined different α values in fitting the available (vapor + liquid) data for binary aqueous salt and alcohol solutions and the experimental LLE data reported in the literature. The suitable values of non-randomness factors which give better quality of fitting were found to be ($\alpha_{wm}=\alpha_{mw}=0.1$, $\alpha_{wca}=\alpha_{caw}=0.1$, $\alpha_{mca}=\alpha_{mca}=0.01$). In fitting LLE data to the modified NRTL and other local composition models and Seteschenow-type equation, the following objective function (Eq. (16)) and equilibrium condition (Eq. (17)) were used:

$$Of = \sum_T\sum_p\sum_l\sum_j(w_{T,p,l,j}^{cal}-w_{T,p,l,j}^{exp})^2$$

$$(16)$$

$$(x_j\gamma_j)^{top}=(x_j\gamma_j)^{bot}$$

$$(17)$$

in which x and γ represent mole fraction and activity coefficient, respectively. The evaluated parameters of different models are listed in Tables 2 to 5 together with the corresponding deviations and the sources of the experimental data. In Table 6 comparison between deviations obtained with different models are given, which

Table 1. Brief Summary of the Characteristic of the Used Alcohols

Material	M (g mol⁻¹)	d (kg m⁻³)			ε (c² J⁻¹ m⁻¹)		
		298.15	308.15	318.15	298.15	308.15	318.15
1-propanol	60.096	799.54	792.27	784.20	20.18	19.05	17.16
2-propanol	60.096	781.10	772.88	763.97	19.85	17.76	16.15
1-butanol	74.123	793.20	765.30	754.20	16.20	15.32	14.20
2-Butanol	74.123	803.35	793.21	788.511	15.90	14.50	13.10
2-methyl-2-propanol	74.123	784.30	768.36	756.327	12.47	10.80	9.87

Table 2. The Parameters of the e-NRTL Model for some {Alcohol (m) + Electrolyte (ca) + Water (w)} Systems at Working Temperature

T/K	τ_{wm}	τ_{mw}	τ_{wca}	τ_{caw}	τ_{mca}	τ_{cam}	Dev[a]
Generalized NRTL($\alpha_{wm} = \alpha_{mw} = 0.1, \alpha_{wca} = \alpha_{caw} = 0.1, \alpha_{mca} = \alpha_{mca} = 0.01$)							
1-propanol + di-sodium hydrogen citrate							
298.15	3.0393[b]	-2.4819[b]	1.5603[d]	-0.2022[d]	10.8878	10.2682	0.03
308.15	1.5658	2.4868	7.5979	16.7112	20.2891	-10.828	0.04
318.15	-0.9579	6.9760	-2.9943	10.9181	-0.8918	-1.8230	1.96
2-propanol + di-sodium hydrogen citrate							
298.15	2.8091[c]	6.6528[c]	1.5603[d]	-0.2022[d]	-10.747	31.225	0.47
308.15	0.6002	2.2569	-24.5115	39.2288	-111.9262	63.7750	0.98
318.15	2.0136	30.0766	-524.113	-5.2630	-0.0046	73.2963	0.23
1-butanol + di-sodium hydrogen citrate							
298.15	1.8636	10.8944	1.5603[d]	-0.2022[d]	-31.2722	87.9262	0.01
308.15	1.2760	4.7165	21.1881	-2.6947	18.3268	-76.9062	0.08
318.15	2.8636	11.0065	16.1023	146.8547	-4.2605	87.6291	0.01
2-butanol + di-sodium hydrogen citrate							
298.15	3.5456	13.3764	1.5603[d]	-0.2022[d]	-33.1109	161.4522	0.03
308.15	-0.810	6.001	3.0020	-0.0854	-14.3002	65.79	0.87
318.15	0.159	3.9984	-139	1299	-526.8444	33.1527	0.08
2-methyl-2-propanol+ di-sodium hydrogen citrate							
298.15	1.9800	2.5047	1.5603[d]	-0.2022[d]	-4.5304	26.2770	0.04
308.15	2.6106	4.5565	17.3855	20.0824	48.769	-47.3063	0.35
318.15	2.6294	-0.4043	-822.1102	8.2483	484100	34.9980	0.19
1-propanol + cesium carbonate							
298.15	3.0393[b]	-2.4819[b]	-10.3903	0.9990	-53.0385	73.1326	0.38
308.15	1.9080	0.2408	-0.026	2.0002	4.365	12.9308	0.45
318.15	2.1104	0.0554	0.0916	2.0185	-9.8492	33.1115	0.52
2-propanol + cesium carbonate							
298.15	2.8091[c]	6.6528[c]	-8.8315	2.3800	-44.71	57.9032	0.18
1-propanol + di-ammonium hydrogen citrate							
298.15	3.0393[b]	-2.4819[b]	-73.9257	2.4622	-458.3416	60.2126	1.69
2-propanol+ di-ammonium hydrogen citrate							
298.15	2.8091[c]	6.6528[c]	5.9729	8.0289	4.5933	1.1871	0.91
2-butanol+ di-ammonium hydrogen citrate							
298.15	-1.3091	5.8764	-89.2394	9.8406	-3765.1	7858.5	1.30
2-methyl-2-propanol+ di-ammonium hydrogen citrate							
298.15	1.3305	4.6088	-2858.7	674.9528	-558.3778	2917.1	0.60
1-propanol + di-sodium tartarate(zafarani)							
298.15	3.0393[b]	-2.4819[b]	0.0107	-8.096	5.7953	13.5320	0.30
2-propanol + di-sodium tartarate(zafarani)							
298.15	2.8091[c]	6.6528[c]	3.022	9.0015	-17.8287	41.3406	0.70
2-butanol + di-sodium tartarate(zafarani)							

Table 2. Continued

298.15	3.4682	5.5619	23.0975	5.174	16.6781	-9.2963	0.27
			2-methyl-2-propanol + di-sodium tartarate(zafarani)				
298.15	2.4526	0.8525	12.9841	296.2679	2.8492	83.3233	0.77
			1-propanol+di-sodium tartarate				
298.15	3.0393^b	-2.4819^b	2.0107	-8.096	5.7953	13.5320	1.22
			2-propanol+di-sodium tartarate				
298.15	2.8091^c	6.6528^c	3.022	11.0015	-17.8287	41.3406	0.26
			2-butanol +di-sodium tartarate				
298.15	0.3682	5.5619	23.0975	5.174	22.6781	-7.2963	0.18
			2-methyl-2-propanol+di-sodium tartarate				
298.15	2.4526	0.8525	12.9841	297.2679	2.8492	83.3233	0.13
			2-propanol + lithium sulfate				
298.15	2.8091^c	6.6528^c	1.8844^e	-1.0759^e	170.1411	-22.1608	0.22
308.15	-0.0087	0.7202	30.9026	-13.1429	10.6891	-33.1463	1.41
318.15	6.1706	50.9911	25.6097	-12.2272	18.597	24.2784	1.52
			1-propanol + manganese sulfate				
298.15	3.0393^b	-2.4819^b	-0.653^f	-0.2844^f	-20.1895	50.6125	0.59
			2-propanol + manganese sulfate				
298.15	2.8091^c	6.6528^c	-0.653^f	-0.2844^f	30.0846	-14.2916	2.65
			2-propanol + sodium carbonate				
298.15	2.8091^c	6.6528^c	22.7685	-8.8318	46.567	-59.9321	0.30
			2-propanol + potassium carbonate				
298.15	2.8091^c	6.6528^c	19.954	-7.7372	108.1749	-74.7695	1.25
			1-propanol + potassium citrate				
298.15	3.0393^b	-2.4819^b	-127.146	8.1192	-872.2601	150.313	0.68
			2-propanol + potassium citrate				
298.15	2.8091^c	6.6528^c	14.3482	6.1414	36.2048	-34.7329	0.77
			2-butanol +potassium citrate				
298.15	2.8803	4.2323	-4239.4	1940.6	-1765.1	367.4527	0.07
			2-methyl-2-propanol + potassium citrate				
298.15	1.6037	2.7832	-2858.7	65.9628	-558.3778	390.5618	1.62
			1-propanol + sodium citrate				
298.15	3.0393^b	-2.4819^b	0.2627^g	-1.0477^g	-18.9613	145.5457	0.66
			2-propanol + sodium citrate				
298.15	2.8091^c	6.6528^c	0.2627^g	-1.0477^g	-19.9171	214.2861	1.99
			2-butanol + sodium citrate				
298.15	0.7684	5.9128	0.2627^g	-1.0477^g	-4.1054	2872	0.68
			2-methyl-2-propanol + sodium citrate				
298.15	3.3875	-2.8597	0.2627^g	-1.0477^g	-3.5394	248.5177	0.15

Table 2. Continued

			1-propanol + di-sodium sccinate				
298.15	3.0393[b]	-2.4819[b]	55.6059	-11.0504	1.5211	-0.6379	0.16
			2-propanol + di-sodium sccinate				
298.15	2.8091[c]	6.6528[c]	10.7627	-6.4327	29.5048	-18.961	0.02
			2-butanol + di-sodium succinate				
298.15	2.8119	4.8145	-0.5367	6.2521	0.6402	17.4852	0.08
			2-methyl-2-propanol + di-sodium succinate				
298.15	1.8847	2.2051	11.1755	5.8316	6.0054	28.1852	0.02
			1-propanol + thiosulfate				
298.15	3.0393[b]	-2.4819[b]	1.8442[h]	-0.7874[h]	60.4795	103.9256	1.96
			2-propanol +thiosulfate				
298.15	2.8091[c]	6.6528[c]	1.8442[h]	-0.7874[h]	1.6279	134.7831	0.40
			2-butanol + thiosulfate				
298.15	5.3928	20.1906	1.8442[h]	-0.7874[h]	1.5561	18.5873	0.06
			2-methyl-2-propanol + thiosulfate				
298.15	1.405	3.2617	1.8442[h]	-0.7874[h]	3.47261	123.8333	1.16

[a] $Dev = \sum_p \sum_l \sum_j \sum_T ((100 w_{p,l,j,T}^{cal} - 100 w_{p,l,j,T}^{exp})^2 / 6N))$, where $w_{p,l,j,T}$ is the mass fraction of the component j (*i.e.* alcohol, salt or water) in the phase p for l th tie-line at temperature T and N represents the number of tie line data. [b]These parameters are obtained from the correlation of the binary vapor-liquid equilibrium data for (1-propanol + water) system reported in Ref. [22]. [c]These parameters are obtained from the correlation of the binary vapor-liquid equilibrium data for (2-propanol + water) system reported in Ref. [23]. [d,e,f,g,h]These parameters are obtained from the correlation of the binary activity coefficient data for binary ($Na_2C_6H_6O_7$ + water) [24], (Li_2SO_4 or $MnSO_4$ + water) [25], ($Na_3C_6H_5O_7$ + water) [21], and (Na_2SO_4 + water) [26] systems.

Table 3. The Parameters of the e-Wilson [6] Model for some {Alcohol (m) + Electrolyte (ca) + Water (w)} Systems at Working Temperature

	e-Wilson						
T/K	H_{wm}	H_{mw}	H_{wca}	H_{caw}	H_{mca}	H_{cam}	Dev
1-propanol +di-sodium hydrogen citrate							
298.15	1.4420[a]	0.4997[a]	2.4543[c]	0.6184[c]	1.0064	-2.788	0.27
308.15	0.813	1.0205	0.9183	1.4139	0.2234	0.8352	0.04
318.15	0.7084	0.8710	0.2285	0.2168	0.0713	1.0641	0.08
2-propanol+di-sodium hydrogen citrate							
298.15	1.3389[b]	0.5808[b]	2.4543[c]	0.6184[c]	1.7977	-2.0613	0.84
308.15	0.830	1.0005	0.9083	1.4039	0.1934	0.8352	0.02
318.15	0.5560	0.8475	0.3228	0.2920	0.3582	0.7804	0.46
1-butanol +di-sodium hydrogen citrate							
298.15	0.440	1.2009	2.4543[c]	0.6184[c]	-2.10	-0.3513	5.48
308.15	0.5090	1.1816	90.0878	-0.1826	-32.1242	-0.0001	0.12
318.15	0.4303	1.418	0.0033	-3.5352	-0.0038	-1.9442	0.01

Table 3. Continued

2-buutanol+di-sodium hydrogen citrate							
298.15	-9.4780	0.005	2.4543^c	0.6184^c	-0.0085	0.5037	1.51
308.15	0.8241	0.9142	0.0572	-2.2829	-0.2964	0.2028	0.06
318.15	0.7639	0.868	1.0006	0.0649	-1.1995	0.0273	0.01
2-methyl-2-propanol +di-sodium hydrogen citrate							
298.15	0.511	1.3433	2.4543^c	0.6184^c	1.1529	1.1529	0.19
308.15	0.6993	0.9447	0.3920	-0.1668	0.5515	-0.5483	2.18
318.15	0.6835	0.8914	0.1883	0.6126	0.0460	0.3859	0.59
1-propanol + cesium carbonate							
298.15	1.4420^a	0.4997^a	99.5024	-0.0684	1.3747	-0.1083	0.46
308.15	0.6532	0.9896	0.7410	0.3195	-0.1407	0.8198	0.11
318.15	0.6243	1.1515	0.7392	0.8248	-0.1927	0.9901	0.12
2-propanol + cesium carbonate							
298.15	1.3389^b	0.5808^b	0.1507	3.2585	-0.0774	1.6089	0.03
1-propanol + di-ammonium hydrogen citrate							
298.15	1.4420^a	0.4997^a	0.1163	4.2299	-0.1197	1.8705	0.35
2-propanol + di-ammonium hydrogen citrate							
298.15	1.3389^b	0.5808^b	0.6365	1.6272	0.1865	0.8868	0.12
2-butanol + di-ammonium hydrogen citrate							
298.15	0.7500	0.8476	0.9779	0.8520	-0.8075	1.3958	0.25
2-methyl-2-propanol+ di-ammonium hydrogen citrate							
298.15	0.7387	0.8365	0.2017	0.4074	0.0174	1.0815	0.08
1-propanol+di-sodium succinate							
298.15	1.4420^a	0.4997^a	0.6863	3.0202	-0.1007	0.6455	0.02
2-propanol+di-sodium succinate							
298.15	1.3389^b	0.5808^b	0.9972	2.3445	0.2859	0.1927	0.09
2-butanol+di-sodium succinate							
298.15	0.6531	0.8428	0.1263	0.3459	0.0353	-1.4616	0.23
2-methyl-2-propanol+di-sodium succinate							
298.15	0.8076	0.8537	0.31	0.6851	-0.2179	1.1179	0.02
1-propanol+di-sodium tartarate							
298.15	1.4420^a	0.4997^a	20.9134	1.738	-17.1211	0.3284	0.09
2-propanol+di-sodium tartarate							
298.15	1.3389^b	0.5808^b	1.059	1.4869	-0.1676	0.7034	0.48
2-butanol+di-sodium tartarate							
298.15	0.8287	0.8709	0.0423	1.0398	-0.2331	2.5723	0.09
2-methyl-2-propanol+di-sodium tartarate							
298.15	0.8541	0.8313	2.1426	1.1334	-0.5187	0.1125	0.08
1-propanol+di-sodium tartarate							
298.15	1.4420^a	0.4997^a	9.9134	0.738	-14.1211	0.3284	0.08
2-propanol+di-sodium tartarate							
298.15	1.3389^b	0.5808^b	2.059	1.4869	-1.1676	0.7034	0.45

Table 3. Continued

2-butanol+di-sodium tartarate(zafarani)							
298.15	0.8287	0.8709	0.0423	1.0398	-0.2331	2.5723	0.02
2-methyl-2-propanol+di-sodium tartarate							
298.15	0.8541	0.8313	2.1426	1.1334	-0.5187	0.1125	0.10
2-propanol+lithium solfate							
298.15	1.3389^b	0.5808^b	2.8993^d	0.7255^d	5.3325	-2.616	0.42
308.15	1.1744	0.2868	1.226	0.5912	-1.1417	0.514	0.60
318.15	1.8329	-0.144	0.8351	2.4585	1.7483	-5.9956	0.05
1-propanol+magnesium solfate							
298.15	1.4420^a	0.4997^a	-7.6197^e	0.0055^e	-0.5461	1.9303	0.08
2-propanol+ magnesium solfate							
298.15	1.3389^b	0.5808^b	-7.6197^e	0.0055^e	-0.3635	-0.2309	0.16
2-propanol+potassium carbonate							
298.15	1.3389^b	0.5808^b	1.7587	1.7019	1.994	-1.2601	0.03
2-propanol+sodium carbonate							
298.15	1.3389^b	0.5808^b	1.2215	1.3071	1.5383	-1.5213	0.18
1-propanol+potassium citrate							
298.15	1.4420^a	0.4997^a	1.3716	6.7485	0.2651	-2.0144	0.03
2-propanol+potassium citrate							
298.15	1.3389^b	0.5808^b	1.7915	4.5876	1.0506	-1.0255	0.03
2-butanol +potassium citrate							
298.15	0.7334	0.8181	0.5708	-0.2849	-2.7245	3.0643	0.02
2-methyl-2-propanol+potassium citrate							
298.15	0.7947	0.8323	0.1602	0.3966	0.0102	-0.0653	0.05
1-propanol+sodium citrate							
298.15	1.4420^a	0.4997^a	0.9758^f	1.2388^f	4.0436	-7.595	0.14
2-propanol+ sodium citrate							
298.15	1.3389^b	0.5808^b	0.9758^f	1.2388^f	5.2993	-7.2158	0.20
2-butanol + sodium citrate							
298.15	0.6218	1.1031	0.9758^f	1.2388^f	-1.3528	1.0878	0.03
2-methyl-2-propanol+ sodium citrate							
298.15	0.9091	0.7634	0.9758^f	1.2388^f	2.4286	-3.4419	0.11
1-propanol+thio sulfate							
298.15	1.4420^a	0.4997^a	3.9414^g	-0.4624^g	-2.7251	-1.1446	0.03
2-propanol+thio sulfate							
298.15	1.3389^b	0.5808^b	3.9414^g	-0.4624^g	5.3695	3.1915	1.10
2-butanol+thio sulfate							
298.15			3.9414^g	-0.4624^g			
2-methyl-2-propanol+thio sulfate							
298.15			3.9414^g	-0.4624^g			

Table 3. Continued

$^a Dev = \sum_p \sum_l \sum_j \sum_T ((100 w_{p,l,j,T}^{cal} - 100 w_{p,l,j,T}^{exp})^2 / 6N)$), where $w_{p,l,j,T}$ *is* the mass fraction of the component j (*i. e.* alcohol, salt or water) in the phase p for $_l$ th tie-line at temperature T and N represents the number of tie line data. ^{b}These parameters are obtained from the correlation of the binary vapor-liquid equilibrium data for (1-propanol + water) system reported in Ref. [22]. ^{c}These parameters are obtained from the correlation of the binary vapor-liquid equilibrium data for (2-propanol + water) system reported in Ref. [23]. ^{d,e,f,g,h}These parameters are obtained from the correlation of the binary activity coefficient data for binary ($Na_2C_6H_6O_7$ + water) [24], (Li_2SO_4 or $MnSO_4$ + water) [25], ($Na_3C_6H_5O_7$ + water) [21], and (Na_2SO_4 + water) [26] systems.

Table 4. The Parameters of the Setschenow-Type Equation [8] for some {Alcohol (m) + Electrolyte (ca) + Water (w)} Systems at Working Temperature

Setschenow- type equation as a independent of temperature (Eq. (5))			
T/K	k_m	k_s	Dev
1-propanol + di-sodium hydrogen citrate			
298.15	0.4337	1.7572	0.07
308.15	0.0128	1.4741	0.06
318.15	1.2171	0.7126	0.08
2-propanol + di-sodium hydrogen citrate			
298.15	1.5001	0.3132	0.05
308.15	0.7113	0.8308	0.02
318.15	0.4563	0.7105	0.02
1-butanol + di-sodium hydrogen citrate			
298.15	3.6050	0.3230	0.06
308.15	3.8254	0.6820	0.02
318.15	-1.1944	-0.7556	0.02
2-butanol + di-sodium hydrogen citrate			
298.15	4.7860	75.6163	0.08
308.15	3.5366	0.5543	0.03
318.15	3.4221	1.3247	0.10
2-methyl-2-propanol + di-sodium hydrogen citrate			
298.15	0.7244	1.8686	0.08
308.15	1.0175	1.5850	0.18
318.15	0.8264	2.6915	0.20
1-propanol + cesium carbonate			
298.15	1.925	0.9542	0.04
308.15	1.5096	0.9686	0.02
318.15	2.0916	0.8292	0.06
1-propanol + cesium carbonate			
298.15	2.1028	0.6588	0.04

Table 4. Continued

1-propanol+ di-ammonium hydrogen citrate			
298.15	1.8699	0.6514	0.25
2-propanol+ di-ammonium hydrogen citrate			
298.15	0.1022	0.9403	0.07
2-butanol + di-ammonium hydrogen citrate			
298.15	2.9279	1.1439	0.05
2-methyl-2-propanol+ di-ammonium hydrogen citrate			
29815	0.8525	1.5068	0.07
1-propanol+ di-sodium tartarate			
298.15	0.8465	1.7095	0.24
2-propanol+ di- sodium tartarate			
298.15	-0.2292	1.6368	0.05
2-butanol + di-sodium tartarate			
298.15	2.7611	1.9622	0.13
2-methyl-2-propanol + di-sodium tartarate			
298.15	0.6312	2.6075	0.02
2-propanol + lithium sulfate			
298.15	0.0533	2.183	0.13
308.15	-0.7607	3.1796	0.19
318.15	-0.9374	3.3535	0.66
1-propanol + manganes sulfate			
298.15	0.7165	1.1894	0.19
2-propanol + manganes sulfate			
298.15	0.6431	1.4698	0.35
2-propanol + potassium carbonate			
298.15	-0.2277	1.7255	0.05
2-propanol + sodium carbonate			
298.15	-1.3637	2.0493	0.01
1-propanol + potassium citrate			
298.15	0.3881	3.8287	0.10
2-propanol + potassium citrate			
298.15	0.0723	3.2436	0.06
2-butanol + potassium citrate			
298.15	1.4793	3.1729	0.03
2-butanol + potassium citrate			
298.15	0.5352	3.5801	0.07
1-propanol + sodium citrate			
298.15	-0.1424	4.0302	0.10
2-propanol + sodium citrate			
298.15	-0.2495	2.4721	0.05
2-propanol + sodium citrate			
298.15	3.4647	-4.755	0.07
2-methyl-2-propanol			
298.15	0.1429	4.349	0.05

Table 4. Continued

1-propanol + thio solfate			
298.15	0.5575	0.9936	0.14
2-propanol + thio solfate			
298.15	6.3158	0.2361	0.01
2-butanol + thio solfate			
298.15	9.2199	-.00090	0.01
2-methyl-2-propanol + thio solfate			
298.15	1.0206	0.8605	0.04
1-propanol + sodium succinate			
298.15	-0.101	2.1077	0.07
2-propanol + sodium succinate			
298.15	0.0915	1.7052	0.09
2-butanol + sodium succinate			
298.15	1.6578	1.5904	0.14
2-methyl-2-propanol + sodium succinate			
298.15	0.8551	2.4184	0.01
1-propanol + di-sodium tartarate			
298.15	0.4261	2.2685	0.04
2-propanol + di-sodium tartarate			
298.15	0.1355	1.3448	1.06
2-butanol + di-sodium tartarate			
298.15	1.473	2.541	0.02
2-methyl-2-propanol + di-sodium tartarate			
298.15	0.2507	3.138	0.08

Table 5. The Parameters of the m-NRTL Model for some {Alcohol (m) + Electrolyte (ca) + Water (w)} Systems at Working Temperature

				m-NRTL			
T/K	τ_{wm}	τ_{mw}	τ_{wca}	τ_{caw}	τ_{mca}	τ_{cam}	Dev
1-propanol + di-sodium hydrogen citrate							
298.15	3.0393[a]	-2.4819[a]	-15.4109[c]	3.2034[c]	-105.0063	-0.3969	0.13
308.15	-0.2940	-2.7203	20.8905	512.5473	21.5662	-16.2467	0.14
318.15	12.4087	-0.7117	19.1509	-6.2830	10.1402	-1.9837	0.03
2-propanol + di-sodium hydrogen citrate							
298.15	2.9480[b]	-2.4490[b]	-15.4109[c]	3.2034[c]	6.2694	-22.5461	0.05
308.15	-0.5082	-5.3295	20.3938	-5.1029	23.6849	-16.4243	0.08
318.15	12.4087	-0.7117	19.1509	-6.2830	10.1402	-1.9837	0.09
1-butanol + di-sodium hydrogen citrate							
298.15	8.7614	-3.4826	-15.4109[c]	3.2034[c]	-15.8101	249.4811	0.01
308.15	2.6271	-3.9321	-2.8640	1.7340	-41.2258	1.9886	0.02
318.15	5.5708	-1.6162	17.7198	32.2122	199.7268	85.9064	0.01
2-butanol + di-sodium hydrogen citrate							
298.15	6.3618	-1.6575	-15.4109[c]	3.2034[c]	34.1676	43.1016	0.01
308.15	7.0121	-2.6471	17.8285	-8.6484	32.1463	-24.4086	0.01
318.15	-10.9159	-3.6803	23.1216	-4.0557	-28.8146	-12.6514	0.17

Table 5. Continued

2-methyl-2-propanol + di-sodium hydrogen citrate							
298.15	1.6262	3.0868	-15.4109[c]	3.2034[c]	-100.2473	-17.2920	0.08
308.15	6.2441	-5.2296	-1.0641	-10.0624	-0.1957	-5.8944	1.70
318.15	-1.2245	6.2918	-15.7137	-12.2558	-12.9533	-90.2571	0.04
1-propanol+cesium carbonate							
298.15	3.0393[a]	-2.4819[a]	7.7341	-7.0609	-4.9465	15.0584	0.01
308.15	-.6940	-2.7203	20.8905	512.5473	21.5662	-16.2467	0.02
318.15	11.1219	-1.0359	19.8452	5.3109	12.9677	-7.8277	0.02
1-propanol+di-ammonium hydrogen citrate							
298.15	3.0393[a]	-2.4819[a]	-0.2167	-10.1469	49.9128	-44.5333	0.09
2propanol+ di-ammonium hydrogen citrate							
298.15	2.9480[b]	-2.4490[b]	-4.2031	-9.9395	3.8650	-0.3559	0.04
2-butanol+ di-ammonium hydrogen citrate							
298.15	5.0296	-5.2432	-5.4341	-0.3631	61.9187	21.1706	0.32
2-methyl-2-propanol + di-ammonium hydrogen citrate							
298.15	2.9507	3.2287	-7.0285	14.5001	-148.0372	-40.4418	0.09
1-propanol+di-sodium tartarate							
298.15	3.0393[a]	-2.4819[a]	19.1653	-12.7592	96.0335	-47.2885	0.07
2-propanol+di-sodium tartarate							
298.15	2.9480[b]	-2.4490[b]	12.3158	195.3942	30.1283	-16.2523	0.05
2-butanol+ di-sodium tartarate							
298.15	3.0326	-3.3243	21.0655	18.6357	71.5449	-27.5386	0.01
2-methyl-2-propanol+ di-sodium tartarate							
298.15	3.0097	-2.1556	19.2503	521.1429	33.9975	-17.8757	0.05
2-propanol+litium sulfate							
298.15	2.9480[b]	-2.4490[b]	-13.4628[d]	0.8505[d]	-62.9803	-10.3053	0.07
308.15	1.7347	8.4437	-13.4628[d]	0.8505[d]	-149.8390	249.5884	0.05
318.15	-2.9131	25.8636	-13.4628[d]	0.8505[d]	19.1707	45.4402	0.05
1-propanol+mangenes sulfate							
298.15	3.0393[a]	-2.4819[a]	-13.277[e]	0.6773[e]	-0.0042	-0.0015	0.62
2-propanol+mangenes sulfate							
298.15	2.9480[b]	-2.4490[b]	-13.277[e]	0.6773[e]	32.6833	-27.7792	0.05
2-propanol+potassium carbonate							
298.15	2.9480[b]	-2.4490[b]	-15.4109	3.2034	0.0265	50.6651	0.10
2-propanol+sodium carbonate							
298.15	2.9480[b]	-2.4490[b]	20.0274	-9.1011	8.7404	6.6688	0.03
1-propanol+sodium succinate							
298.15	3.0393[a]	-2.4819[a]	15.4703	-12.0357	50.5903	-40.0929	0.05
2-propanol+sodium succinate							
298.15	2.9480[b]	-2.4490[b]	-30.0994	-9.6290	-43.2093	-61.1759	0.10
2-methyl-2propanol+sodium succinate							
298.15	3.5782	-2.2820	16.5178	38.9004	46.0148	-22.6207	0.02
2-butanol+sodium succinate							
298.15	6.9941	-2.4833	21.0299	38.6603	60.4402	-34.1142	0.01

Table 5. Continued

1-propanol+di-sodium tartarate							
298.15	3.0393^a	-2.4819^a	-24.1061	54.1616	-2.4780	51.1370	0.60
2-propanol+di-sodium tartarate							
298.15	2.9480^b	-2.4490^b	38.259	194.174	-7.737	-7.493	0.18
2-butanol+ di-sodium tartarate							
298.15	6.7720	-2.7407	23.6674	-11.0086	84.8668	-57.9431	0.01
2-methyl-2propanol+ di-sodium tartarate							
298.15	3.8570	157.3108	-69.5410	5.9225	-55.5523	-65.9456	0.92
1-propanol+pottasiom citrate							
298.15	3.0393^a	-2.4819^a	23.6341	-12.8952	105.1941	-66.2053	0.04
2-propanol+pottasiom citrate							
298.15	2.9480^b	-2.4490^b	17.7162	-11.6521	30.8614	-27.8888	0.07
2-butanol+potasiom citrate							
298.15	8.8771	-4.2985	19.9299	17.6907	88.6507	-25.9134	0.01
2-methyl-2-propanol+potasiom citrate							
298.15	1.9997	3.1278	-86.6017	26.9642	-836.8740	-69.0613	0.05
1-propanol+sodium citrate							
298.15	3.0393^a	-2.4819^a	-41.9391^f	-0.7146^f	-47.6806	145.0777	0.05
2-propanol+sodium citrate							
298.15	2.9480^b	-2.4490^b	-41.9391^f	-0.7146^f	-322.2859	-64.8260	0.25
2-butanol +sodium citrate							
298.15	8.4894	-3.5505	-41.9391^f	-0.7146^f	-126.5147	-30.4129	0.01
2-methyl-2-propanol+sodium citrate							
298.15	3.5548	5.7333	-41.9391^f	-0.7146^f	-326.6711	-68.1348	0.11
1-propanol+thio sulfate							
298.15	3.0393^a	-2.4819^a	1.5603^g	-2.7902^g	104.2761	-51.8643	0.04
2-propanol+thio sulfate							
298.15	2.9480^b	-2.4490^b	1.5603^g	-2.7902^g	46.5852	-43.8118	0.30
2-butanol+thio sulfate							
298.15	11.9547	-3.8692	1.5603^g	-2.7902^g	50.9825	-66.7884	0.22
2-methyl-2-propanol+thio sulfate							
298.15	0.0566	0.0921	1.5603^g	-2.7902^g	17.8202	-2.6339	0.03

[a]These parameters are obtained from the correlation of the binary vapor-liquid equilibrium data for (1-propanol + water) system reported in Ref. [22]. [b]These parameters are obtained from the correlation of the binary vapor-liquid equilibrium data for (2-propanol + water) system reported in Ref. [23]. [c,d,e,f,g]These parameters are obtained from the correlation of the binary activity coefficient data for binary ($Na_2C_6H_6O_7$ + water) [24], (Li_2SO_4 or $MnSO_4$ + water) [25], ($Na_3C_6H_5O_7$ + water) [21], and (Na_2SO_4 + water) [26] systems.

Table 6. The Value of Deviation the m-NRTL, e-NRTL [5], e-Wilson [6] and Setschenow-Type Equation [8] for some {Alcohol (m) + Electrolyte (ca) + Water (w)} Systems at Working Temperature

Systems	T/K	Dev				Ref.
		m-NRTL	e-NRTL	Wilson	Setschenow-type equation	
Alcohols(1)+Di-sodium hydrogen citrate(2)+water(3)						[27]
1-propanol	298.15	0.13	0.03	0.27	0.07	
1-propanol	308.15	0.14	0.04	0.04	0.06	
1-propanol	318.15	0.03	1.96	0.08	0.08	
2-propanol	298.15	0.05	0.47	0.84	0.05	
2-propanol	308.15	0.08	0.98	0.02	0.02	
2-propanol	318.15	0.09	0.23	0.46	0.02	
1-butanol	298.15	0.01	0.01	5.48	0.06	
1-butanol	308.15	0.02	0.08	0.12	0.02	
1-butanol	318.15	0.01	0.01	0.01	0.02	
2-butanol	298.15	0.01	0.03	1.51	0.08	
2-butanol	308.15	0.01	0.87	0.06	0.03	
2-butanol	318.15	0.17	0.08	0.01	0.10	
2-mrthyl-2-propanol	298.15	0.08	0.04	0.19	0.08	
2-mrthyl-2-propanol	308.15	0.70	0.35	2.18	0.18	
2-mrthyl-2-propanol	318.15	0.04	0.19	0.59	0.20	
Alcohols (1) + Di-ammonium hydrogen citrate (2) + water (3)						[28]
1-propanol	298.15	0.09	1.69	0.35	0.25	
2-propanol	298.15	0.04	0.91	0.12	0.07	
2-butanol	298.15	0.32	1.30	0.25	0.05	
2-mrthyl-2-propanol	298.15	0.09	0.60	0.08	0.07	
Alcohols (1) + cesium carbonate (2) + water (3)						[29]
1-propanol	298.15	0.01	0.38	0.46	0.04	
1-propanol	308.15	0.02	0.45	0.11	0.02	
1-propanol	318.15	0.02	0.52	0.12	0.06	
2-propanol	298.15	0.05	0.18	0.03	0.04	
Alcohols (1) + Di-sodium tartarate (2) + water (3)						[6]
1-propanol	298.15	0.60	1.22	0.09	0.24	
2-propanol	298.15	0.18	0.26	0.48	0.05	
2-butanol	298.15	0.01	0.18	0.09	0.13	
2-mrthyl-2-propanol	298.15	0.02	0.13	0.08	0.02	
Alcohols (1) + lithium sulfate (2) + water (3)						[5]
2-propanol	298.15	0.07	0.22	0.42	0.13	
2-propanol	308.15	0.05	1.41	0.60	0.19	
2-propanol	318.15	0.05	1.52	0.10	0.66	
Alcohols (1) + manganese sulfate (2) + water (3)						[5]
1-propanol	298.15	0.62	0.59	0.08	0.19	
2-propanol	298.15	0.05	2.65	0.16	0.35	
Alcohols (1) + potassium carbonate (2) + water (3)						[30]
2-propanol	298.15	0.10	1.25	0.03	0.05	
Alcohols (1) + sodium carbonate (2) + water (3)						[30]
2-propanol	298.15	0.03	0.30	0.18	0.01	

Table 6. Continued

Alcohols (1) + potassium citrate (2) + water (3)					[31]
1-propanol	298.15	0.04	0.68	0.03	0.10
2-propanol	298.15	0.07	0.77	0.03	0.06
2-butanol	298.15	0.01	0.07	0.02	0.03
2-mrthyl-2-propanol	298.15	0.05	1.62	0.05	0.07
Alcohols (1) + sodium citrate (2) + water (3)					[31]
1-propanol	298.15	0.05	0.66	0.14	0.10
2-propanol	298.15	0.25	1.99	0.20	0.06
2-butanol	298.15	0.01	0.68	0.03	0.03
2-mrthyl-2-propanol	298.15	0.05	0.15	0.11	0.07
Alcohols (1) + sodium tiosulfate (2) + water (3)					[32]
1-propanol	298.15	0.04	1.96	0.03	0.14
2-propanol	298.15	0.30	0.40	1.10	0.01
2-butanol	298.15	0.22	0.06	0.02	0.01
2-mrthyl-2-propanol	298.15	0.03	1.16	0.04	0.04
Alcohols (1) + di-sodium tartarate (2) + water (3)					[33]
1-propnol	298.15	0.07	0.30	0.08	0.04
2-propanol	298.15	0.05	0.70	0.45	1.06
2-butanol	298.15	0.01	0.27	0.02	0.05
2-mrthyl-2-propanol	298.15	0.05	0.77	0.10	0.08
Alcohols (1) + sodium succinate(2) + water (3)					[33]
1-propanol	298.15	0.05	0.16	0.02	0.07
2-propanol	298.15	0.10	0.02	0.09	0.09
2-butanol	298.15	0.02	0.08	0.23	0.14
2-mrthyl-2-propanol	298.15	0.01	0.02	0.02	0.01
Overall deviation		0.10	0.62	0.34	0.12

indicates a better quality of fitting LLE data with the proposed m-NRTL model than the other models considered in this work for variety of aqueous alcohol $_+$ salt systems at different temperatures. Overall deviation is 0.10 which is less than deviations calculated for other models. To show the performance of m-NRTL model in a better manner, as

examples, the experimental and correlated tie-line data with m-NRTL and e-NRTL are illustrated in Figs. 1-5 for (1-butanol + di-sodium hydrogen citrate + water), (2-butanol + potassium citrate(s) + water), (2-methyl-2-propanol + di-sodium succinate + water), (1-propanol cesium carbonate + water) and (2-propanol + manganese sulfate + water)
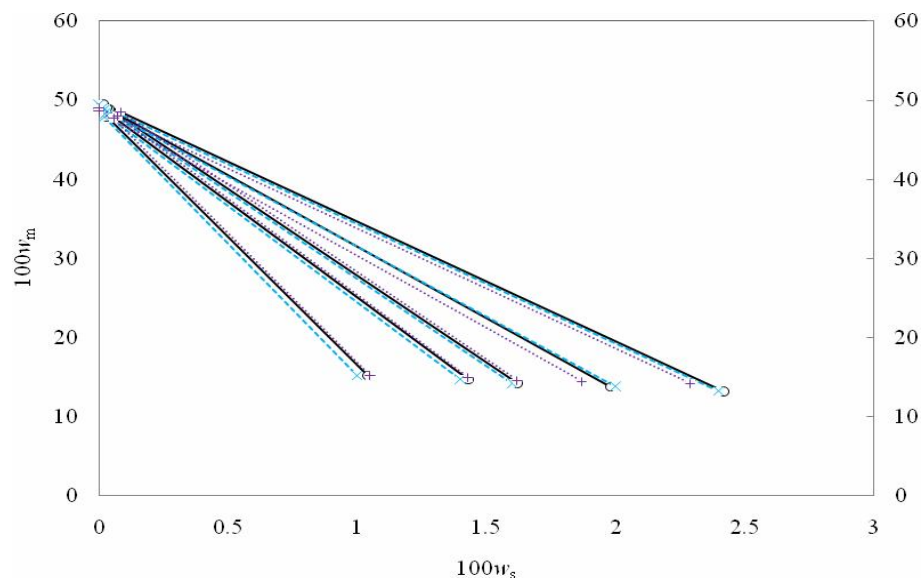
Fig. 1. Plot of mass percent alcohol against mass percent salt to compare the calculated tie-lines of the {1-butanol (m) + di-sodium hydrogen citrate (s) + water (w)} system with m-NRTL and e-NRTL: (─○─) experimental, (--×--) calculated tie-lines from m-NRTL, (··+··) calculated tie-lines from e-NRTL at T = 298.15 K.
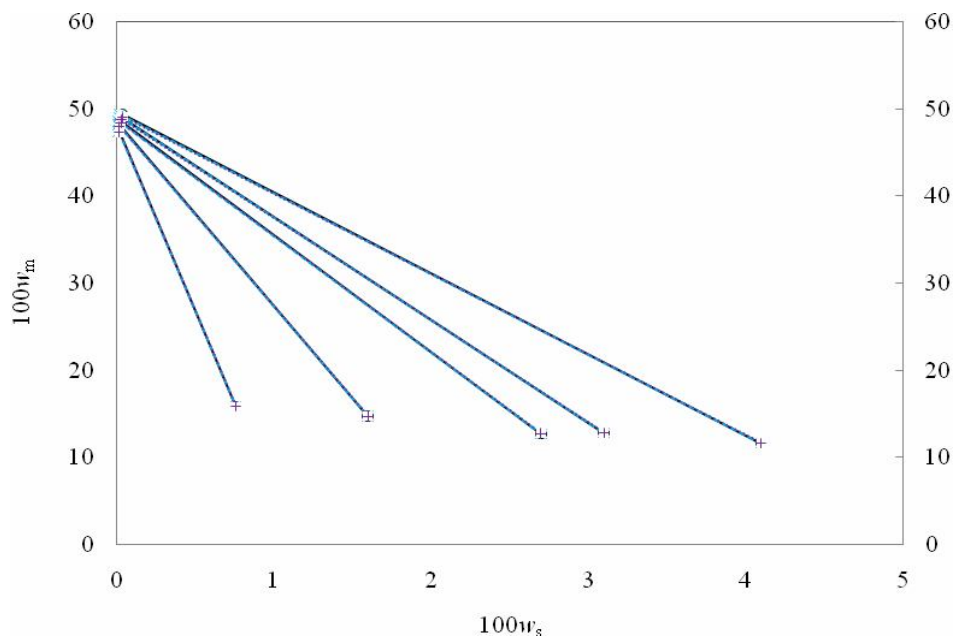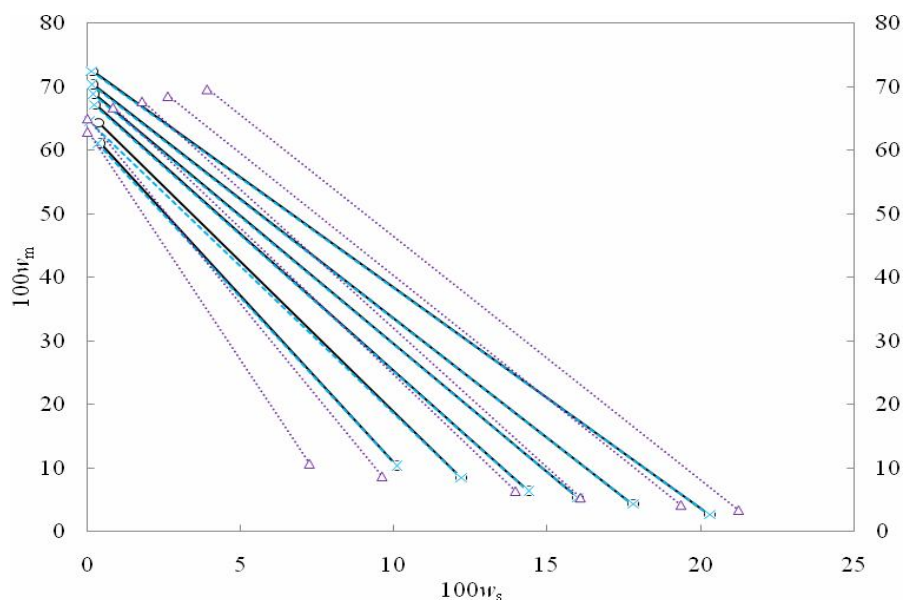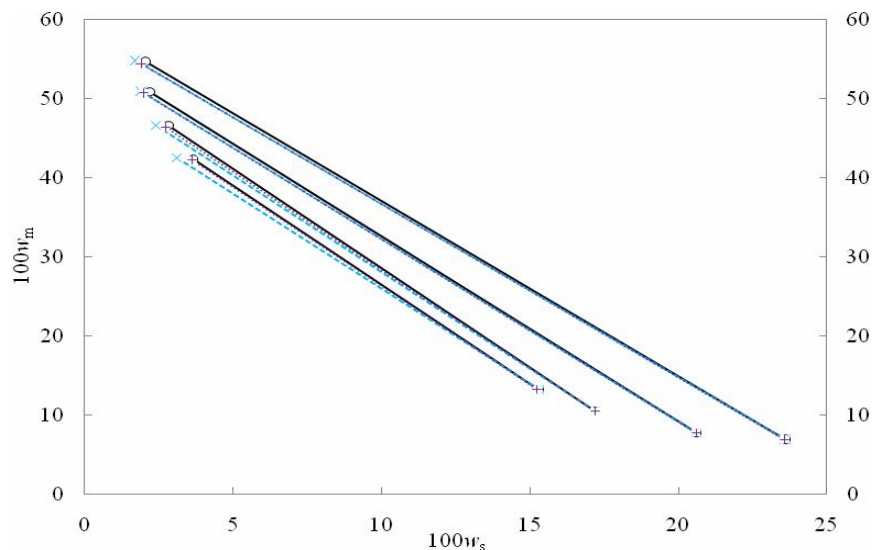

Fig. 2. Plot of mass percent alcohol against mass percent salt to compare the calculated tie-lines of the {2-butanol (m) + potassium citrate (s) + water (w)} system with m-NRTL and e-NRTL: (─○─) experimental, (--×--) calculated tie-lines from m-NRTL, (··+··) calculated tie-lines from e-NRTL at T = 298.15 K.

Fig. 3. Plot of mass percent alcohol against mass percent salt to compare the calculated tie-lines of the {2-metyl-2-propanol (m) + thio sulfate (s) + water (w)} system with m-NRTL and e-NRTL: (─○─) experimental, (--×--) calculated tie-lines from m-NRTL, (··+··) calculated tie-lines from e-NRTL at T = 298.15 K.

Fig. 4. Plot of mass percent alcohol against mass percent salt to compare the calculated tie-lines of the {1-propanol (m) + di-sodium hydrogen citrate (s) + water (w)} system with m-NRTL and e-NRTL: (─○─) experimental, (--×--) calculated tie-lines from m-NRTL, (··+··) calculated tie-lines from e-NRTL at T = 298.15 K.
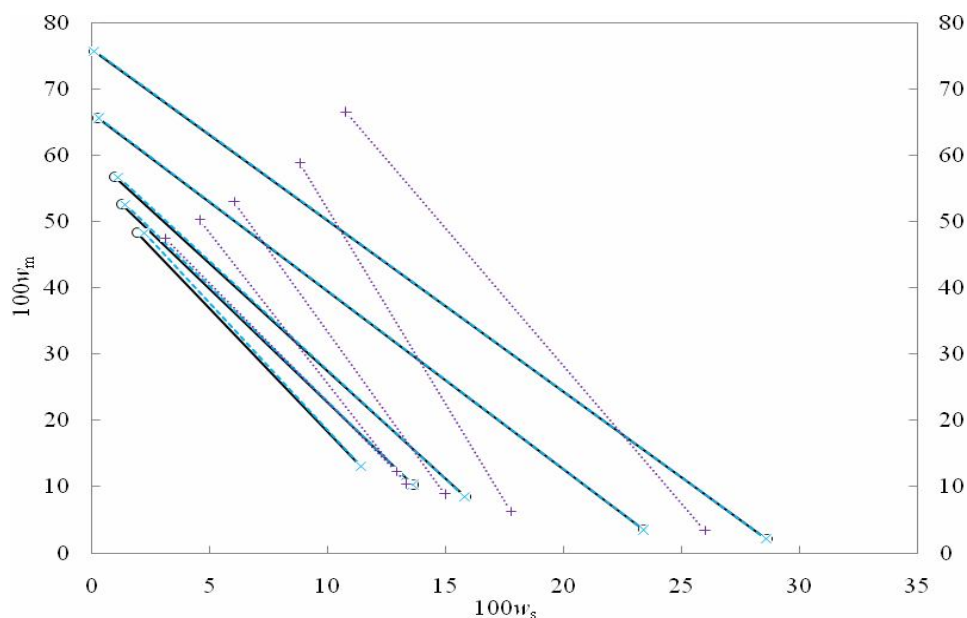
Fig. 5. Plot of mass percent alcohol against mass percent salt to compare the calculated tie-lines of the {2-propanol (m) + manganese sulfate (s) + water (w)} system with m-NRTL and e-NRTL: (━○━) experimental, (--✕--) calculated tie-lines from m-NRTL, (··+··) calculated tie-lines from e-NRTL at T = 298.15 K.

systems, respectively.

REFERENCE

[1]   P.A. Albertsson, Partitioning of Cell Particles and Macromolecules, 3rd rd., Wiley, New York, 1986.

[2]   H. Walter, D.E. Brooks, D. Fisher, Partitioning in Aqueous Two-Phase Systems. Academic Press, New York, 1985.

[3]   B.Y. Zaslavsky, Physical Chemistry and Bio Analytical Application. Marcel Dekker, New York, 1995.

[4]   G.H. Van Bochove, G.J.P. Krooshof, W. Theo, de Loos, Fluid Phase Equilib 171 (2000) 45.

[5]   M.T. Zafarani-Moattar, E. Nemati-Kande, A. Soleimani, Fluid Phase Equilib 313 (2012) 107.

[6]   E. Nemati-Kande, H. Shekaari, S.A. Jafari, J. Chem. Eng. Data 57 (2012) 2336.

[7]   R. Sadeghi, Chem. Eng. Sci. 61 (2006) 7786.

[8]   M.J. Hey, D.P. Jackson, Hong Yan, Polymer. 46 (2005) 2567.

[9]   Zafarani-Moattar, M.T. Sadeghi, R. Fluid Phase Equilibr. 181 (2002) 177.

[10] K.S. Pitzer, J. Am. Chem. Soc. 102 (1980) 2902.

[11] C.C. Chen, Y. Song, AIChE J. 50 (2004) 1928.

[12] C.C. Chen, H.I. Britt, J.F. Boston, L.B. Evans, AIChE J. 28 (1982) 588.

[13] C.C. Chen, L.B. Evans, AIChE J. 32 (1986) 444.

[14] C.C. Chen, Y. Song, AIChE J. 50 (2004) 1928.

[15] J.M. Simonson, K.S. Pitzer, J. Phys. Chem. 90 (1986) 3009.

[16] F.M. Pang, C.E. Seng, T.T. Teng, M.H. Ibrahim, J. Mol. Liq. 136 (2007) 71.

[17] J.M. Resa, C. Gonzalez, M. Juez, S.O. de Landaluce, Fluid Phase Equilib. 217 (2004) 175.

[18] K. Rajagopal, S. Chenthilnath, Indian J. Pure. Appl. Phys. 48 (2010) 326.

[19] E. Nemati-Kande, H. Shekaari, S.A. Jafari, Fluid Phase Equilib. 329 (2012) 42.

[20] D.R. Lide, CRC Handbook of Chemistry and

Physics, 87th ed., Taylor and Francis, Boca Raton, FL, 2007.

[21] R.A. Robinson, R.H. Stokes, Electrolyte Solutions, 2nd ed., Butterworths, London, 1965.

[22] J. Gmehling, U. Onken, Chemistry Data Series, Vol. 1, DECHEMA, Frankfurt, Germany, 1977.

[23] T. Tsuji, K. Hasegawa, T. Hiaki, M. Hongo, J. Chem. Eng. Data 41 (1996) 956.

[24] R. Sadeghi, R.Golabiazar, E. Parsi, J. Chem. Eng. Data 55 (2010) 5874.

[25] R.N. Goldberg, J. Phys. Chem. Ref. Data 10 (1981) 671.

[26] A. Schunk, G. Maurer, J. Chem. Eng. Data 49 (2004) 944.

[27] M.T. Zafarani-Moattar, P. Jafari, Fluid Phase Equilib.

353 (2013) 50.

[28] M.T. Zafarani-Moattar, J. Gasemi. J. Chem. Eng. Data 47 (2002) 525.

[29] M. Hu, L. Jin, Q. Zhai, S. Li, Z. Liu, Fluid Phase Equilib 232 (2005) 57.

[30] Y. Wang, S. Hu, Y. Yan, W. Guan. CALPHAD 33 2009 726.

[31] E. Nemati-Kande, H. Shekaaei. J. Solution Chem. 41 (2012) 1649.

[32] E. Nemati-kande, H. Shekaari, S.A. Jafari, Fluid Phase Equilib. 321 (2012) 64.

[33] M.T. Zafarani-Moattar, V. Hosseinpour-Hashemi, S. Banisaeid, M.A. Shamsi Beirami, Fluid Phase Equilib. 338 (2013) 37.