

Isobaric Vapor–Liquid Equilibria for 2-Methyl-butan-1-ol + 3-Methyl-butan-1-ol + CuCl₂, ZnCl₂, and FeCl₃ Systems at 101.3 kPa

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Isobaric vapor–liquid equilibrium (VLE) data for 2-methyl-butan-1-ol + 3-methyl-butan-1-ol + CuCl₂, ZnCl₂, and FeCl₃ systems were measured, respectively, in a modified Rose recirculation still at 101.3 kPa. The VLE data of binary systems were correlated with the e-NRTL and NRTL models. The ternary systems were predicted with the e-NRTL and NRTL models. The results showed that the VLE of the 2-methyl-butan-1-ol + 3-methyl-butan-1-ol system in the presence of three salts was obviously different from that of the salt-free system. All salts showed a notable salting-out effect and followed the salting-out effect order of ZnCl₂ > FeCl₃ > CuCl₂. The salting-out effect significantly increases the relative volatility of 2-methyl-butan-1-ol.

Introduction

2-Methyl-butan-1-ol and 3-methyl-butan-1-ol are useful solvents and important fine chemicals.¹ They coexist in mixed pentanol (a mixture of 2-methyl-butan-1-ol and 3-methyl-butan-1-ol), which is routinely obtained as a byproduct after wine and similar raw materials are distilled. It is very difficult to separate them with conventional distillation because they are isomeric compounds, and their relative volatility is only 1.078.² Although they can be separated by precise distillation³ and by extractive distillation with glycol,^{4,5} 2,3-dichloropropanol and 2,3-dibromopropanol⁶ as extractant, low productivity in the precise distillation and some disadvantages such as recovery and/or toxicity of extractant in the extractive distillation are noticeable.

Addition of charged species coming from a soluble salt as extractant was found to modify the relative volatility, and so the components can be more easily separated in distillation.⁷ To simulate and design the separation process, the determination of vapor–liquid equilibrium (VLE) data for the ternary system and the research of its correlating models are essential. The VLE data for the binary system 2-methyl-butan-1-ol (1) + 3-methyl-butan-1-ol (2) were reported in the literature.⁵ The saturated vapor pressures and solubilities for the system 2-methyl-butan-1-ol + CuCl₂, ZnCl₂, FeCl₃, and CaCl₂ and for the system 3-methyl-butan-1-ol + CuCl₂, ZnCl₂, and FeCl₃ were reported.^{8–11} However, the VLE data for the ternary system 2-methyl-butan-1-ol (1) + 3-methyl-butan-1-ol (2) + salt (3) are not reported in literature.

This work was carried out as part of a project to simulate the separation of 2-methyl-butan-1-ol from 3-methyl-butan-1-ol by distillation with the salting-out effect. The isobaric VLE data for the ternary system were measured, and the effect of salts on the VLE of the 2-methyl-butan-1-ol + 3-methyl-butan-1-ol system was discussed briefly.

Experimental Section

Materials. 2-Methyl-butan-1-ol and 3-methyl-butan-1-ol were prepared by our lab⁴ and purified twice by distillation. Antoine

coefficients⁴ of 2-methyl-butan-1-ol and 3-methyl-butan-1-ol are summarized in Table 1. The purity of pure liquid used in the present work is more than 0.999 in mass fraction (assay GC). CuCl₂, ZnCl₂, and FeCl₃ (purity is more than 0.99 in mass fraction) purchased from Chengdu Hangjia Biological and Pharmaceutical Tech. Ltd. were recrystallized and dried at 130 °C in the vacuum drying chamber.

Apparatus and Procedure. The modified Rose recirculation still⁴ was used for the VLE determinations. The mixture consisting of 2-methyl-butan-1-ol, 3-methyl-butan-1-ol, and CuCl₂ was weighed with an analytical balance with an accuracy of ± 0.1 mg. First, 90 g of 2-methyl-butan-1-ol, 5 g of 3-methyl-butan-1-ol, and 6 g of CuCl₂ were added into the Rose recirculation still, and then the kettle was heated to a certain temperature. A platinum sensor, with an uncertainty of ± 0.01 K, was used to measure the equilibrium temperature. The pressure was measured by a mercury gauge with an uncertainty of ± 0.0133 kPa. For each analysis, about 10 cm³ of the liquid phase sample was taken out and evaporated in a full-closed minidistiller for isolating salt and liquid and further analyzed with GC, which is similar to others¹² in principle. An amount of 2 cm³ of vapor phase condensate was taken out and directly analyzed with GC. The composition of the solutions was changed, and the same procedure was repeated for the 2-methyl-butan-1-ol + 3-methyl-butan-1-ol and ZnCl₂ or FeCl₃.

The equilibrium compositions of the salt-free liquid and vapor phase were analyzed by GC with a flame ionization detector (FID) and a thermal conductivity conductor (TCD) (SQ-206, Beijing Analysis Instrument Factory) and a chromatographic workstation (FJ2000-NEW, Shanghai Jinzhou Science & Technology Ltd.). A gas chromatograph was used with a 2.5 m stainless steel column (15 % Erythrite on carrier 6201) and an integrator. The temperature of the injector and chamber were 190 °C and 95 °C, respectively. The carrier gas was nitrogen (purity is more than 0.9999 in mass fraction), and the velocity was 0.5 cm³·s⁻¹. The uncertainty of the composition measurement is estimated to be ± 0.0005 in mole fraction after careful calibration (different from previous data due to the difference of the material purity and chromatographic column). The mass fraction of salt was gravimetrically determined after the volatile

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Table 1. Antoine Coefficients of 2-Methyl-butan-1-ol and 3-Methyl-butan-1-ol^a

components	T range/K	Antoine coefficients ^a		
		A	B	C
2-methyl-butan-1-ol	307 to 402	16.2708	2752.19	-116.3
3-methyl-butan-1-ol	298 to 426	16.7127	3026.43	-104.1

$$^a \ln(P_i^0/\text{mmHg}) = A - B/(T/K) + C.$$

components were separated from a known mass of sample by evaporating to dryness.¹²

Results and Discussion

The effect of salt on VLE of the 2-methyl-butan-1-ol + 3-methyl-butan-1-ol system at 101.3 kPa was investigated in this study. The isobaric VLE data for 2-methyl-butan-1-ol + 3-methyl-butan-1-ol systems containing CuCl₂, ZnCl₂, and FeCl₃ at different salt contents (mass fraction as 0.03 and 0.12) were measured. The results are summarized in Tables 2 to 4 and

plotted as *x*-*y* diagrams in Figures 1 to 3, respectively. It should be noted that the mole fractions of liquid components in the tables and figures are on a salt-free basis.

In the literature,⁸⁻¹⁰ the solubilities of salts in 2-methyl-butan-1-ol and 3-methyl-butan-1-ol systems were measured, respectively. Saturated vapor pressures of 2-methyl-butan-1-ol and 3-methyl-butan-1-ol containing salts at different temperatures were determined; however, there was no correlation of experimental data with any model. For the correlation of experimental data of VLE, NRTL¹³ and e-NRTL models are usually used. The e-NRTL model is an extension of the NRTL model which Chen et al.¹⁴ derived as a model for single-solvent + electrolyte systems. Mock et al.¹⁵ extended it to mixed solvent + electrolyte systems.

The VLE data of 2-methyl-butan-1-ol + 3-methyl-butan-1-ol were passed thermodynamic consistency with the integral test of Herington.¹⁶ No consistency test was used for salt-containing systems.

Table 2. Isobaric VLE Data for the 2-Methyl-butan-1-ol (1) + 3-Methyl-butan-1-ol (2) + ZnCl₂ (3) System at Atmospheric Pressure (101.3 kPa)

mass fraction of salt	T/K	<i>x</i> ₁	<i>y</i> ₁	γ_1	γ_2	α_{12}	predicted by e-NRTL		predicted by NRTL		
							ΔT^a	Δy_1^b	ΔT	Δy_1	
0.03	401.95	0.8234	0.8445	1.023	0.955	1.165	-0.27	0.0024	-1.37	0.0204	
	402.25	0.7722	0.7976	1.020	0.954	1.163	-0.25	-0.0004	-1.33	0.0148	
	402.75	0.6371	0.6765	1.031	0.941	1.191	-0.49	0.0067	-1.44	0.0177	
	403.35	0.5569	0.5995	1.024	0.935	1.191	-0.34	0.0017	-1.15	0.0123	
	403.95	0.4974	0.5425	1.017	0.923	1.198	-0.08	-0.0024	-0.75	0.0083	
	404.55	0.4402	0.4838	1.005	0.916	1.192	0.20	-0.0085	-0.31	0.0028	
	405.25	0.3485	0.3897	0.999	0.909	1.194	0.36	-0.0095	0.19	0.0024	
	406.35	0.234	0.2737	1.008	0.887	1.234	0.77	-0.0044	1.16	0.0071	
	ave ^c							0.34	0.0045	0.96	0.0107
	max							0.77	0.0095	1.44	0.0204
	0.12	403.25	0.9629	0.9694	0.961	0.856	1.221	-0.11	0.0039	-0.14	-0.0067
		403.95	0.8359	0.8628	0.963	0.848	1.235	-0.09	0.0043	-0.02	-0.0416
404.45		0.7505	0.7881	0.963	0.847	1.236	-0.05	0.0040	-0.04	-0.0589	
405.25		0.6109	0.6598	0.965	0.849	1.235	-0.03	0.0040	0.07	-0.0752	
405.85		0.5123	0.5653	0.967	0.848	1.238	0.01	0.0041	-0.11	-0.0783	
406.65		0.4172	0.4775	0.977	0.831	1.277	0.26	0.0080	0.37	0.0715	
407.35		0.3201	0.3772	0.983	0.829	1.286	0.38	0.0084	0.54	0.0618	
408.55		0.1989	0.2457	0.991	0.820	1.312	0.83	0.0072	1.13	0.0434	
ave ^c								0.22	0.0084	0.30	0.0547
max ^d								0.83	0.0055	1.13	0.0783

$$^a \Delta T = T_{\text{exp}} - T_{\text{cal}}; ^b \Delta y_1 = y_{1,\text{exp}} - y_{1,\text{cal}}; ^c \text{ave}(y_1) = (1/N) \sum |y_{1,\text{exp}} - y_{1,\text{cal}}|; \text{ave}(T) = (1/N) \sum |T_{\text{exp}} - T_{\text{cal}}|; ^d \text{max}(y_1) = \max(|y_{1,\text{exp}} - y_{1,\text{cal}}|); \text{max}(T) = \max(|T_{\text{exp}} - T_{\text{cal}}|); N = \text{number of data points}.$$

Table 3. Isobaric VLE Data for the 2-Methyl-butan-1-ol (1) + 3-Methyl-butan-1-ol (2) + FeCl₃ (3) System at Atmospheric Pressure (101.3 kPa)

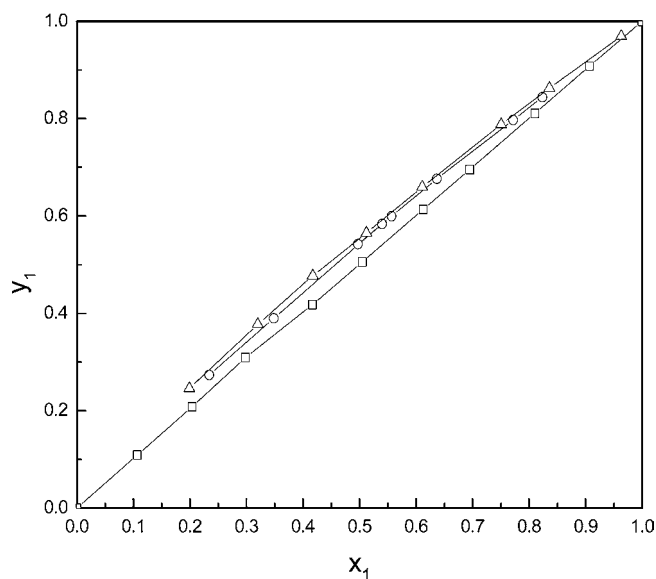
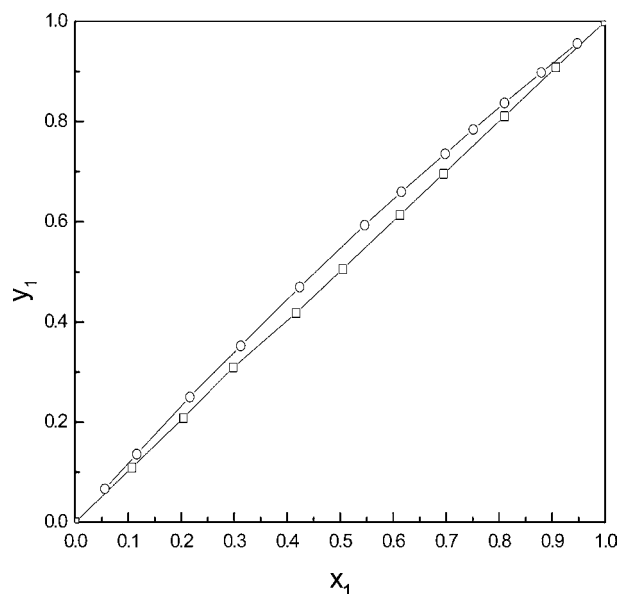
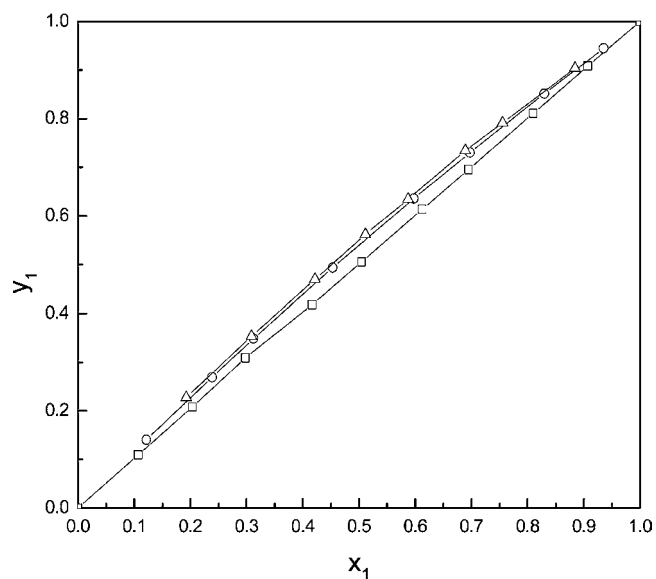
mass fraction of salt	T/K	<i>x</i> ₁	<i>y</i> ₁	γ_1	γ_2	α_{12}	predicted by e-NRTL		predicted by NRTL		
							ΔT^a	Δy_1^b	ΔT	Δy_1	
0.03	402.05	0.9356	0.9446	1.004	0.930	1.174	0.06	0.0012	-0.57	0.0024	
	402.45	0.8296	0.8516	1.007	0.929	1.179	0.17	0.0034	-0.61	0.0163	
	402.95	0.6975	0.73031	1.010	0.935	1.174	0.31	0.0047	-0.69	-0.0299	
	403.35	0.5976	0.6359	1.013	0.936	1.176	0.42	0.0057	-0.71	-0.0338	
	403.85	0.4534	0.4938	1.019	0.942	1.176	0.66	-0.0074	-0.74	-0.0299	
	404.45	0.3125	0.3486	1.023	0.945	1.177	-0.82	0.0064	0.53	0.0227	
	405.05	0.2386	0.2685	1.012	0.939	1.171	0.62	-0.0018	0.06	0.0208	
	405.45	0.1219	0.1405	1.023	0.944	1.178	-0.87	0.0024	0.24	-0.0091	
	ave							0.49	0.0041	0.52	0.0206
	max							0.87	0.0074	0.74	0.0338
	0.12	403.35	0.8846	0.9038	0.972	0.862	1.226	0.60	0.0206	0.03	0.0630
		404.15	0.7555	0.7912	0.970	0.860	1.226	0.43	0.0159	1.05	0.1246
404.55		0.6892	0.7346	0.974	0.849	1.248	0.36	0.0176	1.37	0.1479	
405.05		0.5877	0.6348	0.971	0.865	1.219	0.38	0.0129	1.51	0.1863	
405.55		0.5117	0.5618	0.971	0.862	1.223	0.28	0.0111	1.56	0.2035	
406.05		0.4217	0.4699	0.970	0.866	1.216	0.26	0.0084	1.34	0.2153	
406.75		0.3088	0.3533	0.973	0.864	1.223	0.17	0.0073	0.84	0.2060	
407.45		0.1930	0.2272	0.979	0.864	1.229	0.12	0.0058	1.45	0.1483	
ave								0.32	0.0125	1.14	0.1619
max								0.60	0.0206	1.56	0.2153

$$^a \Delta T = T_{\text{exp}} - T_{\text{cal}}; ^b \Delta y_1 = y_{1,\text{exp}} - y_{1,\text{cal}}.$$

Table 4. Isobaric VLE Data for the 2-Methyl-butan-1-ol (1) + 3-Methyl-butan-1-ol (2) + CuCl₂ (3) System at Atmospheric Pressure (101.3 kPa)

mass fraction of salt	T/K	x_1	y_1	γ_1	γ_2	α_{12}	predicted by e-NRTL		predicted by NRTL		
							ΔT^a	Δy_1^b	ΔT^a	Δy_1^b	
0.12	402.55	0.9474	0.9563	0.987	0.883	1.215	-0.02	0.0037	-0.19	-0.0027	
	402.85	0.8796	0.8978	0.988	0.893	1.202	-0.04	0.0041	-0.17	-0.0109	
	403.15	0.8103	0.8373	0.990	0.893	1.205	0.09	-0.0055	0.15	-0.0146	
	403.35	0.7509	0.7845	0.994	0.895	1.208	0.09	-0.0083	0.18	-0.0139	
	403.55	0.6984	0.7359	0.996	0.900	1.203	0.10	0.0090	-0.19	-0.0141	
	403.95	0.6157	0.6596	0.999	0.898	1.209	-0.20	-0.0100	-0.09	-0.0128	
	404.15	0.5464	0.5931	1.006	0.903	1.210	-0.15	0.0126	-0.13	-0.0086	
	404.65	0.4235	0.4695	1.010	0.911	1.205	0.19	0.0120	-0.04	0.0048	
	405.15	0.3123	0.3525	1.012	0.917	1.199	0.28	-0.0092	-0.08	0.0022	
	405.45	0.2184	0.2489	1.025	0.923	1.206	0.22	0.0064	-0.00	0.0006	
	405.85	0.1161	0.1332	1.028	0.930	1.200	0.23	0.0025	0.22	0.0003	
	406.15	0.0561	0.0649	1.034	0.931	1.206	0.29	0.0011	0.52	0.0001	
	ave							0.16	0.0070	0.16	0.0071
	max							0.29	0.0126	0.52	0.0146

$$^a \Delta T = T_{\text{exp}} - T_{\text{cal}}, \quad ^b \Delta y_1 = y_{1,\text{exp}} - y_{1,\text{cal}}$$

**Figure 1.** Isobaric VLE diagram for the 2-methyl-butan-1-ol (1) + 3-methyl-butan-1-ol (2) + ZnCl₂ (3) system at 101.3 kPa. The symbols were the experimental data: \square , salt-free; \circ , ZnCl₂, mass fraction as 0.03; Δ , ZnCl₂, mass fraction as 0.12.**Figure 3.** Isobaric VLE diagram for the 2-methyl-butan-1-ol (1) + 3-methyl-butan-1-ol (2) + ZnCl₂ (3) system at 101.3 kPa. The symbols were the experimental data: \square , salt-free; \circ , CuCl₂, mass fraction as 0.12.**Figure 2.** Isobaric VLE diagram for the 2-methyl-butan-1-ol (1) + 3-methyl-butan-1-ol (2) + FeCl₃ (3) system at 101.3 kPa. The symbols were the experimental data: \square , salt-free; \circ , FeCl₃, mass fraction as 0.03; Δ , FeCl₃, mass fraction as 0.12.

Calculation of Binary Vapor–Liquid Equilibrium. The binary VLE have been correlated using the NRTL and the e-NRTL models. In these correlations, the nonrandomness parameters α are also adjusted, obtaining better results than fixing them as constants. When these models are used for systems constituted by a solvent + salt, the equilibrium condition has to do only with the solvent, which is the component that is present in both phases. These correlations were made by minimizing the following objective function

$$\text{OF} = \sqrt{\sum_i^n (\gamma_{i,\text{cal}}/\gamma_{i,\text{exp}} - 1)^2/n(n-1)} \quad (1)$$

where $\gamma_{1,\text{exp}}$ and $\gamma_{1,\text{cal}}$ are the experimental activity coefficients and the calculated ones, respectively. The calculated parameters, Δg and α , and average deviations (ARD) of $100 \cdot \Delta \gamma$ for both correlation models are summarized in Table 5. The vapor pressures of the components were calculated using the Antoine equation.

Predication of Ternary Vapor–Liquid Equilibrium. The parameters of the binary system 2-methyl-butan-1-ol (1) +

Table 5. Binary Correlation Parameters, Δg and α , and Average Deviation^a, $100 \cdot \Delta\gamma$, for the Binary Systems 2-Methyl-butan-1-ol (1) + ZnCl₂(2), 3-Methyl-butan-1-ol (1) + ZnCl₂(2), 2-Methyl-butan-1-ol (1) + FeCl₃(2), 3-Methyl-butan-1-ol (1) + FeCl₃(2), 2-Methyl-butan-1-ol (1) + CuCl₂(2), and 3-Methyl-butan-1-ol (1) + CuCl₂ (2) at Atmospheric Pressure (101.3 kPa)

2-Methyl-butan-1-ol (1) + ZnCl ₂ (2)				
NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	8307.92	α	0.44
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	4331.06	$100 \cdot \Delta\gamma$	0.58
e-NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	4835.22	α	0.12
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-7974.51	$100 \cdot \Delta\gamma$	0.56
3-Methyl-butan-1-ol (1) + ZnCl ₂ (2)				
NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	4644.84	α	0.60
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-5543.57	$100 \cdot \Delta\gamma$	0.45
e-NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	2363.89	α	0.21
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-4308.24	$100 \cdot \Delta\gamma$	0.63
2-Methyl-butan-1-ol (1) + FeCl ₃ (2)				
NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	10890.78	α	0.05
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	11082.34	$100 \cdot \Delta\gamma$	0.61
e-NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	2727.11	α	0.43
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-3774.78	$100 \cdot \Delta\gamma$	0.51
3-Methyl-butan-1-ol (1) + FeCl ₃ (2)				
NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	-12934.15	α	0.15
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-19933.76	$100 \cdot \Delta\gamma$	0.96
e-NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	2084.57	α	0.01
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-4392.64	$100 \cdot \Delta\gamma$	1.48
2-Methyl-butan-1-ol (1) + CuCl ₂ (2)				
NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	10137.29	α	0.62
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	9868.52	$100 \cdot \Delta\gamma$	0.60
e-NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	2768.89	α	0.39
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-3904.85	$100 \cdot \Delta\gamma$	0.66
3-Methyl-butan-1-ol (1) + CuCl ₂ (2)				
NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	2423.32	α	0.45
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-3978.19	$100 \cdot \Delta\gamma$	0.57
e-NRTL	$\Delta g_{12}/J \cdot \text{mol}^{-1}$	2607.54	α	0.41
	$\Delta g_{21}/J \cdot \text{mol}^{-1}$	-3837.27	$100 \cdot \Delta\gamma$	0.60

^a Average deviation: $\text{ARD}100 \cdot \Delta\gamma = 100 \times (\sum_i |\gamma_{\text{exp}} - \gamma_{\text{cal}}| / \gamma_{\text{exp}}) / (N)$.

3-methyl-butan-1-ol (2) have been taken from the literature.² The other necessary parameters have been determined in this work. Using these binary parameters determined, the behavior of the ternary systems can be studied using the NRTL and e-NRTL models. The VLE data of the ternary systems and the deviation in temperatures and vapor mole fraction were shown in Tables 2 to 4. These results showed that the NRTL and e-NRTL models could give a good representation of the experimental data.

The effect of salt on the solution nonideality can be expressed by activity coefficient of component i , γ_i , which can be calculated by the following equation

$$\gamma_i = y_i \phi_i P / (x_i \phi_i^s P_i^s) \quad (2)$$

where y_i represents mole fraction of component i in the vapor phase; x_i is the mole fraction of component i in the liquid phase (including salt); P is the total pressure of the equilibrium system, 101.3 kPa; P_i^s is the vapor pressure of pure component i at system temperature, which can be calculated by the Antoine equation and Antoine coefficients taken from the literature;⁴ ϕ_i is the fugacity coefficient of component i in the vapor mixture; and ϕ_i^s is the fugacity coefficient of pure component i in its saturated state. The fugacity coefficients ϕ_i and ϕ_i^s were calculated by the R-K equation of state.¹⁶

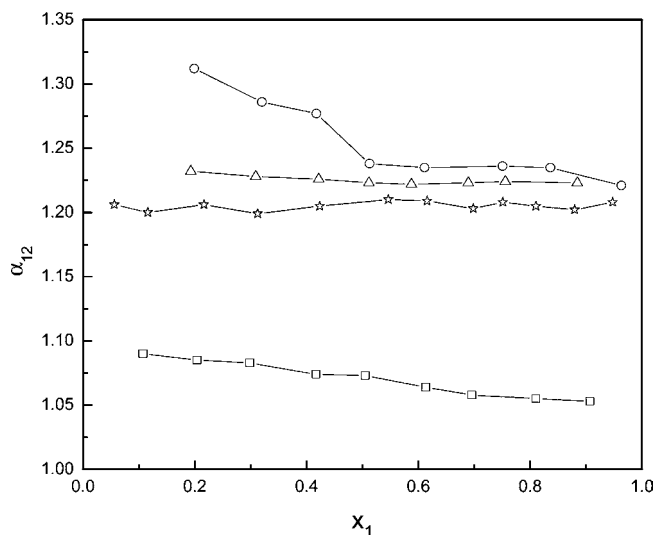


Figure 4. Relative volatility of 2-methyl-butan-1-ol for 2-methyl-butan-1-ol (1) + 3-methyl-butan-1-ol (2) systems containing ZnCl₂, FeCl₃, and CuCl₂ of mass fraction as 0.12. The symbols were the experimental data: □, salt-free; ○, ZnCl₂; △, FeCl₃; ☆, CuCl₂.

It should be noted that salt component does not occur in the vapor phase due to its nonvolatility; however, its mole fraction in the liquid phase should be considered when calculating activity coefficients of 2-methyl-butan-1-ol or 3-methyl-butan-1-ol. In addition to activity coefficient, relative volatility of 2-methyl-butan-1-ol was also calculated in terms of the following equation

$$\alpha_{12} = (y_1/x_1)/(y_2/x_2) \quad (3)$$

where x_1 and x_2 are mole fraction of 2-methyl-butan-1-ol and 3-methyl-butan-1-ol, respectively, on a salt-free basis. The activity coefficients and relative volatilities calculated were also listed in Tables 2 to 4.

As can be seen from Figures 1 to 3, three salts all could increase the relative volatility of 2-methyl-butan-1-ol in the whole concentration range, thus showing a salting-out effect for 2-methyl-butan-1-ol. Relative volatilities of 2-methyl-butan-1-ol were plotted in Figure 4 for the isomeric system containing different salts of mass fraction as 0.12, which clearly shows the salting effect of salts on the isomeric methyl-butan-1-ol system. As can be seen from Figure 4, the salting-out effect follows the order: ZnCl₂ > FeCl₃ > CuCl₂.

The relative volatility of 2-methyl-butan-1-ol can be increased from 1.078 (salt-free system) to 1.31 for the ZnCl₂-containing system, 1.25 for the FeCl₃-containing system, and 1.22 for the CuCl₂-containing system. In the case of mole fraction of 0.20 of 2-methyl-butan-1-ol in a feed and mole fraction of 0.99 of product 2-methyl-butan-1-ol, according to the Fenske equation, the minimum number of theoretical plates would reduce 72% when ZnCl₂ was used. Thus, the results implied that the three salts might be used as promising additives in the separation of 2-methyl-butan-1-ol and 3-methyl-butan-1-ol by salt distillation due to their notable salting-out effect.

Conclusions

Isobaric VLE data for 2-methyl-butan-1-ol + 3-methyl-butan-1-ol + CuCl₂, ZnCl₂, and FeCl₃ systems were measured at 101.3 kPa. The VLE data of the ternary systems were predicted, and the constituent binary systems containing the salts were cor-

related with NRTL and e-NRTL models. Both models give similar results for the binary systems, obtaining satisfactory results. The results indicate that three salts show notable salting-out effect. For the isomeric methyl-butan-1-ol system, the salting-out effect follows the order of: $\text{ZnCl}_2 > \text{FeCl}_3 > \text{CuCl}_2$. As a result, distillation separation of 2-methyl-butan-1-ol from 3-methyl-butan-1-ol is facilitated by the addition of ZnCl_2 , FeCl_3 , and CuCl_2 .

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