

Vapor-Liquid Equilibrium of the Acetone-Water-Salt System

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Isobaric vapor-liquid equilibrium (VLE) data were measured for the binary system acetone-water at 0.2-1.013 bar and for the acetone-water-salt systems at 1.013 bar and at different salt concentrations. All the salts investigated in this work, LiCl, NaBr, KBr, and KI, exhibited a salting out effect which increases with the increasing salt concentration. The obtained data were used for the estimation of the interaction parameters between acetone and the salt ions by applying the extended UNIQUAC method of Sander et al. These estimated interaction parameters were used with other parameters presented in the literature in the VLE calculations. Application of the model to the salt-free system at different pressures and to the acetone-water-salt systems showed that the vapor-phase composition could be represented with good accuracy up to a salt molality of 4 mol/kg of solvent, and that relatively higher deviations were obtained between the experimental and calculated vapor compositions at higher salt molalities. The deviations in vapor-phase mole fractions were 0.02 for the salt-free system over 75 binary data points and 0.037 for mixed solvent-salt systems over 167 ternary data points.

Introduction

Phase equilibria of mixed solvent-salt systems are important for different applications such as the design of extractive distillation columns, where the salt is employed as the separating agent and for the separation of salt-containing mixtures. The addition of small amounts of salt to a mixture has a pronounced effect on the relative volatility of the mixture components. For azeotropic mixtures, the addition of certain salts can eliminate the azeotrope completely, thereby affecting the complete separation of the components of the mixture.

The prediction and correlation of vapor-liquid equilibria (VLE) of mixtures containing strong electrolytes, especially mixed solvent-salt systems, have received considerable attention in recent years. Several methods for the correlation of the activity coefficients of the solvents in the electrolytic mixture have appeared in the literature (1-6). Most of these models are based on the local composition concept with the consideration of the long-range ion-ion interactions and the short-range ion-solvent and solvent-solvent interactions except for the work of Dahl et al. (6) in which the long-range ion-ion interactions are disregarded and the salt is considered as a single solvated molecule. In our work, the extended UNIQUAC model of Sander et al. (2) will be applied for the correlation of the water-acetone-salt VLE data. This model utilizes a Debye-Huckel term to describe the ion-ion interaction and modified UNIQUAC terms for the short-range interactions.

The testing of these models requires accurate experimental data. Previous VLE data on the water-acetone-salt systems were obtained with NaCl, NaNO₃, and CaCl₂ by Sada et al. (7). This work is a contribution to that experimental data base.

Experimental Apparatus and Procedure

The equilibrium still, shown schematically in Figure 1, was supplied by Fischer. The main body of the still consists of a cylindrical flask with a 1-L internal volume and a double-surface condenser. A magnetic stirrer is used to maintain sufficient homogeneity of the liquid, improve salt dissolution, and at the same time decrease irregularities in the boiling behavior such as blanketing. The entire vapor space is surrounded by a vacuum jacket in order to prevent refluxing of vapor condensate in the vapor space of the still due to heat

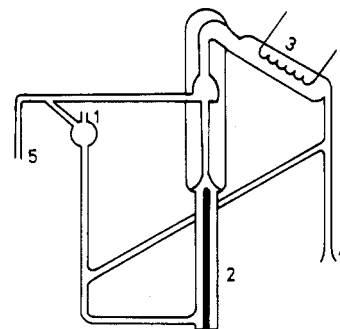


Figure 1. Schematic diagram of the vapor-liquid equilibrium still: (1) filler, (2) circulation heater, (3) condenser, (4, 5) sample receivers.

losses. The vacuum jacket is further silvered to reduce radiation losses.

The temperature was measured with two mercury-in-glass thermometers with 0.1 K accuracy. The pressure was measured with a pressure gauge accurate within 0.005 bar. The composition of the mixture was determined by means of a gas chromatograph (Varian-3300) equipped with a thermal conductivity detector. A Poropak-Q column, 6 ft long, was used. This column was packed with 80/100 mesh size and operated at 80-220 °C with a 20 °C/min temperature programming. The injector temperature was 250 °C, and the detector temperature was 275 °C. The carrier gas was helium flowing at a rate of 30 mL/min. Since the boiling points of the salts used in this work are higher than the injection temperature, only water and acetone enter the column. Therefore, the mole fraction obtained from the analysis of the liquid-phase samples was on a salt-free basis. The actual mole fraction can be obtained through the known molality of the salt. Since the salts were nonvolatile, the vapor samples were salt-free. The conversion of the area percent obtained from the chromatogram to mole percent was obtained by preparing a series of known concentrations of acetone and water. For each concentration the area percent was obtained, and then a calibration curve was prepared. The reported mole fractions are believed accurate to ± 0.002 .

Acetone was supplied by Baker Chemical Co. with a stated purity of 99.5%. The salts had purities of 99.4+% and were supplied by BDH, Baker, and Merck companies. All chem-

Table I. Experimental Vapor-Liquid Equilibrium Data for the Binary Acetone-Water System at Atmospheric and Subatmospheric Pressures

P = 1.013 bar			P = 0.8 bar			P = 0.6 bar			P = 0.4 bar			P = 0.2 bar		
T, K	X ₁	Y ₁	T, K	X ₁	Y ₁	T, K	X ₁	Y ₁	T, K	X ₁	Y ₁	T, K	X ₁	Y ₁
329.85	0.981	0.984	323.75	0.995	0.991	315.25	0.994	0.991	305.55	0.984	0.984	289.55	0.999	0.999
329.95	0.944	0.951	323.95	0.955	0.961	315.35	0.969	0.970	305.65	0.954	0.961	289.95	0.889	0.851
330.00	0.912	0.921	324.05	0.899	0.931	315.95	0.894	0.932	305.85	0.891	0.937	290.15	0.837	0.944
330.50	0.761	0.886	324.15	0.807	0.905	316.15	0.875	0.931	306.45	0.787	0.900	290.65	0.754	0.920
331.70	0.642	0.855	324.55	0.736	0.881	316.45	0.797	0.909	306.85	0.659	0.888	290.95	0.613	0.908
332.00	0.526	0.841	324.75	0.650	0.869	316.75	0.758	0.899	307.55	0.494	0.877	291.25	0.464	0.907
332.60	0.443	0.829	324.95	0.532	0.849	317.15	0.647	0.869	307.85	0.438	0.866	293.55	0.273	0.898
333.70	0.330	0.813	325.15	0.436	0.846	317.75	0.515	0.865	309.35	0.279	0.851	294.95	0.189	0.856
336.95	0.155	0.769	325.75	0.313	0.838	317.95	0.437	0.858	309.75	0.231	0.839	296.15	0.150	0.821
343.25	0.081	0.713	325.95	0.301	0.831	319.25	0.313	0.854	311.95	0.139	0.791	301.95	0.084	0.752
345.00	0.069	0.695	328.05	0.212	0.815	319.75	0.278	0.841	318.15	0.088	0.742	304.15	0.066	0.724
353.00	0.036	0.537	334.55	0.093	0.735	320.15	0.256	0.840	324.25	0.049	0.661	310.95	0.038	0.606
363.15	0.014	0.350	336.15	0.084	0.702	322.25	0.161	0.802	331.55	0.028	0.520	325.75	0.009	0.233
363.50	0.013	0.252	342.05	0.052	0.630	323.75	0.130	0.788	338.95	0.014	0.327			
368.95	0.004	0.129	344.95	0.039	0.571	332.75	0.067	0.662						
			355.05	0.018	0.358	341.85	0.029	0.524						
						348.25	0.016	0.394						

Table II. Vapor-Liquid Equilibrium Data for Acetone (1)-Water (2)-Salt Systems at 2 m Concentration of Salt

2 m LiCl			2 m NaBr			2 m KBr			2 m KI		
T, K	X ₁ ^a	Y ₁	T, K	X ₁ '	Y ₁	T, K	X ₁ '	Y ₁	T, K	X ₁ '	Y ₁
329.55	0.675	0.902	327.65	0.746	0.900	344.85	0.054	0.732	339.35	0.118	0.758
329.65	0.636	0.897	328.05	0.612	0.889	341.05	0.072	0.783	336.25	0.161	0.800
330.15	0.493	0.890	328.45	0.573	0.887	338.05	0.104	0.811	335.15	0.181	0.811
330.45	0.450	0.888	329.05	0.476	0.873	334.95	0.142	0.835	333.65	0.216	0.816
330.95	0.412	0.887	329.45	0.436	0.870	334.75	0.169	0.836	333.25	0.230	0.823
330.85	0.401	0.885	329.75	0.381	0.870	333.25	0.213	0.857	331.55	0.297	0.838
331.25	0.379	0.873	329.95	0.323	0.869	331.85	0.261	0.856	331.25	0.309	0.839
331.65	0.322	0.869	330.25	0.308	0.863	330.95	0.301	0.857	330.45	0.358	0.857
333.05	0.256	0.864	330.45	0.272	0.858	330.25	0.339	0.858	330.05	0.390	0.859
333.25	0.252	0.863	331.35	0.254	0.856	329.85	0.367	0.859	329.65	0.421	0.871
333.75	0.222	0.861	332.65	0.217	0.846	329.75	0.374	0.861	329.45	0.439	0.879
335.15	0.186	0.856	333.25	0.182	0.842	329.25	0.424	0.876	328.75	0.534	0.889
335.65	0.175	0.841	336.05	0.161	0.835	328.55	0.512	0.881	328.15	0.629	0.892
336.45	0.160	0.832	336.15	0.156	0.833				327.75	0.699	0.911
336.55	0.137	0.815	337.15	0.127	0.814						
338.35	0.115	0.802	340.15	0.084	0.797						
340.35	0.094	0.793	343.45	0.064	0.760						
			352.65	0.031	0.683						

^a Concentration on a salt-free basis

icals were used without further purification.

A solution of the desired composition was prepared. About 50–80 mL of this solution was poured into the apparatus at the filler. After the pressure was adjusted the immersion heater was switched on. Equilibrium was achieved by circulating the liquid and the condensed vapor samples. The first samples were taken from the liquid and vapor sample receivers after a circulation time of 30 min. More samples were then taken after 10–15 min to ensure that equilibrium had been reached. For measurements with salts, a solution of known molality was prepared. The amount of dissolved salt was carefully controlled so that no salt would precipitate out during the course of the measurements. The salts LiCl, NaBr, KI, and KBr were chosen for this study. All of the above salts are very soluble in water and extremely insoluble in acetone. Isobaric VLE data were measured at salt molalities ranging from 2 to 6 m.

Results

A check on the reliability of the experimental technique and apparatus was done by carrying out phase equilibrium measurements on the acetone-water system at 1.013 bar. The close agreement between the measured and literature data (8) is shown in Figure 2. Hence, the accuracy of the data was established.

Isobaric VLE data on the binary acetone-water system were measured at 0.2, 0.4, 0.6, 0.8, and 1.013 bar. The

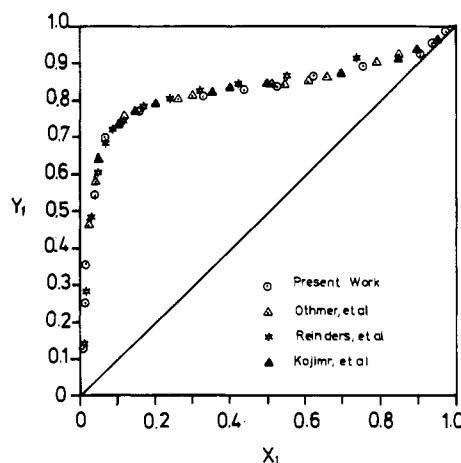


Figure 2. Vapor-liquid equilibrium data for the acetone (1)-water (2) system at atmospheric pressure.

experimental results are presented in Table I. The x - y diagram for the acetone-water mixture at atmospheric pressure is slightly concave upward at high acetone mole fraction, indicating deviation from ideality. At subatmospheric pressures the relative volatility of acetone with respect to water increases.

VLE data at 1.013 bar were measured for the acetone-water system with the salts LiCl and NaBr at salt molalities

Table III. Vapor-Liquid Equilibrium Data for Acetone (1)-Water (2)-Salt Systems at 4 m Concentration of Salt

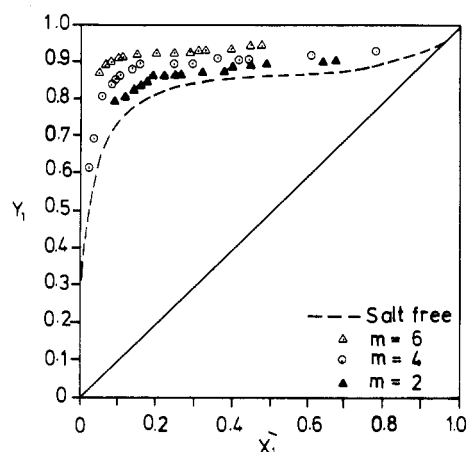
4 m LiCl			4 m NaBr			4 m KBr			4 m KI		
T, K	X ₁ '	Y ₁	T, K	X ₁ '	Y ₁	T, K	X ₁ '	Y ₁	T, K	X ₁ '	Y ₁
356.15	0.026	0.609	352.25	0.031	0.701	362.95	0.011	0.350	360.15	0.024	0.352
351.15	0.039	0.687	343.45	0.075	0.789	350.15	0.035	0.700	348.95	0.045	0.673
344.65	0.064	0.804	338.15	0.092	0.827	345.05	0.053	0.781	346.75	0.065	0.704
340.65	0.088	0.843	336.85	0.111	0.845	340.85	0.069	0.792	341.95	0.107	0.778
339.75	0.095	0.853	334.85	0.152	0.868	338.35	0.087	0.800	340.05	0.122	0.797
339.25	0.099	0.856	333.45	0.173	0.880	337.65	0.111	0.835	337.75	0.146	0.807
335.45	0.141	0.876	332.15	0.195	0.883	336.15	0.122	0.858	336.45	0.161	0.818
334.15	0.160	0.888	328.95	0.293	0.889	332.85	0.171	0.860	333.25	0.219	0.839
333.05	0.252	0.888	327.15	0.376	0.887	330.95	0.210	0.864	330.55	0.295	0.850
332.15	0.293	0.894	326.35	0.423	0.904	330.85	0.211	0.871	328.45	0.380	0.872
331.05	0.363	0.907	325.45	0.506	0.900	329.55	0.245	0.873	327.55	0.423	0.873
330.45	0.417	0.903	325.25	0.570	0.901	328.35	0.288	0.882	327.05	0.443	0.877
330.25	0.441	0.912	324.85	0.635	0.905	327.65	0.318	0.888	326.35	0.483	0.881
329.35	0.609	0.919	324.45	0.722	0.906	326.05	0.407	0.894	325.95	0.504	0.890
328.85	0.780	0.933							324.65	0.647	0.892
									324.05	0.717	0.919
									323.75	0.755	0.923
									323.55	0.783	0.936
									322.45	0.951	0.987
									322.35	0.967	0.989

Table IV. Vapor-Liquid Equilibrium Data for Acetone (1)-Water (2)-Salt Systems at 6 m Concentration of Salt

6 m LiCl			6 m NaBr		
T, K	X ₁ '	Y ₁	T, K	X ₁ '	Y ₁
347.75	0.052	0.872	356.15	0.025	0.766
342.75	0.071	0.893	348.25	0.044	0.834
341.25	0.080	0.894	342.05	0.067	0.864
338.65	0.104	0.908	339.75	0.078	0.866
337.55	0.114	0.910	338.75	0.083	0.867
333.65	0.151	0.913	337.45	0.091	0.868
330.95	0.199	0.914	336.25	0.103	0.875
330.85	0.252	0.918	336.15	0.108	0.876
330.75	0.291	0.920	335.65	0.125	0.887
330.55	0.306	0.925	332.75	0.168	0.894
330.05	0.332	0.928	329.95	0.219	0.895
329.95	0.401	0.932	328.15	0.262	0.893
329.85	0.454	0.936	327.45	0.275	0.898
329.75	0.481	0.938	326.55	0.312	0.906
			324.25	0.421	0.915

of 2, 4, and 6 m and with the salts KBr and KI at 2 and 4 m. Although the knowledge of salt concentration is necessary, it is convenient to express the concentration of the volatile components in both the liquid and vapor phases on a salt-free basis (x'). This makes it easy to compare the degree of the effect of salt presence on the VLE behavior of the salt-free systems. The effect of 2 m concentrations of LiCl, NaBr, and KI on the VLE of the acetone-water system is illustrated by the data in Table II. The presence of these salts increases the relative volatility of acetone; hence, these salts have a "salting out" effect. When a salt is dissolved in a homogeneous liquid mixture, it will form liquid-phase associations or complexes with one species in the liquid more than the other. This interaction will reduce the activity of the more attracted component in solution and increase the activity of the less attracted component. Hence, the less attracted component is expelled or salted out from the liquid solution. In our case the acetone molecules are less attracted to the salt ions and tend to go into the vapor phase.

As the salt concentration is increased, the effect on the partial pressure of acetone is more pronounced, as can be seen from the data in Tables III and IV. The effect of the salt molality is shown in Figure 3. As the salt molality increases the ionic strength increases and the interaction between the ions and water increases. The attraction will cause a reduction in the activity coefficient of water at the higher salt concentration. Thus, the relative volatility of acetone with respect to water increases.

**Figure 3. Effect of salt concentrations on the vapor-liquid equilibrium for the acetone (1)-water (2)-LiCl system at atmospheric pressure.**

According to the electrostatic theories, the salt effect increases as the ionic radius decreases (9). When the ion radius is smallest, the electrostatic field of the ion is greatest, causing a maximum attraction for the highly polar water molecules. Since the lithium ion (0.6-Å radius) is smaller than the sodium ion (0.95 Å) which is smaller than the potassium ion (1.33 Å), one would expect a greater effect with lithium ion than sodium or potassium ions. The experimental work confirms this result as shown in Figure 4.

Data Correlation

The presence of the salt affects the VLE behavior through the interactions between the ions and the solvents and their influence on the activity coefficients of the solvents. The data of this work were correlated using the extended UNIQUAC activity coefficient model of Sander et al. (2). In this model, the long-range ion-ion interactions are described by the Debye-Huckel expression, and the short-range ion-ion, ion-solvent, and solvent-solvent interactions are described using a modified UNIQUAC expression; thus

$$\ln \gamma_n = \ln \gamma_n^{DH} + \ln \gamma_n^c + \ln \gamma_n^R \quad (1)$$

where γ_n is the activity coefficient of solvent n , γ_n^{DH} is the Debye-Huckel term, γ_n^c is the combinatorial term, and γ_n^R is the residual term.

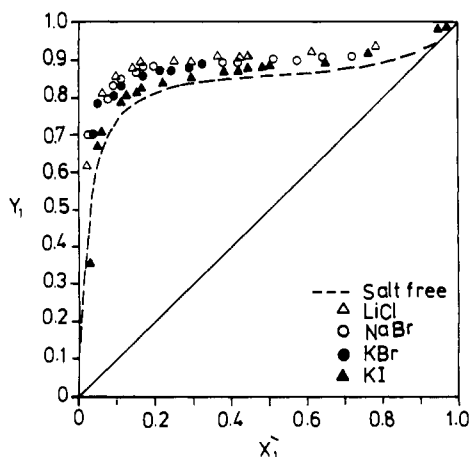


Figure 4. Effect of the decreasing ionic radius of salts on the vapor-liquid equilibrium for the acetone (1)-water (2) system at 4 *m* salt concentrations and atmospheric pressure.

Table V. UNIQUAC Volume (r_k) and Surface Area (q_k) Parameters

	Li ⁺	Na ⁺	K ⁺	Cl ⁻	I ⁻	Br ⁻	C ₃ H ₆ O	H ₂ O
r_k	1.0	3.0	3.0	0.9861	1.6759	1.2331	2.57	0.92
q_k	1.0	3.0	3.0	0.9917	1.4123	1.151	2.34	1.40

The combinatorial term provides the contribution due to differences in molecular size, and the residual term provides the contribution due to energy interactions between molecules. For salt-free mixtures this equation reduces to the usual UNIQUAC equation. The original reference should be consulted for the expressions for each term. While the calculation of the Debye-Huckel and combinatorial terms requires only pure component data and concentrations of compounds, the residual term also incorporates the energy interaction parameters; specifically the term ψ_{kl} in the residual part contains the model parameters a_{kl} :

$$\psi_{kl} = e^{-a_{kl}/T} \quad (2)$$

where k and l may be an ion or a solvent species. For the interaction between ion i and solvent m , the parameter a is considered concentration-dependent:

$$a_{im} = a_{im}^* + \theta_i \sum_{j \neq i} \delta_{ij,m} \theta_j \quad (3)$$

$$a_{mi} = a_{mi}^* + \theta_i \sum_{j \neq i} \delta_{ij,m} \theta_j \quad (4)$$

where a_{im}^* and a_{mi}^* are reference interaction parameters, $\delta_{ij,m}$ is the interaction parameter between the salt and the solvent m , θ_j is the surface area fraction of component j which is obtained from the concentration, x_j , and surface area parameter, q_j , and the summation is over all ionic species except i .

For the application of the mathematical model, 14 binary interaction parameters are needed for each single salt-binary

solvent system. Fortunately, the interaction parameters with water for some of the cations and anions studied in this work were presented by Sander et al. (2). Other parameters were estimated by minimizing the following objective function with the experimental data of this work:

$$F = \sum_N [(\ln \gamma_{1,\text{exptl}} - \ln \gamma_{1,\text{calcd}})^2 + (\ln \gamma_{2,\text{exptl}} - \ln \gamma_{2,\text{calcd}})^2] \quad (5)$$

γ_{exptl} and γ_{calcd} refer to the experimentally obtained and calculated activity coefficients, respectively, and N is the number of data points. The Powell minimization technique was utilized to estimate the values of the interaction parameters. The calculated and experimental activity coefficients were obtained assuming that the vapor phase is ideal. Since the pressure is atmospheric and considering other sources of uncertainties in the experimental measurements, this assumption is acceptable. The UNIQUAC volume and surface area parameters are given in Table V, and the UNIQUAC reference interaction parameters a_{kl}^* and the $\delta_{ij,m}$ parameters are presented in Tables VI and VII.

In order to test the model, isobaric bubble point temperature VLE calculations were performed. The computer program calculates the temperature and vapor composition from the experimental pressure and liquid composition using a Newton-Raphson iteration scheme. The activity coefficients were calculated using the extended UNIQUAC model with the above parameters. The vapor pressures of acetone and water were estimated from the Antoine equation.

A comparison between the experimental and calculated temperatures and vapor mole fractions of acetone is presented in Table VIII. The results for the salt-free mixtures of acetone-water gave a mean absolute deviation in the vapor composition of 0.02 over 75 data points at different pressures. For the data of the mixed solvent-salt systems, the mean absolute deviation in vapor composition was 0.037 over 167 ternary data points. The relatively greater error is due to the data at the high salt concentration of LiCl and NaBr (molality 6). When the data points at this salt concentration are removed, the mean deviation in the vapor phase mole fraction drops to 0.029 over 138 ternary data points. For the ternary data, the mean absolute deviation in the calculated temperatures is on the order of 1-2 K. The data with the NaBr at 6 *m* gave the maximum mean deviation in the vapor-phase mole fractions. Sander et al. (2) also found that the data for the system 2-propanol-water with the salt NaBr could not be correlated satisfactorily.

Conclusions

All salts used in this work have a salting out effect. This effect increases as the salt concentration increases. The model used in this work combines the Debye-Huckel term with a modified UNIQUAC equation using concentration-dependent

Table VI. UNIQUAC Reference Interaction Parameters a_{kl}^* (K) (ref 2 and this work)

	Li ⁺	Na ⁺	K ⁺	Cl ⁻	Br ⁻	Br ⁻	C ₃ H ₆ O	H ₂ O
Li ⁺	0.0	0.0	0.0	0.0	na ^a	na	851.4 ^b	-484.2
Na ⁺	0.0	0.0	0.0	76.2	na	-362.1	996.8 ^b	-209.4
K ⁺	0.0	0.0	0.0	-470.3	0.0	-63.1	1267.5 ^b	-220.7
Cl ⁻	0.0	-11.2	-60.9	0.0	na	0.0	596.1 ^b	-524.9
I ⁻	na	na	0.0	na	0.0	na	883.5 ^b	-281.0
Br ⁻	na	265.2	210.0	0.0	na	0.0	277.1 ^b	-128.8
C ₃ H ₆ O	851.4 ^b	996.8 ^b	1267.5 ^b	596.1 ^b	883.5 ^b	277.1 ^b	0.0	530.99
H ₂ O	-59.2	330.6	458.4	-190.2	-281.0	-43.5	-100.71	0.0

^a Not available. ^b Estimated from the data of this work.

Table VII. $\delta_{ij,m}$ Parameters (K) ($\delta_{ij,m} = \delta_{ji,m}$) (ref 2 and this work)

	$m = \text{H}_2\text{O}$	$m = \text{C}_3\text{H}_8\text{O}$		$m = \text{H}_2\text{O}$	$m = \text{C}_3\text{H}_8\text{O}$
LiCl	6548	868 280 ^a	KI	19 582 ^b	60 226 ^b
NaBr	6624	899 994 ^a	KBr	5668	555 599 ^b

^a Estimated from the data of this work.

Table VIII. Comparison between the Experimental and Calculated Temperature and Vapor Mole Fractions

system	P , bar	molality, mol/kg of solvent	no. of data points	ΔT , ^a K	ΔY_1 ^b
acetone-water	1.013	0	15	0.65	0.015
acetone-water	0.800	0	16	0.70	0.15
acetone-water	0.600	0	17	0.84	0.012
acetone-water	0.400	0	14	0.79	0.027
acetone-water	0.200	0	13	0.74	0.038
acetone-water-LiCl	1.013	2	17	0.92	0.016
acetone-water-LiCl	1.013	4	15	1.20	0.061
acetone-water-LiCl	0.400	4	13	1.40	0.037
acetone-water-LiCl	1.013	6	14	1.19	0.068
acetone-water-NaBr	1.013	2	18	1.38	0.028
acetone-water-NaBr	1.013	4	14	1.81	0.042
acetone-water-NaBr	1.013	6	15	1.58	0.082
acetone-water-KBr	1.013	2	13	1.63	0.025
acetone-water-KBr	1.013	4	14	1.59	0.035
acetone-water-KI	1.013	2	14	2.28	0.008
acetone-water-KI	1.013	4	20	2.11	0.020

^a $\Delta T = \sum |T_{\text{calcd}} - T_{\text{exptl}}| / \text{no. of data points}$. ^b $\Delta Y_1 = \sum |Y_{1,\text{calcd}} - Y_{1,\text{exptl}}| / \text{no. of data points}$.

parameters. The application of the model to acetone-water-salt mixtures has shown that the change in vapor-phase composition on addition of a salt can be represented with

good accuracy. A total of 167 ternary data points have been correlated with a total mean absolute deviation in the vapor-phase mole fraction of 0.037.

Due to the mathematical nature of the UNIQUAC activity coefficient model, the parameters obtained are highly correlated and other sets of parameters might give equally good results.

The new model developed by Dahl et al. (6) uses a reduced number of parameters which can be easily obtained from VLE data. It can be deduced that models are constantly being improved, but effort has to be directed toward obtaining more accurate experimental VLE data in order to obtain more accurate model parameters.

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