Measurement and Correlation of Isothermal Vapor−Liquid Equilibrium Data for the System Ethanol + 2-Propanol + Barium Iodide

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Isothermal vapor−liquid equilibrium data for the system ethanol + 2-propanol + barium iodide at three constant salt molalities (0.5, 1.0 and 1.5 mol·kg^{-1}) have been measured with the help of headspace gas chromatography at 40.3, 55.3, and 70.6 °C. The experimental data were correlated using four electrolyte models: an electrolyte NRTL model, an extended UNIQUAC model, an electrolyte UNIFAC model, and the LIQUAC model.

Introduction

The synthesis and design of industrial separation processes such as extractive distillation using salt as an extractant,[1] extractive and antisolvent crystallization of salts,[2] and simulation of unit operations for salt-containing systems require an accurate description of the phase equilibrium behavior of electrolyte systems. The quality of the description of the phase equilibrium behavior for electrolyte systems strongly depends on the thermodynamic model [g^E model, equation of state (EOS), EOS + g^E mixing rules] and the quality of the parameters used. This has been the incentive for the development of a database and thermodynamic models suitable for the correlation and prediction of phase equilibria of electrolyte systems.

The addition of salt solvent mixtures may affect the boiling point, the mutual solubility of the two liquid components, and the relative volatility of solvents. Many experimental data [about 2500 vapor−liquid equilibrium (VLE) and 3000 salt solubility data sets] concerning the salt effect on the phase equilibrium behavior have been stored in the Dortmund Data Bank (DDB). Whereas many data exist for water and low alcohols, much less data are available for salts in other organic solvents or their mixtures because of the low salt solubility, which results in a negligible salt effect. Furthermore, most of the data are reported for isobaric, rather than isothermal, conditions. For systems with salts and two solvents, the temperature for isobaric data may change drastically, and thus data correlation is complicated unless it is assumed that the model parameters are independent of temperature or unless an explicit temperature dependence is incorporated into the model. No such difficulty exists for isothermal data. It is an excellent assumption to neglect the pressure dependence of the activity coefficients at low or moderate pressure.

The aim of this work is to determine systematically the effect of barium iodide on the vapor−liquid equilibrium of the ethanol + 2-propanol system at three temperatures (40.3, 55.3, and 70.6 °C) and different constant salt concentrations (0.5, 1.0, and 1.5 mol·kg^{-1}) with the help of headspace gas chromatography. Presently no VLE data are available for these systems. The experimental data presented in this work were correlated using four different models based on the local composition concept or group contribution concept. Several new interaction parameters for each model were obtained and are presented in this work.

Experimental Section

Materials. Ethanol (99.9 wt %) and 2-propanol (99.5 wt %) were dehydrated with the help of 3 Å molecular sieves. The water content for ethanol and 2-propanol was determined using a 684 KF coulometer (Ω Metrohm). The water contents were 0.01 wt % for ethanol and 0.02 wt % for 2-propanol. The purity was checked by gas chromatography. The purities were >99.9 wt % for ethanol and >99.6 wt % for 2-propanol. Barium iodide (99.0 wt %, Fluka) was recrystallized using an ethanol + 2-propanol mixed solvent and dried at 65 °C in a vacuum oven until a constant mass was reached.

Apparatus. Liquid mixtures consisting of ethanol, 2-propanol, and barium iodide were prepared gravimetrically by using a Sartorius analytical balance with an accuracy of ±0.1 mg. For each experimental point, ~8 cm^3 of sample solution was charged into the 22 cm^3 sample vial. After the sample vials were tightly closed by means of a special aluminum lid, with a washer and a Teflon disk, they were brought to the desired temperature in the thermostatic bath controlled within ±0.1 °C. The measurements were started after the samples were held at a constant temperature for at least 12 h, to ensure phase equilibrium.

For the determination of the vapor-phase composition, a vapor sample was automatically withdrawn using a Perkin-Elmer F45 GLC vapor analyzer and analyzed by an F22 gas chromatograph with the help of a thermal conductivity detector and an integrator (Hewlett-Packard 3390A). For separation, a 1.2 m stainless steel column filled with Porapak Q 80/100 was used. The optimum operating conditions were as follows: injection temperature, 190 °C; oven temperature, 170 °C; detector temperature, 190 °C; carrier gas, helium (purity = 99.9%) with a flow rate of 0.40 cm^3·s^{-1}. Because of negligible amounts in the vapor phase (small vapor volume, moderate pressure), it was reasonable to assume that the liquid phase composition is the same as the feed composition. A detailed description of the experimental setup has already been given by Weidlich and Gmehling.[3]

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Table 1. Vapor−Liquid Equilibrium Data for the System Ethanol (1) + 2-Propanol (2) + Barium Iodide (3)

x_1' [a]	y_1	γ_1 [b]	γ_2 [b]
$m = 0.500$ mol·kg^{-1}; $T = 40.3$ °C			
0.3000	0.3075	0.8606	1.0597
0.3000	0.3080	0.8606	1.0597
0.4208	0.4308	0.8823	1.0725
0.4958	0.5096	0.8970	1.0778
0.5688	0.5836	0.9117	1.0807
0.6034	0.6167	0.9187	1.0812
0.6506	0.6671	0.9281	1.0811
0.7006	0.7207	0.9380	1.0798
0.7566	0.7756	0.9488	1.0770
0.7991	0.8150	0.9568	1.0738
0.9001	0.9099	0.9745	1.0626
0.9499	0.9584	0.9825	1.0552
$m = 1.000$ mol·kg^{-1}; $T = 40.3$ °C			
0.4208	0.4002	0.8009	1.1248
0.4958	0.4786	0.8227	1.1404
0.5688	0.5389	0.8444	1.1537
0.6034	0.5786	0.8547	1.1593
0.6506	0.6302	0.8688	1.1662
0.7006	0.6818	0.8837	1.1725
0.7566	0.7424	0.9003	1.1784
0.7991	0.7894	0.9128	1.1820
0.9001	0.8996	0.9420	1.1874
0.9499	0.9499	0.9560	1.1885
$m = 1.500$ mol·kg^{-1}; $T = 40.3$ °C			
0.5688	0.5242	0.7679	1.1969
0.6034	0.5538	0.7807	1.2080
0.6506	0.6068	0.7983	1.2226
0.7006	0.6618	0.8172	1.2374
0.7566	0.7248	0.8385	1.2532
0.7991	0.7695	0.8547	1.2645
0.9001	0.8853	0.8936	1.2895
0.9499	0.9441	0.9129	1.3007
$m = 0.500$ mol·kg^{-1}; $T = 55.3$ °C			
0.3000	0.3025	0.8747	1.0624
0.4208	0.4280	0.8928	1.0769
0.4958	0.5060	0.9055	1.0837
0.5688	0.5803	0.9184	1.0883
0.6034	0.6123	0.9246	1.0898
0.6506	0.6630	0.9332	1.0911
0.7006	0.7152	0.9422	1.0913
0.7566	0.7709	0.9522	1.0903
0.7991	0.8129	0.9596	1.0885
0.9001	0.9079	0.9763	1.0809
0.9499	0.9557	0.9840	1.0752
$m = 1.000$ mol·kg^{-1}; $T = 55.3$ °C			
0.4208	0.3967	0.8126	1.1293
0.4958	0.4760	0.8325	1.1465
0.5688	0.5360	0.8524	1.1616
0.6034	0.5753	0.8620	1.1683
0.6506	0.6279	0.8752	1.1766
0.7006	0.6783	0.8892	1.1847
0.7566	0.7405	0.9050	1.1926
0.7991	0.7878	0.9169	1.1978
0.9001	0.8971	0.9450	1.2074
0.9499	0.9481	0.9587	1.2106
$m = 1.500$ mol·kg^{-1}; $T = 55.3$ °C			
0.6506	0.6048	0.8055	1.2334
0.7006	0.6573	0.8235	1.2501
0.7566	0.7216	0.8439	1.2681
0.7991	0.7666	0.8596	1.2813
0.9001	0.8842	0.8975	1.3111
0.9499	0.9425	0.9164	1.3248
$m = 0.500$ mol·kg^{-1}; $T = 70.6$ °C			
0.3000	0.3007	0.8876	1.0654
0.4208	0.4282	0.9025	1.0813
0.4958	0.5045	0.9134	1.0893
0.5688	0.5807	0.9248	1.0955
0.6034	0.6147	0.9304	1.0977
0.6506	0.6638	0.9381	1.1002
0.7006	0.7127	0.9464	1.1018
0.7566	0.7686	0.9556	1.1023
0.7991	0.8116	0.9624	1.1019
0.9001	0.9080	0.9783	1.0973
0.9499	0.9542	0.9857	1.0932
$m = 1.000$ mol·kg^{-1}; $T = 70.6$ °C			
0.4208	0.3934	0.8238	1.1342
0.4958	0.4734	0.8420	1.1526
0.5688	0.5315	0.8603	1.1693
0.6034	0.5716	0.8693	1.1768
0.6506	0.6242	0.8816	1.1864
0.7006	0.6753	0.8948	1.1959
0.7566	0.7377	0.9098	1.2056
0.7991	0.7858	0.9212	1.2123
0.9001	0.8951	0.9484	1.2255
0.9499	0.9464	0.9617	1.2307
$m = 1.500$ mol·kg^{-1}; $T = 70.6$ °C			
0.6506	0.6028	0.8128	1.2439
0.7006	0.6573	0.8300	1.2621
0.7566	0.7183	0.8497	1.2821
0.7991	0.7644	0.8649	1.2969
0.9001	0.8826	0.9018	1.3309
0.9499	0.9407	0.9204	1.3469

[a] Liquid phase mole fraction on a salt-free basis. [b] Activity coefficients calculated by the LIQUAC model with the parameters listed in Table 4.

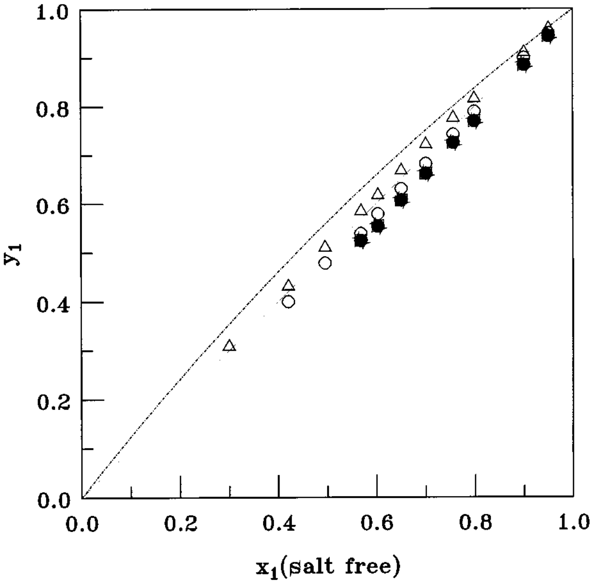

Figure 1. $x-y$ VLE diagram for the system ethanol (1) + 2-propanol (2) + BaI_2 at 40.3 °C: △, $m = 0.5$; ○, $m = 1.0$; ●, $m = 1.5$ mol kg^{-1}; − • − ($m = 0.0$ mol kg^{-1}), calculated by the UNIQUAC model (parameters taken from Gmehling et al.[5]).

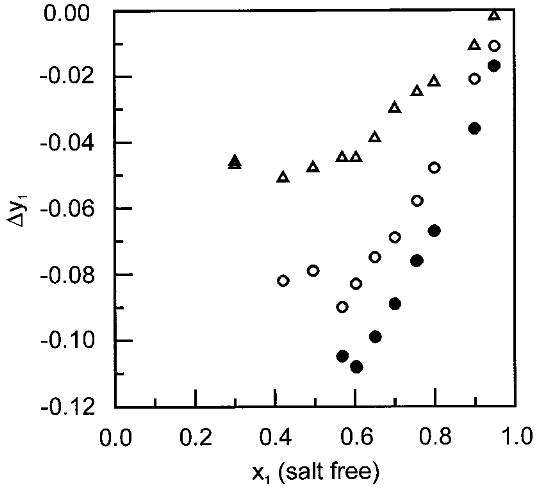

Figure 2. Δy values for the system ethanol (1) + 2-propanol (2) + BaI_2 at 40.3 °C; △, $m = 0.5$; ○, $m = 1.0$; ●, $m = 1.5$ mol kg^{-1}; deviation calculated using the UNIQUAC model (parameters taken from Gmehling et al.[5]).

Calibration was necessary before the peak areas could be used to determine the vapor phase composition. To obtain the calibration curve, various ethanol + 2-propanol mixtures were prepared and injected. With the help of a calibration curve, the required mole fractions and area fractions were correlated using a fifth-order polynomial (mean deviation = 0.07%). The vapor phase composition was determined with this calibration curve. The average uncertainty in the measurement of the mole fraction is ±0.0016, which has been obtained by comparing the known composition of the made-up liquid samples with the composition calculated from the calibration curve.

Results

Experimental Data. Isothermal vapor−liquid equilibrium data for the system ethanol (1) + 2-propanol (2) + barium iodide (3) have been measured at three different temperatures (40.3, 55.3, and 70.6 °C) and various salt concentrations ($m = 0.5$, 1.0, and 1.5 mol·kg^{-1}). The experimental results are given in Table 1. As a typical example, experimental data at 40.3 °C are shown in Figures 1 and 2. Whereas in Figure 1 the $y-x$ diagram is shown, in Figure 2 the deviations in vapor phase mole fraction of the ternary and binary systems on a salt-free basis are given. It is obvious that a considerable increase of the 2-propanol mole fraction in the vapor phase is observed by the addition of barium iodide when compared with the salt-free system calculated using the UNIQUAC model.

Calculation of VLE for Salt-Containing Systems. To describe the observed VLE behavior, the experimental data are correlated using the following four models.

1. Electrolyte NRTL Model of Mock et al.[4] The electrolyte NRTL model used to correlate the VLE data is an extension of the Chen model for single-solvent electrolyte systems to mixed-solvent electrolyte systems, neglecting the long-range interaction contribution term.[4] The two fundamental assumptions about the local composition of an electrolyte solution are (1) the repulsion of ions of the

Table 2. Energy Parameters (Δg_{ij} and Δg_{ji}, $J \cdot mol^{-1}$) and Nonrandomness Factors (α_{ij}) for the Electrolyte NRTL Model

I	*j*	α_{ij}	Δg_{ij}	Δg_{ji}
ethanol	2-propanol	0.3789	411.812	−419.995
ethanol	BaI_2	0.2	−651.098 (f)[a]	−132.425 (f)
2-propanol	BaI_2	0.211 (f)	346.077 (f)	99.546 (f)

[a] (f) means that these interaction parameters have been fitted in this work.

same sign, which results in the fact that the local composition of cations (anions) around a central cation (anion) is zero, and (2) local electroneutrality, which means that the sum of the charges of cations and anions around a central molecule is zero.

The model parameters are specific for the solvent−solvent and solvent−salt pairs. For a system with two solvents, m_1 and m_2, and one salt, six energy parameters ($\Delta g_{m1,m2}$, $\Delta g_{m1,m2}$, $\Delta g_{m1,ca}$, $\Delta g_{ca,m1}$, $\Delta g_{m2,ca}$, and $\Delta g_{ca,m2}$) and three nonrandomness factors ($\alpha_{m1,m2}$, $\alpha_{ca,m1}$, and $\alpha_{ca,m2}$) are required. The binary parameter τ_{ij} is expressed by

$$\tau_{ij} = \Delta g_{ij}/RT \tag{1a}$$

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij}) \tag{1b}$$

To minimize the number of parameters, the binary solvent−solvent parameters ($\Delta g_{m1,m2}$, $\Delta g_{m1,m2}$, and $\alpha_{m1,m2}$) were directly taken from the literature.[5] Moreover, as pointed out by Mock et al.,[4] the nonrandomness factor for the salted-in solvent and salt was set arbitrarily to 0.2. The remaining parameters for the binary pairs ethanol + barium iodide and 2-propanol + barium iodide were fitted by minimization of the following objective function *F* using the Simplex−Nelder−Mead method[6]

$$F(\Delta g_{i,j},\Delta g_{j,i},\alpha_{i,j}) = \sum_{\text{nt}}\sum_{\text{np}}(y_{i,1(\text{exptl})} - y_{i,1(\text{calcd})})^2 = \min \tag{2}$$

where *y* represents the vapor phase mole fraction. nt and np are the number of data sets and the number of data points for each data set, respectively. The subscripts exptl and calcd denote experimental data and calculated values, respectively. The vapor phase compositions can be calculated by solving iteratively the equilibrium condition

$$y_i P = x_i \gamma_i P_i^{\,s} \Phi_i \tag{3}$$

where

$$P = x_1\gamma_1 P_1^{\,s}\Phi_1 + x_2\gamma_2 P_2^{\,s}\Phi_2 \tag{4}$$

$$\Phi_i = \varphi_i^{\,s}\text{Poy}_i/\varphi_i^{\,v} \tag{5}$$

and x_i is the liquid phase mole fraction of solvent *i* based on the assumption of total dissociation of the salt. The saturation vapor pressure of the pure solvent *i*, P_i^s, at system temperature was calculated with the Antoine equation using Antoine constants from the literature.[5] In eq 5, φ_i^v is the fugacity coefficient of solvent *i* in the vapor phase, φ_i^s is the fugacity coefficient of pure solvent *i* at saturation pressure and Poy_i is the Poynting term. φ_i^s is approximately equal to φ_i^v, and Poy_i is approximately equal to one at atmospheric pressure, so Φ_i is equal to one, respectively. The activity coefficient of solvent *i* was calculated as described by Mock et al.[4] The NRTL energy parameters and the nonrandomness factors are given in Table 2.

Table 3. UNIQUAC Reference Interaction Parameters a_{ij}* (K), Concentration-Dependent Parameters $\delta_{ij,m}$, Volume Parameters r_i, and Surface Area Parameters q_i for the Extended UNIQUAC Model of Macedo[7]

	ethanol	2-propanol	Ba^{2+}	I^-
		a_{ij}*		
ethanol	0.0	−176.5	641.1	−244.2
2-propanol	241.9	0.0	730.73 (f)[a]	−51.09 (f)
Ba^{2+}	168.81	−390.56 (f)	0.0	−132.06 (f)
I^-	−574.2	103.75 (f)	494.43 (f)	0.0
		r_i and q_i		
r_i	2.1005	2.7791	3.0	1.6807
q_i	1.9720	2.5080	3.0	1.4198
		$\delta_{ij,m}$		
$Ba^{2+}-I^-$	377.80 (f)	−299.88 (f)		

[a] (f) means that these interaction parameters have been fitted in this work.

2. Extended UNIQUAC Model of Macedo et al.[7] Sander et al.[8] presented a model for the calculation of salt effects on the vapor−liquid equilibrium. The model combines a Debye−Hückel term with a modified UNIQUAC term. To ensure a rigorous expression of a Debye−Hückel term, Macedo et al.[7] modified the Debye−Hückel term of Sander's model according to the McMillan−Mayer solution theory.[9] The interaction parameters between an ion *i* and a solvent *m* (a_{im} and a_{mi}) are considered to be dependent on concentration in the same way as proposed by Sander et al.[8]

$$a_{im} = a_{im}{}^* + \theta_i \sum_{j \neq i} \delta_{ij,m}\theta_j \tag{6}$$

$$a_{mi} = a_{mi}{}^* + \theta_i \sum_{j \neq i} \delta_{ij,m}\theta_j \tag{7}$$

where $a_{im}{}^*$ and $a_{mi}{}^*$ represent reference interaction parameters, $\delta_{ij,m}$ is a parameter, the summation is over all ionic species except *i*, and θ_i represents the surface area fraction of ion *i*.

For two solvents and one salt system, 14 parameters are needed: 2 solvent−solvent interaction parameters, 2 ion−ion interaction parameters, 8 ion−solvent reference interaction parameters, and 2 salt−solvent interaction parameters. The binary solvent−solvent interaction parameters have been obtained directly from Gmehling et al.[5] For the ethanol + 2-propanol + barium iodide system, a few interaction parameters were available in literature.[7] The remaining model parameters were fitted to the experimental data. All UNIQUAC parameters are given in Table 3.

3. LIQUAC Model of Li et al.[10] The LIQUAC model for the excess Gibbs energy was proposed by Li et al.[10] to describe the behavior for both single- and mixed-solvent electrolyte systems.[11] This model consists of three contributions: (1) a Debye−Hückel term to account for long-range electrostatic interaction, (2) the UNIQUAC equation for the description of short-range interaction between all species, and (3) a middle-range contribution to include all indirect effects of the charge interactions.

For a two-solvent and one-salt system, 12 short-range interaction parameters (a_{ij}) and 10 middle-range interaction parameters (b_{ij} and c_{ij}) are required. However, a large number of parameters have been published already.[10] Therefore, in this work 14 parameters were directly taken from the published parameter matrix. The remaining interaction parameters between 2-propanol−Ba^{2+} and 2-propanol−I^- were fitted to the new experimental data with the help of the Simplex−Nelder−Mead method men-

Table 4. Binary Interaction Parameters, Volume Parameters, and Surface Area Parameters for the LIQUAC Model[10]

i	*j*	a_{ij}	a_{ji}	b_{ij}	c_{ij}	r_i	q_i
ethanol	2-propanol	−176.5	241.9				
ethanol	Ba^{2+}	1082.0	−276.80	−5.0970	1.9210		
ethanol	I^-	314.32	194.5	−3.4340	−1.3400		
2-propanol	Ba^{2+}	448.45 (f)[a]	−28.80 (f)	2.4721(f)	0.4277 (f)		
2-propanol	I^-	449.51 (f)	105.36 (f)	−8.9090 (f)	−0.5816 (f)		
Ba^{2+}	I^-	−660.30	128.00	0.4980	1.7440		
ethanol						2.106	1.972
2-propanol						2.779	2.508
Ba^{2+}						1.000	1.000
I^-						1.000	1.000

[a] (f) means that these interaction parameters have been fitted in this work.

Table 5. UNIFAC Group Interaction Parameters a_{ij}, Subgroup Volume Parameters R_i, and Surface Area Parameters Q_i for the Electrolyte UNIFAC Model[12]

a_{ij}

	CH_2	OH	Ba^{2+}	I^-
CH_2	0.0	986.5	1744.4	−1796.4
OH	156.4	0.0	−296.21	31892.6
Ba^{2+}	982.91	−248.49	0.0	−7562.32 (f)[a]
I^-	9183.5	−864.67	1243.57 (f)	0.0

R_i and Q_i

	CH_2	CH_3	OH	Li^+	I^-
R_i	0.6744	0.9011	1.000	3.0	1.6807
Q_i	0.5400	0.8480	1.200	3.0	1.4118

[a] (f) means that these interaction parameters have been fitted in this work.

Table 6. Mean Absolute Deviations of Vapor Phase Composition for the Different Electrolyte Models

		$\overline{\lvert\Delta y\rvert}$[a]			
T/°C	data points	NRTL[4]	UNIQUAC[7]	LIQUAC[10]	UNIFAC[12]
40.3	30	0.010	0.009	0.004	0.039
55.3	27	0.009	0.007	0.003	0.031
70.6	27	0.008	0.008	0.005	0.027
av deviation		0.009	0.008	0.004	0.032

[a] $\overline{|\Delta y|} = (1/n)\sum_i^n |y_{i,1}(\text{exptl}) - y_{i,1}(\text{calcd})|$, where n represents the number of data points.

tioned above. The used interaction parameters with the volume and surface area parameters are given in Table 4. As suggested by Li et al.,[10] the volume and surface area parameters for the ions were set arbitrarily to 1.0.

4. Electrolyte UNIFAC Group Contribution Model of Kikic et al.[12] The first electrolyte model based on the group contribution method was published by Kikic et al.[12] This model combines a modified Debye−Hückel term according to the McMillan−Mayer solution theory as described by Cardoso and O'Connell[9] with the original UNIFAC group contribution method for short-range physical interactions[13] with concentration-independent group interaction parameters.

For a system with three solvent groups and two ions, there are 20 UNIFAC group interaction parameters. The group interaction parameters between solvent groups are the same as those published by Hansen et al.[14] Some parameters between solvent group and ion or between ions were taken from the literature.[12] In this work only two group interaction parameters had to be fitted. The fitted UNIFAC group interaction parameters a_{ij}, subgroup volume parameters R_i, and surface area parameters Q_i are listed in Table 5.

Discussion

The VLE behavior of the system ethanol−2-propanol−barium iodide have been investigated between 40.3 and 70.6 °C at three different salt concentrations. As expected, it was found that the addition of barium iodide increases the relative volatility of the less polar component 2-propanol. The VLE behavior can be described with the help of electrolyte models. All models except UNIFAC model proposed by Kikic et al.[4] represent the experimental data with the required accuracy, but superior results are obtained for the LIQUAC model.

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