

Measurement and Correlation of Isobaric Vapor–Liquid Equilibrium Data for the System Acetone + Methanol + Zinc Chloride

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Isobaric vapor–liquid equilibrium data for the system acetone (1) + methanol (2) + zinc chloride (3) at constant salt molalities have been measured with the help of a modified Scott ebulliometer at 66.66 and 101.33 kPa. The measured data were correlated using the electrolyte UNIQUAC (Sander et al., 1986) and the LIQUAC (Li et al., 1994) model. A comparison of the correlations with the experimental data shows superior results for the LIQUAC model.

1. Introduction

A reliable knowledge of the phase equilibria of electrolyte systems is essential for the design and simulation of different chemical processes including wastewater treatment, extractive distillation, extractive crystallization of salts, gas scrubbing, etc. The description of the phase equilibrium behavior of 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.

To obtain reliable model parameters for predictive methods, a large database should be applied. The Dortmund data bank (DDB) formed the basis for the development of various thermodynamic models in our research group. It is a steadily growing database, which today contains more than 1860 VLE and 1230 salt solubility data sets for electrolyte systems besides other data. But still, VLE data for a large number of systems are missing in the literature.

The aim of this investigation is the systematic study of the effect of zinc chloride on the vapor–liquid equilibrium of the azeotropic system acetone + methanol. Presently, only data at saturated salt concentrations in the liquid phase are available for this system (Avcia et al., 1993). The measurements were carried out at 66.66 and 101.33 kPa and different constant salt concentrations with a modified Scott ebulliometer.

In addition, the experimental data were correlated using two local composition models: the modified electrolyte UNIQUAC model of Sander et al. (1986) and the LIQUAC model of Li et al. (1994).

2. Experimental Section

2.1. Materials. Acetone (99.5 wt %, Scharlau) and methanol (99.5 wt %, Scharlau) were purified by fractional distillation on a 1.0 m Vigreux column, dried, and stored over 3 Å molecular sieves. The water content was determined using the Karl Fischer method. Acetone had a final

purity of 99.9 wt % and methanol of 99.7 wt % determined by GC using an FID detector. Zinc chloride (99.0+ wt %, Fluka) was dried at 120 °C in a vacuum oven until constant mass was reached.

2.2. Apparatus. The experimental apparatus used for the VLE measurements is schematically shown in Figure 1. The modified Scott ebulliometer used in this work is similar to the one used by Dallinga et al. (1993). However, some modifications have been carried out. (1) A liquid sampling port (B1) and a vapor sampling port (B2) now allow to determine the liquid-phase and the vapor-phase compositions analytically. The volume (ca. 0.5 cm³) of the vapor sampling port is small compared with the large volume (ca. 300 cm³) of the liquid phase. (2) A vertically adjustable quartz thermometer (C) ensures that the equilibrium temperature can be measured accurately. (3) A primary pressure controller (L, Vacuubrand vacuum controller CVC 24) was used to keep the pressure constant in the 50 L ballast tank in order to improve the temperature stability of the system (± 0.01 °C).

The total pressure was measured and controlled by an MKS pressure controller consisting of a 390 HA transducer sensor head (G), a 250 controller, and a 270 signal conditioner. Dry air in the 50 L ballast tank entered the system via an automatically controlled needle valve (H1). The system pressure was indicated on a digital display with a resolution of 1.33×10^{-2} kPa and kept constant within $\pm 1.33 \times 10^{-2}$ kPa during the complete measurement cycle. A magnetic stirrer/heater (E, IKA-MAG RH) heats the content of the ebulliometer to the boiling point at the given pressure, ensures thorough mixing, and prevents the occurrence of bumping.

All liquid mixtures, consisting of acetone, methanol, and zinc chloride, were prepared gravimetrically with a Sartorius analytical balance with an accuracy of ± 0.1 mg. For each experimental point approximately 300 cm³ was filled into the ebulliometer. The pressure was set either to 101.33 or 66.66 kPa before the ebulliometer was heated, and a steady-state boiling condition was observed. The equilibrium temperature was measured using a Hewlett-Packard quartz thermometer (model 2804 A) with an accuracy of ± 0.02 °C.

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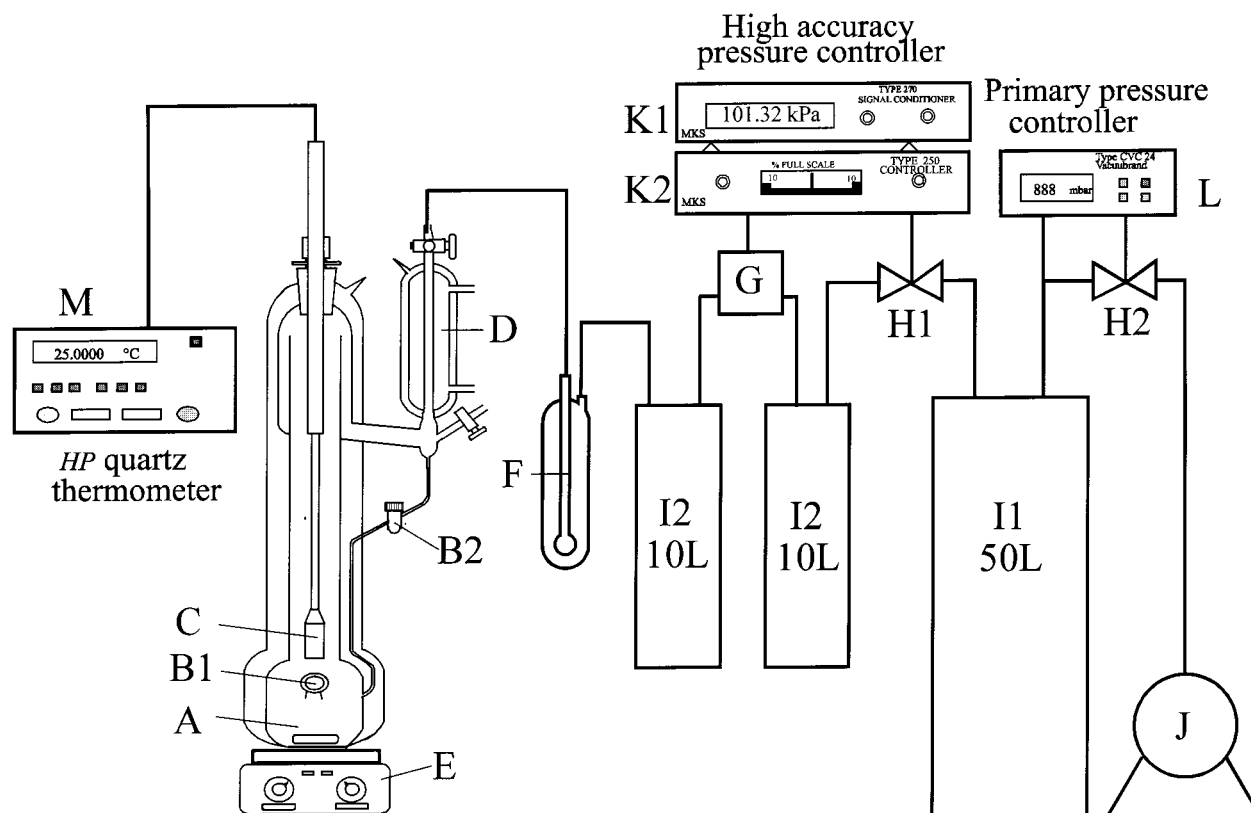


Figure 1. Schematic diagram of the experimental apparatus: A, ebullimeter; B, liquid and vapor sampling ports; C, quartz thermometer sensor; D, condenser; E, magnetic stirrer/heater (IKA-MAG RH); F, cold trap; G, pressure sensor head (MKS type 390 HA); H, needle valve; I, ballast tank; J, vacuum pump; K, high-accuracy pressure controller (MKS pressure controller); L, primary pressure controller (Vacubrand vacuum controller CVC 24); M, HP quartz thermometer (HP model 2804 A).

2.3. Sample Analysis. The vapor-phase composition was determined using a Hewlett-Packard (mode 6890) gas chromatograph with the help of a thermal conductivity detector connected to a computer with HP ChemStation software. A 30 m glass capillary column (stationary phase HP 19091-133) was used with the following conditions: inlet temperature, 100 °C; oven temperature, 80 °C; detector temperature, 250 °C. Helium was used as carrier gas, which passed through the column at a flow rate of 1.3 cm³/min. The calibration was carried out by injection of acetone + methanol mixtures of known composition prepared gravimetrically. The accuracy of the measured mole fraction was ± 0.001 , which was confirmed by comparing the known composition of the made-up sample with the composition measured by GC.

The presence of the nonvolatile salt in the liquid-phase precluded direct solvent analysis via gas chromatography (GC). Therefore, the liquid-phase composition was calculated by material balance. Since the vapor-phase volume of the ebullimeter is known, it is easy to calculate the amount of each component in the vapor phase according to the vapor-phase composition measured by GC. Then the liquid-phase composition can be estimated by subtracting the amount in the vapor phase and the condensed mass in the vapor sampling port (B2) from the known composition of the made-up samples. The mean deviation between calculated and weight liquid-phase composition was found to be ± 0.0002 in mole fraction. To validate the experimental method, experiments for the binary system acetone + methanol without salt were also performed whereby the liquid-phase composition was estimated by material balance and compared to that analyzed by gas chromatography. The uncertainty was found to be within ± 0.0012 in mole fraction.

Table 1. Vapor-Liquid Equilibrium Data of the Acetone (1) + Methanol (2) System at $P = 101.33$ kPa

liquid phase		vapor phase		temperature	
x_1	y_1	Δy_1^a	$\Delta y_1\%^b$	$t/^\circ\text{C}$	$\Delta t/^\circ\text{C}^c$
0.0338	0.0817	0.0069	8.45	63.24	0.07
0.0927	0.1923	0.0100	5.20	61.56	0.12
0.1473	0.2662	0.0034	1.28	60.33	0.12
0.1956	0.3254	0.0025	0.77	59.42	0.13
0.2931	0.4255	0.0030	0.71	57.87	0.24
0.4000	0.5126	0.0016	0.31	56.75	0.23
0.4995	0.5886	0.0056	0.95	56.06	0.16
0.6036	0.6544	0.0001	0.02	55.53	0.14
0.6889	0.7139	0.0001	0.01	55.24	0.15
0.7461	0.7528	0.0034	0.45	55.16	0.13
0.8943	0.8779	0.0046	0.52	55.37	0.04
mean deviation		0.003	1.70		0.13

^a $\Delta y_1 = y_{1,\text{exp}} - y_{1,\text{calc}}$. ^b $\Delta y_1\% = (y_{1,\text{exp}} - y_{1,\text{calc}}) \times 100/y_{1,\text{exp}}$. ^c $\Delta t = t_{\text{exp}} - t_{\text{calc}}$ calculated values using the UNIQUAC equation (parameters taken from Gmehling et al., 1977).

2.4. Consistency of the Experimental Data. To confirm the reliability of the experimental VLE data, each experimental point for the salt-free system acetone (1) + methanol (2) was measured twice at 101.33 kPa. The mean values of the experimental data obtained are given in Table 1 and shown in Figure 2. They were also compared with published data (Amer et al., 1956) and the smoothed values calculated by the UNIQUAC equation (parameters taken from Gmehling et al., 1977). The mean deviation between experimental and smoothed values was 0.003 in the vapor-phase mole fraction and 0.13 °C in the temperature. The thermodynamic consistency of the experimental data was examined by the Redlich-Kister area test (Redlich and Kister, 1948). The average area deviation was 0.1%.

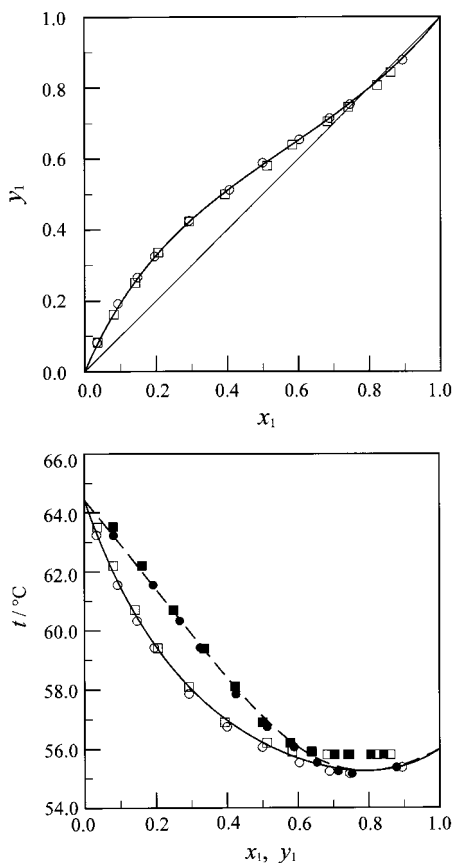


Figure 2. Vapor-liquid equilibrium diagram for the system acetone (1) + methanol (2) at 101.33 kPa: (○,●) this work; (□,■) Amer et al., 1956; (continuous line and dashed line) calculated by UNIQUAC equation (parameters taken from Gmehling et al., 1977).

Table 2. Vapor-Liquid Equilibrium Data for the Acetone (1) + Methanol (2) + Zinc Chloride (3) System at $P = 66.66$ kPa

x_1^a	y_1^b	$t/^\circ\text{C}^c$	α_{12}^d	x_1^a	y_1^b	$t/^\circ\text{C}^c$	α_{12}^d
$m = 1.082 \text{ mol kg}^{-1}$				$m = 1.502 \text{ mol kg}^{-1}$			
0.903	0.962	45.62	2.697	0.903	0.970	46.59	3.489
0.830	0.917	45.43	2.259	0.827	0.933	46.34	2.899
0.776	0.879	45.47	2.093	0.701	0.848	46.44	2.372
0.630	0.767	45.72	1.936	0.572	0.742	46.72	2.152
0.535	0.695	46.10	1.984	0.517	0.703	47.06	2.206
0.428	0.618	46.81	2.165	0.461	0.659	47.24	2.265
0.319	0.527	47.94	2.386	0.403	0.608	47.72	2.298
0.209	0.389	49.62	2.407	0.341	0.558	48.32	2.432
0.112	0.267	51.69	2.887	0.278	0.498	49.15	2.584
				0.215	0.437	50.01	2.824
				0.162	0.355	51.14	2.857
$m = 1.751 \text{ mol kg}^{-1}$				$m = 2.000 \text{ mol kg}^{-1}$			
0.902	0.972	46.53	3.805	0.155	0.347	51.28	2.907
0.801	0.920	46.39	2.871	0.074	0.205	53.17	3.209
0.722	0.872	46.42	2.619				
0.648	0.821	46.62	2.497				
0.572	0.759	46.88	2.356	0.900	0.975	46.84	4.271
0.496	0.693	47.46	2.294	0.800	0.934	46.79	3.555
0.417	0.628	47.94	2.363	0.700	0.872	46.83	2.922
0.336	0.563	48.74	2.543	0.601	0.795	47.11	2.567
0.259	0.493	49.81	2.792	0.501	0.715	47.63	2.509
0.192	0.415	50.84	2.985	0.400	0.627	48.35	2.530
0.087	0.228	53.06	3.092	0.305	0.552	49.16	2.813
0.073	0.205	53.40	3.290	0.225	0.455	50.26	2.884
				0.101	0.274	52.92	3.366

^a Salt-free liquid-phase mole fraction. ^b Vapor-phase mole fraction. ^c System temperature ($^\circ\text{C}$). ^d Relative volatility $\alpha_{12} = (y_1/x_1)/(y_2/x_2)$.

Accordingly, it can be deduced that reliable and thermodynamically consistent vapor-liquid equilibrium data can

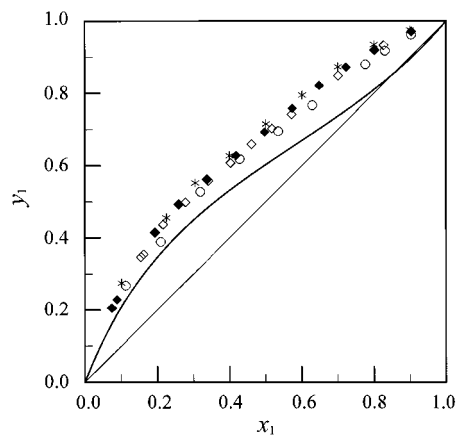


Figure 3. x - y vapor-liquid equilibrium diagram for the system acetone + methanol + zinc chloride at 66.66 kPa: (○) $m = 1.082$, (◇) $m = 1.502$, (◆) $m = 1.751$, (*) $m = 2.000 \text{ mol kg}^{-1}$; (—) $m = 0.0 \text{ mol kg}^{-1}$ calculated by the UNIQUAC model (parameters taken from Gmehling et al., 1977).

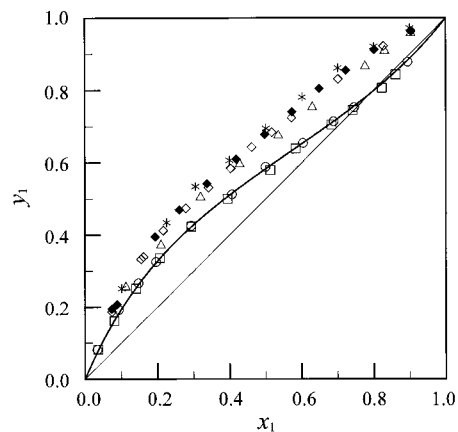


Figure 4. x - y vapor-liquid equilibrium diagram for the system acetone + methanol + zinc chloride at 101.33 kPa: (○) $m = 0.0$, (△) $m = 1.082$, (◇) $m = 1.502$, (◆) $m = 1.751$, (*) $m = 2.000 \text{ mol kg}^{-1}$; (—) $m = 0.0 \text{ mol kg}^{-1}$ calculated by the UNIQUAC model (parameters taken from Gmehling et al., 1977); (□) $m = 0.0 \text{ mol kg}^{-1}$ (Amer et al., 1956).

be measured with the experimental apparatus described in section 2.2.

3. Results and Discussion

3.1. Experimental Data. Isobaric vapor-liquid equilibrium data for the system acetone (1) + methanol (2) + zinc chloride (3) were measured at two pressures (66.66 and 101.33 kPa) and various constant salt concentrations. The experimental results are given in Tables 2 and 3. In Figures 3 and 4 these experimental data are plotted in form of an x - y diagram on a salt-free basis. From these figures it can be seen that the addition of zinc chloride to the system acetone + methanol increases the amount of acetone in the vapor phase. A salting-out effect of acetone occurs, and the azeotropic point disappears at all investigated salt concentrations. The salt effect slightly decreases with increasing system pressure.

3.2. Calculation of VLE for the Systems Containing ZnCl_2 . To describe the observed vapor-liquid equilibrium behavior, the experimental data were correlated using the extended electrolyte UNIQUAC (Sander et al., 1986) and the LIQUAC (Li et al., 1994) model.

3.2.1. Extended Electrolyte UNIQUAC Model of Sander et al. (1986). Sander et al. (1986) presented an

Table 3. Vapor–Liquid Equilibrium Data for the Acetone(1) + Methanol(2) + Zinc Chloride (3) System at $P = 101.33$ kPa^a

x_1	y_1	$t/^\circ\text{C}$	α_{12}	x_1	y_1	$t/^\circ\text{C}$	α_{12}
$m = 1.082$ mol kg ⁻¹				$m = 1.502$ mol kg ⁻¹			
0.903	0.957	57.17	2.408	0.904	0.964	57.70	2.827
0.830	0.908	57.00	2.013	0.827	0.922	57.50	2.459
0.776	0.865	57.03	1.849	0.701	0.831	57.59	2.093
0.630	0.753	57.23	1.793	0.572	0.724	57.82	1.963
0.535	0.675	57.49	1.803	0.517	0.684	58.01	2.022
0.428	0.595	57.97	1.969	0.461	0.643	58.29	2.110
0.319	0.504	58.86	2.173	0.403	0.584	58.63	2.086
0.209	0.371	60.21	2.226	0.341	0.531	59.23	2.188
0.112	0.255	62.40	2.703	0.278	0.474	60.09	2.347
				0.215	0.412	61.01	2.554
				0.161	0.339	61.94	2.667
$m = 1.751$ mol kg ⁻¹				$m = 2.000$ mol kg ⁻¹			
0.902	0.965	57.88	2.962	0.155	0.333	62.07	2.724
0.801	0.913	57.71	2.592	0.074	0.187	63.41	2.866
0.722	0.857	57.77	2.299				
0.648	0.805	57.86	2.250				
0.572	0.741	58.05	2.139	0.900	0.972	58.48	3.793
0.496	0.679	58.28	2.152	0.800	0.921	58.31	2.907
0.417	0.611	58.72	2.191	0.700	0.861	58.39	2.659
0.336	0.543	59.04	2.347	0.601	0.781	58.73	2.367
0.259	0.471	60.13	2.549	0.501	0.695	59.13	2.272
0.192	0.395	61.25	2.743	0.400	0.607	59.39	2.317
0.088	0.208	63.21	2.740	0.305	0.534	60.24	2.621
0.073	0.195	63.58	3.089	0.225	0.434	61.35	2.646
				0.101	0.252	63.86	2.991

^a See footnotes a, b, c, d in Table 2.

Table 4. UNIQUAC Reference Interaction Parameters a_{ij}^* (K), Concentration-Dependent Parameters $\delta_{ij,m}$, Relative van der Waals Volume Parameters r_i , and Surface Area Parameters q_i for the Extended UNIQUAC Model of Sander (Sander et al., 1986)

	CH ₃ OH	CH ₃ COCH ₃	Zn ²⁺	Cl ⁻
		a_{ij}^*		
CH ₃ OH	0.0	-54.2	-242.76 ^a	-426.3
CH ₃ COCH ₃	223.8	0.0	390.57 ^a	-166.15 ^a
Zn ²⁺	-343.21 ^a	-367.89 ^a	0.0	-1729.85 ^a
Cl ⁻	788.7	1472.57 ^a	816.25 ^a	0.0
		r_i and q_i		
r_i	1.4311	2.5735	3.0	0.9861
q_i	1.4322	2.3360	3.0	0.9917
		$\delta_{ij,m}$		
Zn ²⁺ -Cl ⁻	8.959 ^a	298.07 ^a		

^a These interaction parameters have been fitted in this work.

extension of the UNIQUAC equation for mixed solvents with salts. The activity coefficient of a solvent is calculated as the sum of a long-range and a short-range contribution. The first term is calculated by a simplified Debye–Hückel term for mixed solvents, and the short-range interaction is given by an extended UNIQUAC equation. The UNIQUAC parameters (a_{im} and a_{mi}) between an ion i and the

solvent m are regarded as concentration-dependent and are given by

$$a_{im} = a_{im}^* + \theta_i \sum_{j \neq 1} \delta_{ij,m} \theta_j \quad (1a)$$

$$a_{mi} = a_{mi}^* + \theta_i \sum_{j \neq 1} \delta_{ij,m} \theta_j \quad (1b)$$

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

For a system with two solvents and one salt, 14 parameters are needed: 2 solvent–solvent, 2 ion–ion, 8 ion–solvent, and 2 salt–solvent interaction parameters. The binary solvent–solvent interaction parameters have been obtained directly from Gmehling et al. (1977). For the acetone + methanol + zinc chloride system, two interaction parameters were directly taken from literature (Sander et al., 1986). The remaining 10 parameters were fitted to the experimental data by minimization of the objective function F using the simplex–Nelder–Mead method (Nelder and Mead, 1965):

$$F(a_{ij}, a_{ji}, \delta_{j,m}) = \sum_{nt} \sum_{np} \omega_y (y_{i,1(\text{exp})} - y_{i,1(\text{calc})})^2 + \sum_{nt} \sum_{np} \omega_T (T_{i(\text{exp})} - T_{i(\text{calc})})^2 \quad (2)$$

where y_i represents the vapor-phase mole fraction, T the system temperature (K), ω_y and ω_T the weighting factors, nt the number of data sets, and np the number of data points for each data set. The subscripts exp and calc denote experimental and calculated values. The vapor-phase mole fractions y_i and the boiling points can be calculated by solving iteratively the equilibrium condition

$$y_i P = x_i \gamma_i P_i^s \Phi_i \quad (3)$$

where

$$P = \sum_i x_i \gamma_i P_i^s \Phi_i \quad (4)$$

$$\Phi_i = \varphi_i^s(\text{Poy}) / \varphi_i^v \quad (5)$$

and where x_i is the liquid-phase mole fraction of the solvent i based on the assumption of total dissociation of the salt. The saturation vapor pressure of the pure solvent i at system temperature, P_i^s was calculated using Antoine constants from the literature (Gmehling et al., 1977). In eq 5, φ_i^v is the fugacity coefficient of solvent i in the vapor

Table 5. Binary Interaction Parameters, Relative van der Waals Volume Parameters, and Surface Area Parameters for the LIQUAC Model^a

i	j	a_{ij}	a_{ji}	b_{ij}	c_{ij}	r_i	q_i
CH ₃ OH	CH ₃ COCH ₃	-54.2	223.8				
CH ₃ OH	Zn ²⁺	386.98 ^b	346.91 ^b	10.6202 ^b	2.1227 ^b		
CH ₃ OH	Cl ⁻	-378.2	-231.6	-5.620	-1.006		
CH ₃ COCH ₃	Zn ²⁺	1225.85 ^b	800.43 ^b	4.3993 ^b	2.1866 ^b		
CH ₃ COCH ₃	Cl ⁻	739.9	-333.3	-2.653	-1.206		
Zn ²⁺	Cl ⁻	-72.91	-126.7	0.2042	-0.00557		
CH ₃ OH						1.431	1.432
CH ₃ COCH ₃						2.574	2.336
Zn ²⁺						1.000	1.000
Cl ⁻						1.000	1.000

^a Units: a_{ij} is K. b_{ij} and c_{ij} are mol kg⁻¹. ^b These interaction parameters have been fitted in this work.

Table 6. Mean Absolute Deviations of Vapor-Phase Composition and Boiling Point for Both Electrolyte Models

P/kPa	molality	Δy		$\Delta t/^{\circ}\text{C}$	
		Sander	LIQUAC	Sander	LIQUAC
66.66	1.082	0.015	0.010	0.23	0.17
	1.502	0.019	0.007	0.33	0.29
	1.751	0.021	0.008	0.26	0.18
	2.000	0.025	0.010	0.25	0.22
101.33	1.082	0.014	0.009	0.24	0.21
	1.502	0.017	0.006	0.18	0.20
	1.751	0.019	0.008	0.47	0.35
	2.000	0.023	0.009	0.27	0.18
average deviation		0.019	0.008	0.28	0.23

phase, φ_i^s is the saturation fugacity coefficient of pure solvent i at system temperature, and $(\text{Poy})_i$ is the Poynting factor. φ_i^s becomes approximately equal to φ_i^v , and $(\text{Poy})_i$ is approximately equal to unity at atmospheric pressure, so Φ_i becomes approximately equal to 1. Therefore, the activity coefficient of the solvent γ_i was calculated using eq 3, assuming $\Phi_i = 1$.

3.2.2. LIQUAC Model of Li et al. (1994). The LIQUAC model for the excess Gibbs energy was presented by Li et al. (1994). It is able to describe the behavior for both single and mixed solvent electrolyte systems (Polka et al., 1994). This model consists of three contributions: (1) a Debye-Hückel term to consider long-range electrostatic interactions, (2) the UNIQUAC equation to describe the short-range interactions between all species, and (3) a middle-range contribution to include all indirect effects of the charge interactions.

For a system with 2 solvents and 1 salt, 12 short-range interaction parameters (a_{ij}) and 10 middle-range interaction parameters (b_{ij} and c_{ij}) are required. A large number of parameters have already been published (Li et al., 1994). Therefore, in this work 14 parameters were directly taken from the published parameter matrix. The remaining eight interaction parameters were fitted to the new experimental data with the help of the Simplex-Nelder-Mead method

using the same objective function (eq 2). The obtained interaction parameters, relative volumes, and surface areas are given in Table 5. As suggested by Li et al. (1994), the relative volumes and surface areas for the ions were arbitrarily set to 1.0.

For both models the new interaction parameters are listed in Tables 4 and 5 together with the parameters directly taken from literature. Mean absolute deviations in the vapor-phase mole fraction and boiling points for both models are listed in Table 6. It can be seen that both models are able to present the experimental data. However, slightly better results are obtained using the LIQUAC model (Li et al. 1994).

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