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PREDICTION OF VAPOR–LIQUID EQUILIBRIUM FROM TERNARY LIQUID–LIQUID EQUILIBRIUM DATA BY MEANS OF LOCAL COMPOSITION EQUATIONS

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ABSTRACT

Ternary vapor–liquid equilibrium can be predicted by use of the extended UNIQUAC and LEMF equations whose energy parameters are obtained from the correlation of the corresponding liquid–liquid equilibrium data. Three objective functions are used in parameter estimation, and objective functions are usually preferred defined in terms of liquid-phase mole fractions than in terms of activities. The extended UNIQUAC equation shows better performance than the LEMF equation. Prediction of binary vapor–liquid equilibrium from ternary liquid–liquid equilibrium data confirms the same trends as observed in ternary vapor–liquid equilibrium predictions.

INTRODUCTION

The correlation of the ternary liquid–liquid equilibrium (LLE) data with an appropriate expression for the activity coefficient leads to the evaluation of the parameters for the corresponding binary systems. These parameters can be used in the calculation of the vapor–liquid equilibrium (VLE) relation of the same systems or in the prediction of ternary (or multicomponent) VLE relation, combined with parameters obtained from VLE for other binary systems.

Joy and Kyle [1] used the NRTL equation [2] in the correlation of LLE data for four ternary systems and the parameters obtained were applied to the prediction of binary and ternary VLE. Their approach worked well for three systems and failed for the fourth one. By means of the Black [3] and NRTL equations, Newsham and Vahdat [4] computed ternary VLE from LLE data for three systems including water and two alcohols with reasonable accuracy. Yee et al. [5] presented a more comprehensive study of the prediction of binary and ternary VLE from LLE data for eight systems using

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TABLE 1

Ternary systems studied

System	LLE data			VLE data		
	No. and type	Temp. (°C)	Ref.	Pressure (or temp. (°C))	Data points	Ref.
Acetonitrile(1)–benzene(2)–*n*-heptane(3)	1A	45	13	(45)	33	13
n-Pentane(1)–benzene(2)–sulfur dioxide(3)	2A	−17.8	14	(−17.8)	41	14
Water(1)–1-butanol(2)–1-propanol(3)	3A	90–92	15	98.53 kPa	9	15
Water(1)–methanol(2)–ethyl acetate(3)	4B	70	16	101.33 kPa	65	16
Water(1)–ethanol(2)–ethyl acetate(3)	5B	70	17	(70)	9	20
Benzene(1)–ethanol(2)–water(3)	6C	25	18			
Benzene(1)–1-propanol(2)–water(3)	7C	37.7	19	(30)	22	21

the NRTL, LEMF [6] and UNIQUAC [7] equations and concluded that the LEMF equation appears to give somewhat better results for both binary and ternary VLE predictions.

This paper presents another study of the prediction of binary and ternary VLE from ternary LLE data for seven type I systems which include one partially miscible binary and two completely miscible binaries for each

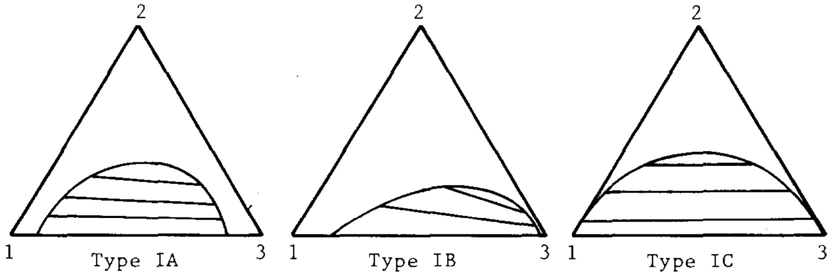

Fig. 1. Classification of ternary solubility envelopes.

ternary. Table 1 gives LLE and VLE data sources for the seven ternary systems, which are arbitrarily classified into three types. Figure 1 shows schematically these three types: type IA, with a binary solubility gap in the range 0.05–0.95 mole fraction; type IB, with a solubility gap whose one point remains within the afore-mentioned range and the other point outside this composition range; type IC, with a large solubility gap outside the same range. Two local composition equations, LEMF and extended UNIQUAC [8], are used to obtain the proper binary parameters in evaluating binary parameters from ternary LLE data, since several sets of binary parameters could be obtained from different objective functions in the regression procedure.

ACTIVITY COEFFICIENT EQUATIONS

The LEMF equation gives the activity coefficient of any component in a multicomponent system by

$$\ln \gamma_i = \frac{\sum_j \tau_{ji} G_{ji} x_j}{\sum_k G_{ki} x_k} + \sum_j \frac{x_j G_{ij}}{\sum_k G_{kj} x_k} \left[\tau_{ij} - \frac{\sum_r x_r \tau_{rj} G_{rj}}{\sum_k G_{kj} x_k} \right] \tag{1}$$

where x is the liquid-phase mole fraction. τ_{ji} and G_{ji} are related to the binary parameter a_{ji}:

$$\tau_{ji} = a_{ji}/T \tag{2}$$

$$G_{ji} = \exp(\tau_{ji}) \tag{3}$$

The extended UNIQUAC equation expresses $\ln \gamma_i$ by

$$\ln \gamma_i = \ln\left(\frac{\phi_i'}{x_i}\right) + 1 - \frac{\phi_i'}{x_i} - \left(\frac{Z}{2}\right) q_i \left[\ln\left(\frac{\phi_i}{\theta_i}\right) + 1 - \frac{\phi_i}{\theta_i}\right]$$

$$-q_i^* \ln\left(\sum_j \theta_j \tau_{ji}\right) + q_i \sum_j \left(\frac{q_j^*}{q_j}\right) \theta_j - q_i \sum_j \frac{(q_j^*/q_j)\theta_j \tau_{ij}}{\sum_k \theta_k \tau_{kj}} \tag{4}$$

where Z is the coordination number (taken as 10). ϕ', ϕ, θ and τ are expressed by

$$\phi_i' = x_i r_i^{2/3} / \sum_j x_j r_j^{2/3} \tag{5}$$

$$\phi_i = x_i r_i / \sum_j x_j r_j \tag{6}$$

$$\theta_i = x_i q_i / \sum_j x_j q_j \tag{7}$$

$$\tau_{ji} = \exp(-a_{ji}/T) \tag{8}$$

r, q and q^* are the pure-component molecular constants. The values of r and q were taken from Prausnitz et al. [9], and those of q^* were empirically taken as follows: 0.96 for water; 0.95 for methanol; 0.92 for ethanol; 0.89 for propanols; 0.88 for butanols; $q^* = q^{0.1}$ for other components studied in this work [8].

COMPUTATIONAL PROCEDURE

All experimental ternary tie lines were checked by use of Hand's plot [10] and Othmer-Tobias's plot [11]. Tie lines deviating greatly from these plots were rejected. Various objective functions have been proposed for the evaluation of the binary parameters from the ternary LLE data. We used the following three objective functions as described in the supplement to ref. 12 (eqn. (9) in terms of activities; eqns. (10) and (11) in terms of mole fractions):

$$F_1 = \sum_k \sum_i \left[\frac{a_{ik}^{\mathrm{I}} - a_{ik}^{\mathrm{II}}}{a_{ik}^{\mathrm{I}} + a_{ik}^{\mathrm{II}}} \right]^2 + Q \sum_n P_n^2 \qquad (9)$$

where $i = 1, 2, \ldots\ N$ (components), $k = 1, 2, \ldots\ M$ (tie lines), P_n = parameter value in Kelvin, a_{ik}^{I} = activity given by $x_{ik}^{\mathrm{I}} \gamma_{ik}^{\mathrm{I}}$, x_{ik}^{I} is the experimental mole fraction of component i in phase I at tie line k. The calculated activity coefficients depend on the experimental mole fractions and the parameters. Q is a penalty factor set as 10^{-6}.

$$F_2 = \sum_k \min \sum_i \sum_j \left[x_{ijk} - \hat{x}_{ijk} \right]^2 + Q \sum_n P_n^2 \qquad (10)$$

where $i = 1, 2\ \ldots,\ N$ (components), $j = \mathrm{I}, \mathrm{II}$ (phases), $k = 1, 2, \ldots, M$ (tie lines), x_{ijk} is the mole fraction of component i in phase j at tie line k. The calculated mole fractions $\hat{x}_{ijk}$ depend on the parameters. Q is taken as 10^{-10} in eqns. (10) and (11).

$$F_3 = \sum_k \min \sum_i \sum_j \left[x_{ijk} - \hat{x}_{ijk} \right]^2 + Q \sum_n P_n^2 + \left[\ln \left(\frac{a_{2,\infty}^{\mathrm{I}}}{a_{2,\infty}^{\mathrm{II}}} K_{\mathrm{D}2,\infty} \right) \right]^2 \qquad (11)$$

∞ = infinite dilution

$K_{\mathrm{D}2,\infty}$ = calculated limiting distribution coefficient defined by

$$\lim_{\substack{x^{\mathrm{I}} \to 0 \\ x^{\mathrm{II}} \to 0}} K_{\mathrm{D}2}, \text{ where } K_{\mathrm{D}2} = x_2^{\mathrm{I}} / x_2^{\mathrm{II}} = \gamma_2^{\mathrm{II}} / \gamma_2^{\mathrm{I}} \qquad (12)$$

$a_{2,\infty}^{\mathrm{I}} / a_{2,\infty}^{\mathrm{II}}$ is calculated using the parameters evaluated from objective function (9) and $K_{\mathrm{D}2,\infty}$ is derived from the parameters obtained by objective function (11).

Both the extended UNIQUAC and LEMF equations have two binary parameters per binary mixture. For a ternary mixture these equations have generally six parameters. This means that we may fit a total of six binary parameters of the extended UNIQUAC (or LEMF) equation to a set of ternary LLE data. For a type I mixture, we can prefix the two parameters obtained from the mutual solubility data for the partially miscible system and then we may determine the remaining four parameters. Five methods were used to evaluate which method gives the most acceptable parameters to predict ternary or binary VLE: method I, objective function (9) and four parameters; method II, objective function (9) and six parameters; method III, objective function (10) and four parameters; method IV, objective function (10) and six parameters; method V, objective function (11) and six parameters. Our experiences showed that objective function (9) gave a set of similar parameters, regardless of the various starting values and, in the other methods, the initial estimates of the binary parameters lead to many sets of the final parameters obtained in regression. The parameters derived from objective function (9) are not always the suitable starting parameters for methods III–V. In such cases the binary parameters for the two completely miscible binaries, 1–2 and 2–3, are estimated from the UNIFAC method [22,23] whenever the pertinent interaction parameters are available. The estimated UNIFAC binary parameters can be converted to the corresponding extended UNIQUAC or LEMF parameters as the starting values in regression using the infinite dilution activity coefficients only [24]. The initial values of the partially miscible binary 1–3 are the parameters obtained from the binary mutual solubilities.

RESULTS AND DISCUSSION

Table 2 shows predicted results of ternary and binary VLE obtained by use of the extended UNIQUAC equation with either four or six binary parameters derived from the correlation of ternary LLE data, indicating that one may use six binary parameters for correlating ternary LLE data in order to obtain a better prediction of ternary or binary VLE and method V gives much more reasonable parameters than method I does whenever the convergence is obtained. VLE calculations included vapor-phase non-ideality. The fugacity coefficients were calculated by use of the volume-explicit virial equation of state, truncated after the second virial coefficients. The second virial coefficients were estimated from the correlation of Hayden and O'Connell [27] with the related parameters tabulated by Prausnitz et al. [9]. The Poynting correction was taken into account using pure-liquid molar volumes calculated by the modified Rackett equation [28]. Pure-component vapor pressures were calculated from the Antoine equation whose constants were taken from the literature [29–31]. Table 3 gives the extended UN-

TABLE 2

Prediction of ternary or binary vapor–liquid equilibrium obtained from the extended UNIQUAC equation

System	Temp. (°C)		Absolute arithmetic mean deviations					Ref.
			I [a]	II [b]	III [c]	IV [d]	V [e]	
Acetonitrile(1)– benzene(2)– *n*-heptane(3)	45	Δy_1 [f]	0.0391	0.0355	0.0216	0.0183	0.0079	13
		Δy_2	0.0361	0.0173	0.0269	0.0219	0.0041	
		Δy_3	0.0160	0.0270	0.0098	0.0093	0.0070	
		ΔP(kPa)	5.720	4.093	4.106	3.493	0.973	
Water(1)– ethanol(2)– ethyl acetate(3)	70	Δy_1	0.0181	0.0278	0.0998	0.1090	0.0152	20
		Δy_2	0.0432	0.0390	0.1242	0.1344	0.0144	
		Δy_3	0.0416	0.0511	0.1006	0.1142	0.0073	
		ΔP(kPa)	11.519	13.906	38.544	41.770	3.040	
Benzene(1)– ethanol(2)– water(3)	25	Binary 1–2						25
		Δy_1	0.0546	0.0476	0.0070	0.0063		
		ΔP(kPa)	1.627	1.533	0.173	0.160		
	25	Binary 2–3						26
		Δy_1	0.0750	0.0533	0.0090	0.0115		
		ΔP(kPa)	0.907	0.627	0.093	0.093		

[a] I = method I whose objective function is eqn. (9) and four parameters are estimated.

[b] II = method I whose objective function is eqn. (9) and six parameters are estimated.

[c] III = method III whose objective function is eqn. (10) and four parameters are estimated.

[d] IV = method IV whose objective function is eqn. (10) and six parameters are estimated.

[e] V = method V whose objective function is eqn. (11) and six parameters are estimated.

[f] Δy_1 = deviation in vapor-phase mole fraction given by $\Delta y_1 = \Sigma_i^N |y_{1_i}(\text{exp}) - y_{1_i}(\text{calc})|/N$. ΔP = deviation in pressure given by $\Delta P = \Sigma_i^N |P_i(\text{exp}) - P_i(\text{calc})|/N$.

TABLE 3

Binary parameters obtained in fitting the extended UNIQUAC equation to ternary liquid–liquid equilibria

System	Temp. (°C)	Prefixed parameters for binary 1–3 (K)			Parameters for binaries 1–2 and 2–3 (K)			
		a_{13}	a_{31}		a_{12}	a_{21}	a_{23}	a_{32}
Acetonitrile(1)– benzene(2)– sulfur dioxide(3)	45	330.96	974.93	I [a]	9.95	80.44	6.10	6.74
				III [b]	−127.37	282.57	9.82	−25.18
Water(1)– ethanol(2)– ethyl acetate(3)	70	307.92	421.38	I	−10.34	−30.09	−0.73	23.11
				III	−61.58	−343.42	−4.43	−737.49
Benzene(1)– ethanol(2)– water(3)	25	1238.8	352.43	I	175.13	285.51	23.60	−180.53
				III	828.05	63.09	62.30	66.13

[a] I = method I.

[b] III = method III.

IQUAC parameters obtained with methods I and III. Table 4 presents predicted results of ternary or binary VLE obtained from the extended UNIQUAC and LEMF equations with six parameters, which are listed in Table 5. For the extended UNIQUAC equation, method IV is better than method II for the four systems, except for the water–methanol–ethyl acetate and water–ethanol–ethyl acetate systems. However, method V gives much improved results for these two systems and the acetonitrile–benzene–*n*-heptane system. Only method II gives a set of the acceptable parameters for

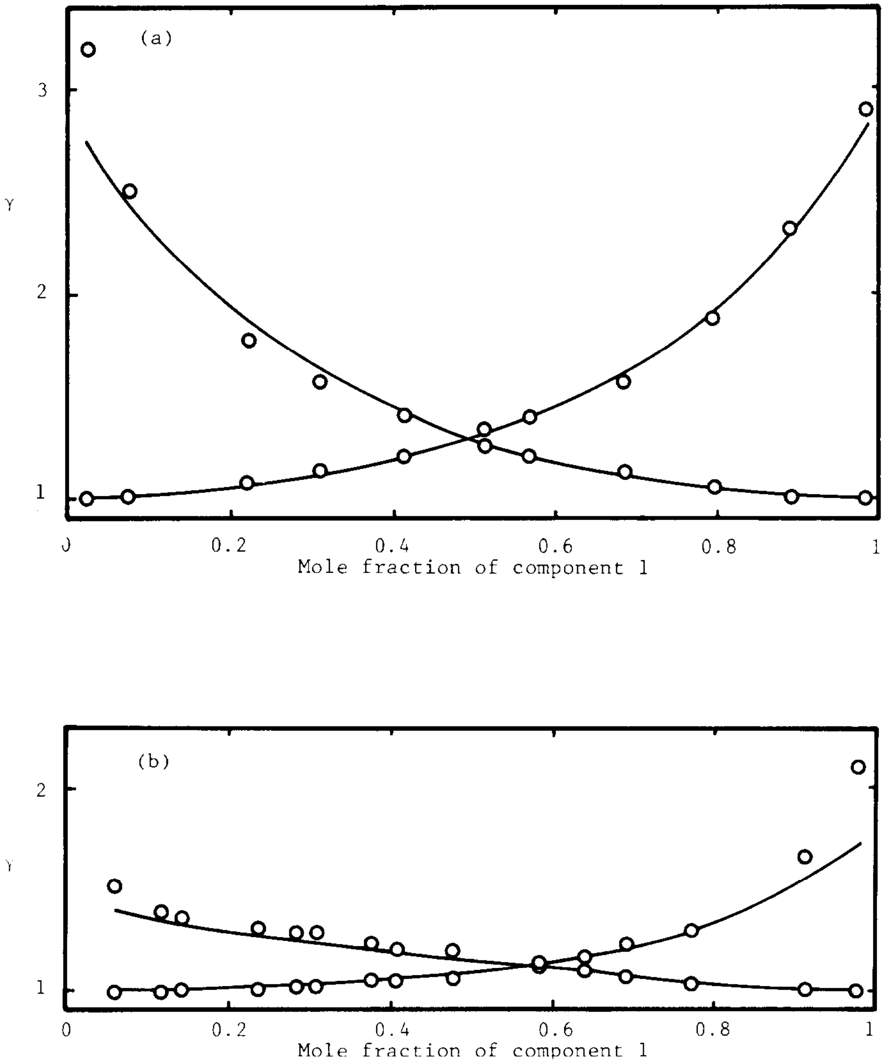

Fig. 2. Predicted activity coefficients obtained from the extended UNIQUAC equation with method V for (a) acetonitrile(1)–benzene(2) and (b) benzene(1)–*n*-heptane(2) at 45 °C. Experimental (○), ref. 13; calculated (———).

TABLE 4

Prediction of ternary or binary vapor–liquid equilibrium obtained from the extended UNIQUAC and LEMF equations by use of six parameters

System	Temp. (°C)		Absolute arithmetic mean deviations						Ref.
			II [a]		IV [b]		V [c]		
			A [d]	B [e]	A	B	A	B	
Acetonitrile(1)–	45	Δy_1	0.0355	0.0282	0.0183	0.0335	0.0079	0.0203	13
benzene(2)–		Δy_2	0.0173	0.0339	0.0219	0.0401	0.0041	0.0232	
n-heptane(3)		Δy_3	0.0270	0.0091	0.0093	0.0098	0.0070	0.0075	
		ΔP(kPa)	4.093	5.000	3.493	5.533	0.973	3.440	
n-Pentane(1)–	−17.8	Δy_1	0.0122	0.0248	0.0042	0.0067	0.0041	0.0054	14
benzene(2)–		Δy_2	0.0009	0.0027	0.0011	0.0054	0.0011	0.0041	
sulfur dioxide(3)		Δy_3	0.0131	0.0274	0.0048	0.0048	0.0047	0.0046	
		ΔP(kPa)	3.506	1.427	1.987	1.960	1.933	1.587	
Water(1)–	88–100	Δy_1	0.0207	0.0167					15
1-butanol(2)–		Δy_2	0.0299	0.0084					
1-propanol(3)		Δy_3	0.0094	0.0246					
		ΔP(kPa)	5.306	1.080					
Water(1)–	68–74	Δy_1	0.0199	0.0209	0.0427	0.0280	0.0139	0.0213	16
methanol(2)–		Δy_2	0.0327	0.0430	0.1364	0.0940	0.0205	0.0655	
ethyl acetate(3)		Δy_3	0.0389	0.0370	0.1083	0.0838	0.0252	0.0581	
		ΔP(kPa)	14.066	14.852	38.543	28.984	16.959	19.945	

Water(1)– ethanol(2)– ethyl acetate(3)	70	Δy_1	0.0278	0.0233	0.1090	0.0184	0.0152	0.0193	20
		Δy_2	0.0390	0.0417	0.1344	0.0258	0.0144	0.0241	
		Δy_3	0.0511	0.0504	0.1142	0.0218	0.0073	0.0173	
		ΔP(kPa)	13.906	12.839	41.770	3.733	3.040	3.706	
Benzene(1)– ethanol(2)– water(3)	25	Binary 1–2							25
		Δy_1	0.0479	0.0309	0.0063	0.0449			
		ΔP(kPa)	1.533	1.240	0.160	1.613			
	25	Binary 2–3							26
		Δy_1	0.0533	0.0250	0.0115	0.0452			
		ΔP(kPa)	0.627	0.280	0.093	0.493			
Benzene(1)– 1-propanol(2)– water(3)	30	Δy_1	0.0647	0.0661	0.0407	0.0694			21
		Δy_2	0.0420	0.0385	0.0333	0.0376			
		Δy_2	0.0310	0.0371	0.0345	0.0370			
		ΔP(kPa)	2.586	2.253	1.920	2.133			

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[a] II = method II.

[b] IV = method IV.

[c] V = method V.

[d] A = extended UNIQUAC equation.

[e] B = LEMF equation.

TABLE 5

Binary parameters obtained in fitting the extended UNIQUAC and LEMF equations to ternary liquid–liquid equilibria by use of six parameters

System	Method	Eqn.	Parameters (K)					
			a_{12}	a_{21}	a_{13}	a_{31}	a_{23}	a_{32}
Acetonitrile(1)–	II	1 [a]	32.78	189.60	412.32	586.36	22.72	16.21
benzene(2)–		2 [b]	68.00	63.69	273.19	308.34	−41.60	−56.44
n-heptane(3)	IV	1	−105.93	294.03	344.85	967.31	−39.65	25.40
		2	19.59	86.47	281.15	310.21	−22.45	−104.18
	V	1	4.15	281.22	323.82	985.80	3.45	84.66
		2	100.02	89.49	280.73	310.96	−45.51	23.32
n-Pentane(1)–	II	1	76.81	46.41	466.68	407.35	18.22	−11.29
benzene(2)–		2	20.67	15.37	254.36	185.18	−9.84	−20.06
sulfur dioxide(3)	IV	1	73.77	106.74	636.47	420.19	3.43	−28.75
		2	324.34	76.79	256.60	204.26	147.89	116.64
	V	1	77.23	106.96	636.58	420.14	3.26	−24.76
		2	293.02	86.29	256.71	203.99	141.26	92.42
Water(1)–	II	1	−58.55	−54.95	327.06	222.83	77.84	65.15
methanol(2)–		2	−6.66	42.69	131.52	404.32	13.08	10.37
ethyl acetate(3)	IV	1	110.10	−554.85	500.91	373.61	−446.63	−36.57
		2	−316.44	359.10	211.38	426.14	328.20	221.54
	V	1	368.94	−226.60	148.86	452.35	−310.45	636.81
		2	−61.36	286.01	210.54	420.05	256.50	244.76
Water(1)–	II	1	1.23	8.91	340.33	225.41	8.34	2.34
ethanol(2)–		2	38.54	195.42	137.43	407.68	−25.89	−33.54
ethyl acetate(3)	IV	1	−13.27	−438.09	395.41	471.89	−252.45	−709.18
		2	−470.78	336.16	281.30	406.46	358.63	−699.22
	V	1	535.76	−146.56	89.67	488.04	−59.81	423.58
		2	−471.03	333.21	259.13	408.93	343.07	−701.43
Benzene(1)–	II	1	240.29	212.28	761.94	729.54	75.89	−153.93
ethanol(2)–		2	57.74	261.93	478.12	338.57	254.17	−54.84
water(3)	IV	1	871.32	56.61	1600.3	371.85	4.72	162.30
		2	166.71	164.78	412.21	326.98	170.03	−2.81
Benzene(1)–	II	1	135.44	111.38	653.36	583.55	145.96	15.26
1-propanol(2)–		2	48.23	216.40	446.31	356.19	293.33	33.23
water(3)	IV	1	668.02	−0.30	1534.6	573.03	−19.33	386.48
		2	62.31	200.50	458.82	348.50	286.54	68.57
Water(1)–	II	1	307.95	122.71	136.15	72.10	−74.73	−84.27
1-butanol(2)–		2	45.45	416.50	28.76	351.47	−21.76	−20.08
1-propanol(3)								

[a] 1 = extended UNIQUAC equation.

[b] 2 = LEMF equation.

TABLE 6

Prediction of binary vapor–liquid equilibrium obtained from the extended UNIQUAC and LEMF equations by use of the best parameters

Ternary system	Binary system (1–2)	Temp. (°C)	No. of data points	Absolute arithmetic mean deviations				Ref.
				$\Delta y_1(\times 10^3)$		ΔP (kPa)		
				I [a]	II [b]	I	II	
1	Acetonitrile–benzene	45	11	7.1	23.0	0.107	2.373	13
	Benzene–*n*-heptane	45	15	6.0	40.7	0.253	2.466	13
2	*n*-Pentane–benzene	−17.8	18	5.6	31.1	0.160	0.587	14
	Benzene–sulfur dioxide	−17.8	19	0.9	2.5	2.800	5.053	14
3	1-Butanol–1-propanol	100–115	6	30.3	11.0	7.666	2.013	32
	1-Propanol–water	90	12	28.8	14.7	7.093	3.146	33
4	Ethyl acetate–ethanol	70	15	6.8	24.7	0.640	3.053	20
	Ethanol–water	70	13	19.8	34.0	3.280	5.520	20
5	Ethyl acetate–methanol	62.1–74.8	19	26.5	100.1	6.586	28.638	16
	Methanol–water	65	10	4.5	56.5	0.787	7.013	34
6	Benzene–ethanol	25	11	6.3	45.0	0.160	1.613	25
	Ethanol–water	25	10	11.5	45.2	0.093	0.507	26
7	Benzene–1-propanol	45	11	22.0	31.3	1.755	2.028	35
	1-Propanol–water	90	12	32.2	14.0	1.320	0.867	33

[a] I = extended UNIQUAC equation.

[b] II = LEMF equation.

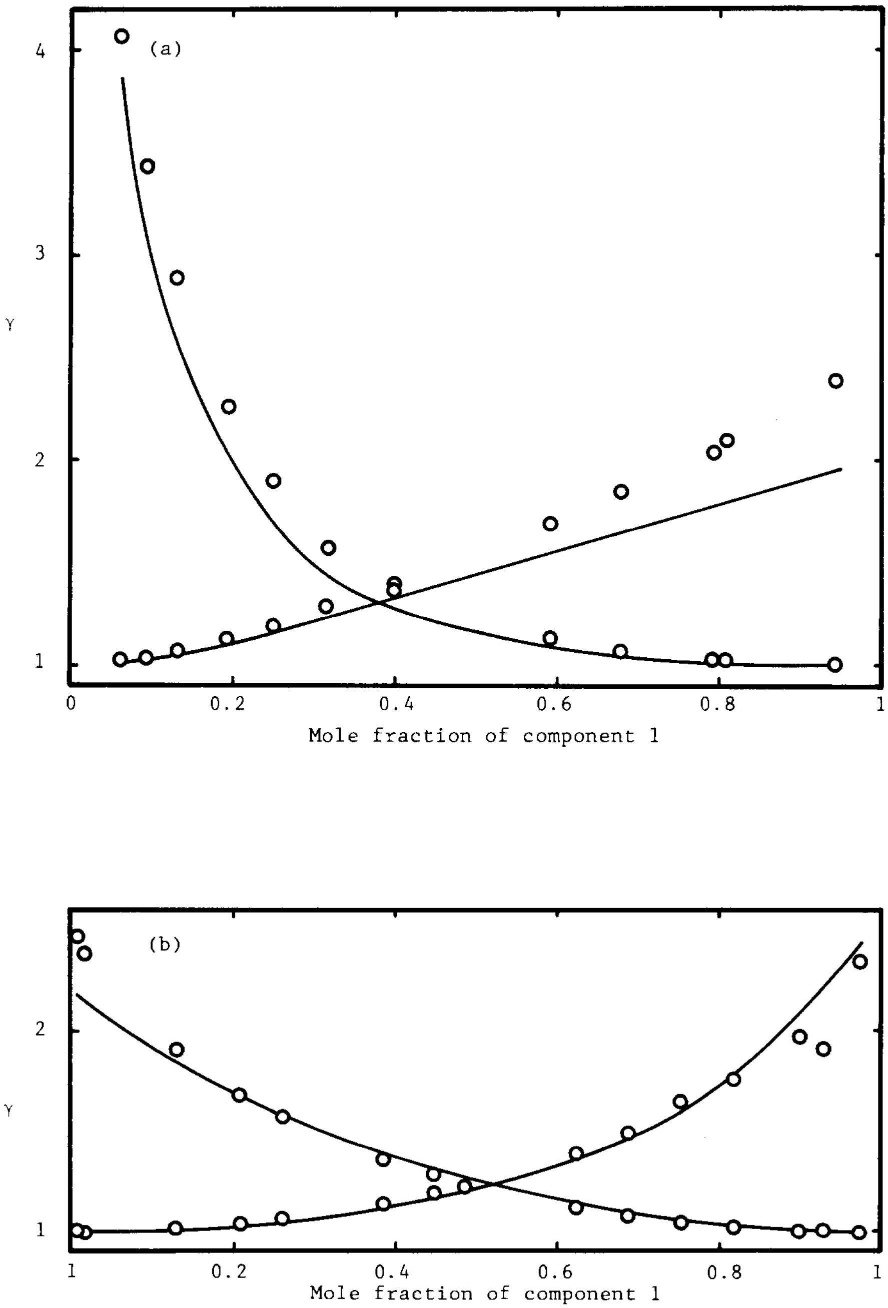

Fig. 3. Predicted activity coefficients obtained from the extended UNIQUAC equation with method V for (a) ethanol(1)–water(2) and (b) ethyl acetate(1)–ethanol(2) at 70°C. Experimental (○), ref. 20; calculated (———).

the water–1-butanol–1-propanol system and the other methods did not work, probably because the solubility envelope for this system is too small to evaluate six parameters. For the benzene–ethanol–water and benzene–1-propanol–water systems method II provided too erroneous values of the calculated limiting distribution coefficients $K_{D2,\infty}$, so that method V was not applied for these two systems and method IV is recommended for use. For the LEMF equation, method II sometimes gives better results than the other methods as shown in the water–methanol–ethyl acetate and benzene–ethanol–water systems. The best results obtained from the extended UNIQUAC equation are better than those from the LEMF equation if the water–1-butanol–1-propanol system is excluded. The parameters which best predicted ternary VLE were used to predict binary VLE for the two completely miscible systems constituting each ternary system. Table 6 shows that the extended UNIQUAC equation provides smaller deviations in vapor-phase mole fraction and pressure than the LEMF equation does, except for the 1-butanol–1-propanol and 1-propanol–water systems. Figures 2 and 3 compare the calculated values with the experimental results of the activity coefficients for four systems.

CONCLUSIONS

Ternary VLE predictions are reasonable when made with the extended UNIQUAC and LEMF equations, whose parameters are obtained by using the LLE data. VLE predictions for the completely miscible binary systems are of a similar accuracy as those for the ternary systems. The extended UNIQUAC equation gives somewhat better results in binary and ternary VLE predictions than the LEMF equation does.

NOMENCLATURE

a	activity
a_{ij}	extended UNIQUAC or LEMF parameter
F	objective function
G_{ij}	coefficient defined by eqn. (3)
K_{D2}	distribution coefficient defined by x_2^{I}/x_2^{II}
P_n	parameter value
Q	penalty factor
q, q^*	pure-component surface parameters in the extended UNIQUAC equation
R	universal gas constant
r	pure-component size parameter in the extended UNIQUAC equation

T	absolute temperature
x	liquid-phase mole fraction
Z	liquid-phase coordination number, taken as 10

Greek letters

γ	activity coefficient
ϕ	segment fraction
θ	surface fraction
τ	coefficient related to binary parameter defined by eqn. (2) or (8)

Superscripts

I, II	phases
E	excess

Subscripts

1, 2, 3	components
i, j	components
j	phase
k	tie line
∞	infinite dilution

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