740 *J. Chem. Eng. Data* **2002,** *47,* 740−747

Vapor−Liquid Equilibrium Measurements for Three Binary Mixtures: Allyl Alcohol/Acetonitrile, 2-Butoxyethanol/Acetic Acid, and 1-Methoxy-2-Propanol/2,3-Epoxy-1-Propanol

W. Vincent Wilding,* Karen L. Adams, Alexander E. Carmichael, Jeffery B. Hull, Thomas C. Jarman, and Tonya L. Marshall

Department of Chemical Engineering, Brigham Young University, Provo, Utah 84602

Vapor−liquid equilibrium measurements using the *PTx* method have been made on three binary mixtures: allyl alcohol/acetonitrile, 2-butoxyethanol/acetic acid, and 1-methoxy-2-propanol/2,3-epoxy-1-propanol. Each binary mixture was studied at two temperatures. Equilibrium vapor- and liquid-phase compositions were derived from the *PTx* data using the Soave−Redlich−Kwong equation of state to represent the vapor phase and the NRTL activity coefficient model to represent the liquid phase.

Introduction

Experimental vapor−liquid equilibrium data are essential to process design and optimization. These measurements, sponsored by the Design Institute for Physical Property Data (DIPPR) of the American Institute of Chemical Engineers (AIChE), provide accurate binary vapor−liquid equilibrium data on systems of industrial importance. Each system was studied at two temperatures to determine the temperature dependence of the activity coefficient model. The data are also useful for determining parameters for group contribution correlations. Table 1 shows the systems studied and the temperatures at which they were studied.

Table 1. Experimental Systems and Temperatures

system	isotherm, °C
1. allyl alcohol/acetonitrile	40, 80
2. 2-butoxyethanol/acetic acid	50, 100
3. 1-methoxy-2-propanol/2,3-epoxy-1-propanol	70, 120

Table 2. Sources and Purities of Chemicals

substance	source	purity, %
allyl alcohol	Aldrich	99.9+
acetonitrile	Mallinckrodt	99.90
2-butoxyethanol	Aldrich	99+
acetic acid	Aldrich	99.70
1-methoxy-2-propanol	Aldrich	99.70
2,3-epoxy-1-propanol	Aldrich	98.60

Experimental Section

Chemicals. The sources and purities of the chemicals used in the measurements are given in Table 2.

The purities listed here are obtained from lot analyses performed by the manufacturer. The chemicals were degassed to remove any dissolved light contaminants. Degassing was performed by boiling off and discarding approximately 10% of the chemical. No further purification of these chemicals was performed.

Experimental Apparatus. An isothermal, binary *PTx* experiment consists of measuring the total pressure as a function of composition. Measurements can be made across the entire composition range. By using an equation of state for vapor fugacity coefficients and an activity model for liquid-phase activity coefficients, the *PTx* data can be used to determine equilibrium phase compositions. Measurements were made at two temperatures to determine the temperature dependence of the activity coefficients.

The apparatus used for the *PTx* measurements is shown in Figure 1. The cell is made of thick-walled Pyrex with a Teflon cap and has an internal volume of approximately 300 cm^3. The cap screws into the cell and forms a seal with an O-ring. Small-bore tubing connected through the cap permits adding components and degassing. A thermowell, into which a platinum resistance thermometer is inserted, also extends into the cell.

The platinum thermometer was calibrated using ice and steam points and was referenced to a NIST traceable standard. Temperatures in this apparatus were measured with an accuracy of ±0.1 K. During the course of a run, the temperature was held constant to within ±0.05 K with the use of a temperature controller.

The pressures were measured with a mercury manometer, which extends into the side of the cell. The manometer is connected to a McLeod gauge for cell pressures below about 50 kPa or is open to room pressure for higher pressures. The mercury levels in the cell manometer were read by using a cathetometer with an accuracy of ±0.05 kPa. Atmospheric pressure was measured with a barometer located adjacent to the experimental apparatus. Measured pressures were corrected for the temperature dependence of the density of mercury and for the vapor pressure of mercury.

Experimental Procedure. In a *PTx* experiment, the entire composition range was traversed at each temperature. This required at least two runs. To initiate the first run, the cell was charged with a known amount of one component. The cell contents were then degassed by removing vapor into a weighed, evacuated cell or a weighed syringe fitted with a valve. On the order of 1% of the cell charge was removed in a degas sample. The cell contents

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* E-mail: wildingv@byu.edu. Fax: (801) 378-7799.

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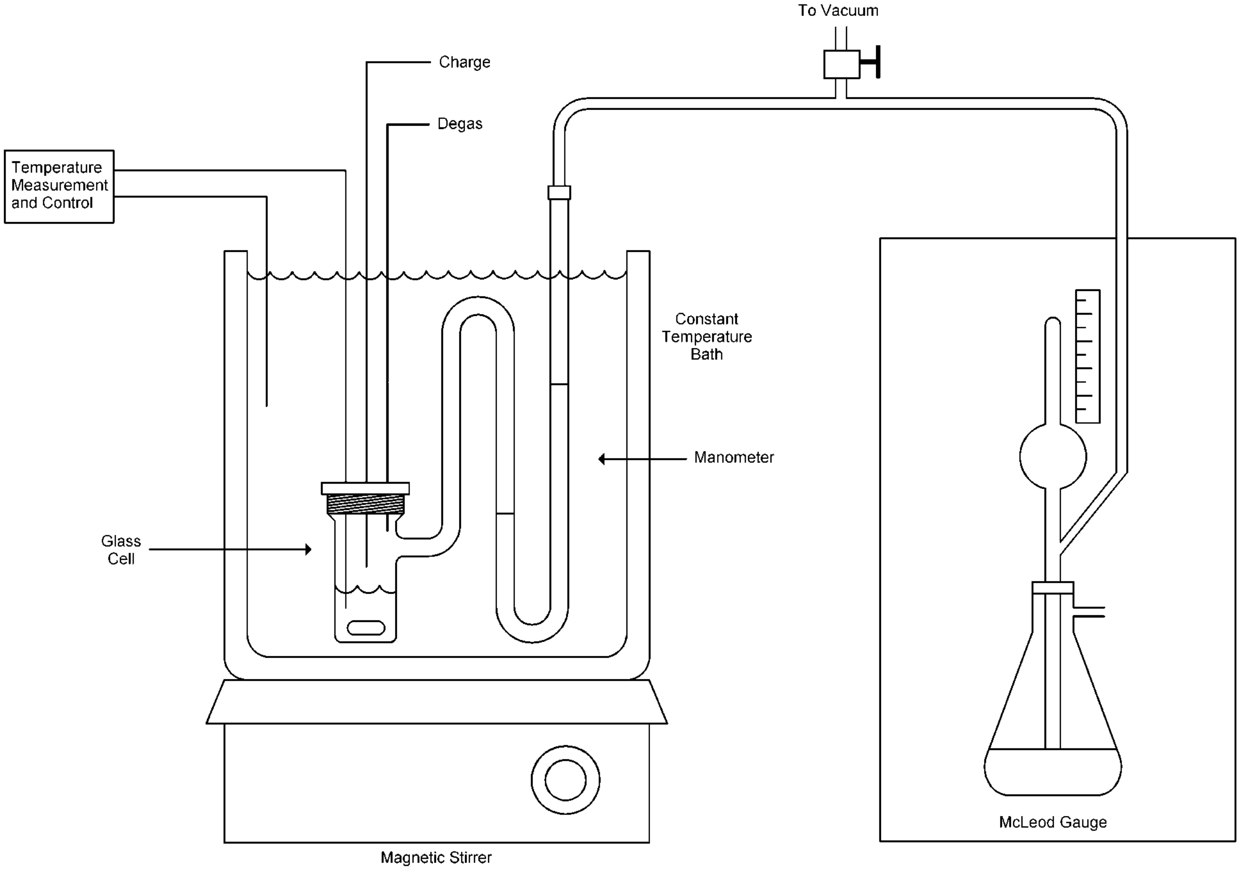

Figure 1. Glass *PTx* apparatus.

Table 3. Vapor Pressure Comparison

		vapor pressure/kPa		% deviation
compound	t/°C	meas	DIPPR 801	100(meas − lit.)/meas
allyl alcohol	40	7.81	7.99	−2.30
	80	52.33	52.53	−0.38
acetonitrile	40	22.83	23.14	−1.36
	80	96.24	96.74	−0.52
2-butoxyethanol	50	0.63	0.719	−14.1
	100	8.53	9.119	−6.91
acetic acid	50	7.67	7.58	1.17
	100	56.67	56.56	0.19
1-methoxy-2-propanol	70	15.86	15.85	0.063
	120	101.0	100.07	0.92
2,3-epoxy-1-propanol	70	2.95	2.76	6.44
	120	25.21	25.56	−1.39

were stirred with the magnetic stirrer until equilibrium was attained, and the pure-component vapor pressure was measured. The cell contents were again degassed and the pressure measured. This process was repeated until the vapor pressure no longer changed upon further degassing. Two or three degasses were generally sufficient. The measured pressure is thus an accurate pure-component vapor pressure.

After the pure-component vapor pressure was measured, increments of the second component were then charged to the cell. After each increment, the cell contents were again degassed and allowed to equilibrate before the pressure was measured. Increments of the second component were added until over half of the composition range was traversed. The cell was then emptied and cleaned in preparation for the second run.

The second run was similar to the first except that the second component was charged to the cell before adding increments of the first component. The ranges of compositions covered in the runs were designed to overlap in the midcomposition range to check for consistency between the runs.

Data Reduction Procedure. The *PTx* measurements result in data for total pressure as a function of charge composition at constant temperature. Using these values, equilibrium phase compositions and activity and fugacity coefficients were then calculated, with the Soave−Redlich−Kwong equation[1] of state representing the vapor phase and the NRTL activity coefficient model[2] representing the liquid phase. The SRK equation binary interaction parameters were assumed to be zero. The pure-component critical constants and densities were taken from the DIPPR 801 database.[3]

To derive equilibrium phase compositions from *PTx* data, an iterative process was used to solve the fundamental equation of vapor−liquid equilibrium,

$$y_i\phi_i P = x_i\gamma_i P_i^{\circ}\phi_i^{\circ}\exp\left[\left(\frac{\bar{V}_i}{RT}\right)(P - P_i^{\circ})\right] \qquad (1)$$

where y_i is the vapor mole fraction of component i, ϕ_i is the fugacity coefficient of component i in the vapor phase, P is the total pressure, x_i is the liquid mole fraction of component i, γ_i is the activity coefficient of component i, P_i° is the vapor pressure of component i at the system temperature, ϕ_i° is the fugacity coefficient of pure component i at the system temperature and corresponding vapor pressure of pure i, and the exponential term is the Poynting correction in which $\bar{V}_i$ is the liquid molar volume of component i. This volume is calculated using pure-component density data adjusted to the temperature of the measurements using the Rackett equation.

Table 4. Results of Vapor−Liquid Equilibrium Measurements by the *PTx* Method for the Allyl Alcohol (A)/Acetonitrile (B) System at 40 °C[a]

	mol % A			pressure/kPa		activity coefficient		fugacity coefficient		relative volatility
run no.	charge	liquid	vapor	meas	calc	*A*	*B*	*A*	*B*	*B*/*A*
1	100.00	100.00	100.00	7.81	7.81	1.000	2.290	0.997	0.997	6.701
1	97.39	97.40	85.42	8.95	8.92	1.001	2.186	0.997	0.997	6.394
1	94.11	94.13	72.67	10.21	10.16	1.003	2.067	0.996	0.996	6.030
1	88.09	88.13	57.79	12.10	12.08	1.013	1.876	0.995	0.995	5.423
1	78.07	78.11	43.89	14.44	14.53	1.043	1.625	0.995	0.994	4.561
1	68.04	68.08	35.62	16.24	16.34	1.091	1.437	0.994	0.994	3.854
1	58.33	58.37	29.89	17.69	17.71	1.156	1.299	0.993	0.993	3.288
2	51.76	51.78	26.62	18.54	18.50	1.212	1.226	0.993	0.993	2.959
1	48.59	48.61	25.15	18.96	18.85	1.243	1.196	0.993	0.993	2.815
2	42.12	42.14	22.25	19.56	19.53	1.314	1.142	0.993	0.993	2.544
1	38.08	38.10	20.47	19.93	19.92	1.363	1.114	0.993	0.992	2.391
2	31.34	31.36	17.47	20.58	20.55	1.458	1.075	0.992	0.992	2.158
2	20.68	20.69	12.41	21.52	21.47	1.639	1.031	0.992	0.992	1.841
2	10.30	10.30	6.76	22.30	22.29	1.862	1.008	0.992	0.991	1.584
2	4.95	4.95	3.43	22.61	22.68	1.998	1.002	0.992	0.991	1.467
2	2.62	2.62	1.86	22.67	22.84	2.063	1.000	0.991	0.991	1.420
2	0.00	0.00	0.00	23.00	23.00	2.139	1.000	0.991	0.991	1.368

[a] NRTL parameters: $\tau_{AB} = 0.6365$, $\tau_{BA} = 0.1998$, and $\alpha = 0.2$.

Table 5. Results of Vapor−Liquid Equilibrium Measurements by the *PTx* Method for the Allyl Alcohol (A)/Acetonitrile (B) System at 80 °C[a]

	mol % A			pressure/kPa		activity coefficient		fugacity coefficient		relative volatility
run no.	charge	liquid	vapor	meas	calc	*A*	*B*	*A*	*B*	*B*/*A*
1	100.00	100.00	100.00	52.33	52.33	1.000	1.819	0.986	0.986	3.303
1	97.28	97.34	91.97	54.95	55.46	1.000	1.760	0.985	0.985	3.193
1	95.01	95.10	86.22	58.06	57.90	1.002	1.713	0.985	0.984	3.105
1	85.47	85.68	68.44	66.86	66.63	1.013	1.540	0.983	0.982	2.760
1	65.15	65.36	46.66	79.25	79.48	1.076	1.278	0.979	0.978	2.157
2	62.93	62.96	44.78	80.61	80.62	1.087	1.255	0.979	0.978	2.096
1	57.55	57.73	40.93	82.86	82.93	1.114	1.209	0.978	0.977	1.971
2	54.26	54.30	38.56	84.47	84.31	1.134	1.182	0.978	0.977	1.893
1	46.95	47.07	33.82	86.85	86.94	1.182	1.133	0.977	0.976	1.741
2	44.24	44.29	32.05	88.25	87.85	1.202	1.116	0.977	0.976	1.686
1	36.79	36.86	27.38	90.12	90.07	1.264	1.079	0.976	0.975	1.549
2	31.90	31.94	24.26	90.94	91.37	1.311	1.058	0.976	0.975	1.465
2	21.58	21.60	17.43	93.67	93.67	1.427	1.026	0.975	0.974	1.305
2	11.18	11.19	9.77	95.41	95.34	1.570	1.007	0.975	0.974	1.164
2	5.91	5.91	5.41	95.98	95.89	1.654	1.002	0.975	0.974	1.100
2	2.74	2.74	2.59	96.17	96.12	1.709	1.000	0.975	0.974	1.063
2	0.00	0.00	0.00	96.24	96.24	1.760	1.000	0.975	0.974	1.032

[a] NRTL parameters: $\tau_{AB} = 0.4467$, $\tau_{BA} = 0.1567$, and $\alpha = 0.2$.

The data reduction procedure consists of fitting the pressure data to eq 1 across the entire composition range by adjusting the parameters of the activity coefficient model. The NRTL equation[2] was used in the data reduction procedure,

$$\ln(\gamma_1) = x_2^{\,2}\left[\frac{\tau_{21}G_{21}^{\;2}}{(x_1 + x_2G_{21})^2} + \frac{\tau_{21}G_{12}}{(x_2 + x_1G_{12})^2}\right]$$

$$\ln(\gamma_2) = x_1^{\,2}\left[\frac{\tau_{12}G_{12}^{\;2}}{(x_2 + x_1G_{12})^2} + \frac{\tau_{21}G_{21}}{(x_1 + x_2G_{21})^2}\right] \qquad (2)$$

$$G_{21} = \exp(-\alpha\tau_{21}) \qquad G_{12} = \exp(-\alpha\tau_{12})$$

where γ_1 and γ_2 are activity coefficients, x_1 and x_2 are component liquid mole fractions, and α, τ_{12}, and τ_{21} are experimentally determined parameters.

To begin the data reduction procedure, the ideal-solution parameters of the activity coefficient model are selected. Then, assuming the liquid composition is the same as the

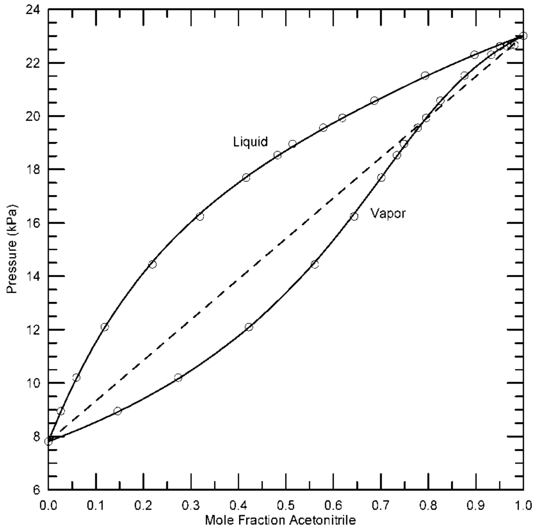

Figure 2. *PTx* results for the allyl alcohol/acetonitrile system at 40 °C.

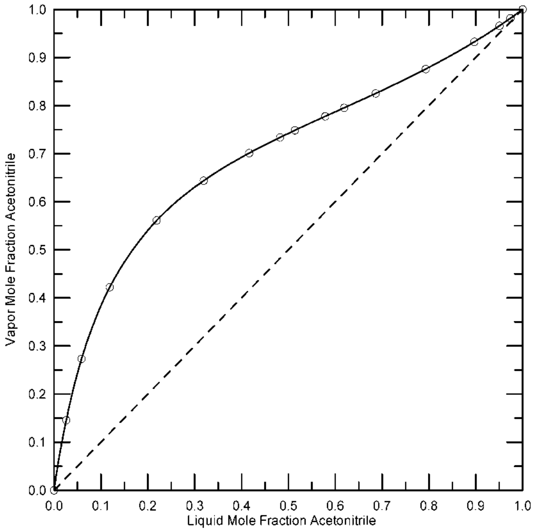

Figure 3. *y*−*x* plot for the allyl alcohol/acetonitrile system at 40 °C.

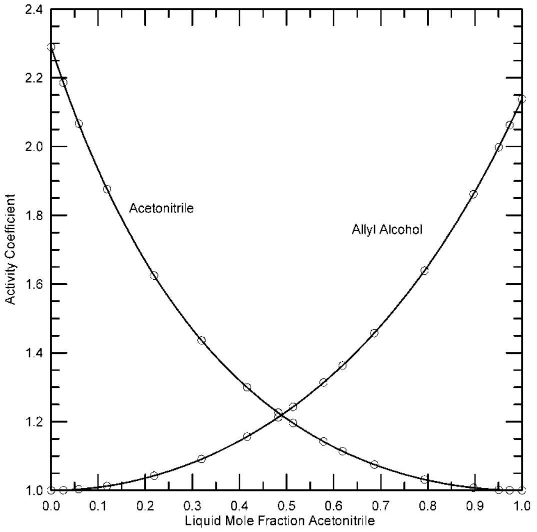

Figure 4. Activity coefficients for the allyl alcohol/acetonitrile system at 40 °C.

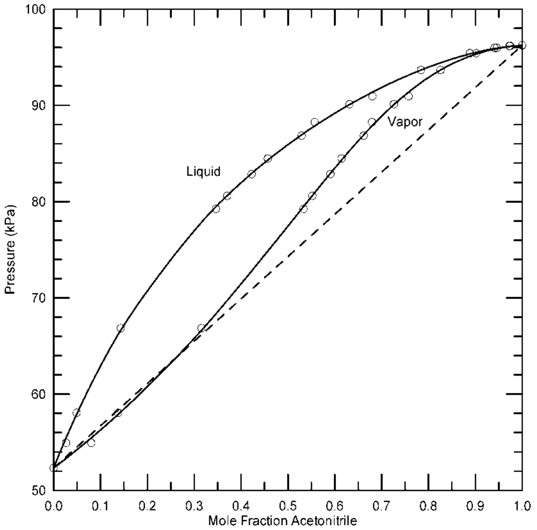

Figure 5. *PTx* results for the allyl alcohol/acetonitrile system at 80 °C.

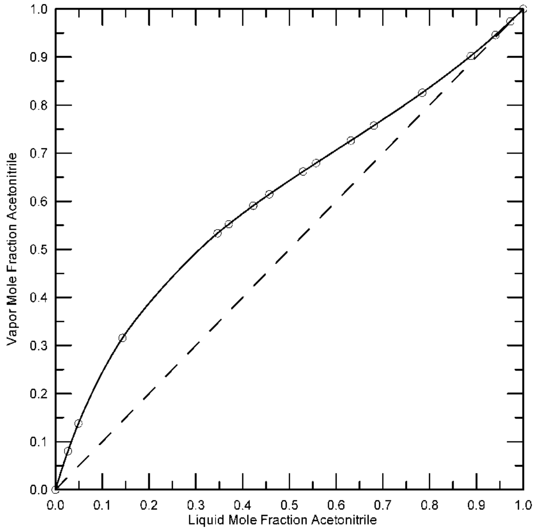

Figure 6. *y*−*x* plot for the allyl alcohol/acetonitrile system at 80 °C.

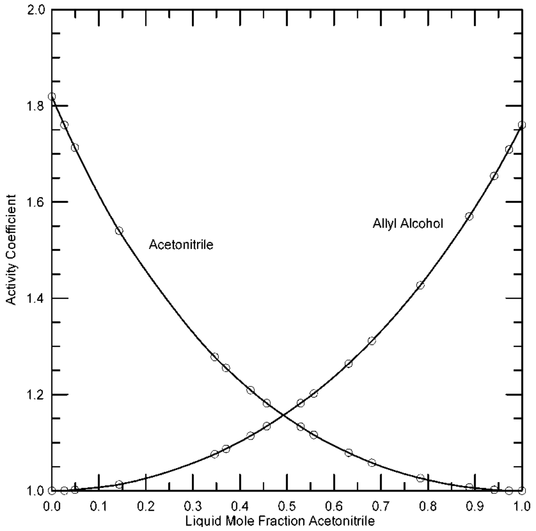

Figure 7. Activity coefficients for the allyl alcohol/acetonitrile system at 80 °C.

charge composition and the fugacity coefficients are unity, eq 1 is solved for the product Py_i for each component. The calculated pressure is then the sum of these products,

$$P_{\text{calc}} = \sum Py_i \tag{3}$$

The vapor mole fraction for each component is then determined from the relation

$$y_i = \frac{(Py_i)}{P_{\text{calc}}} \tag{4}$$

By using values for the vapor-phase composition, fugacity coefficients can be calculated from the equation of state.

The next step is to correct the liquid composition for the amount of each component in the vapor and to return to the step in which the activity coefficients were calculated and continue iterating until the calculated pressure converges. As part of each iteration step, the amount of material taken out of the cell degas is subtracted from the total charge at the calculated vapor composition.

This procedure is performed for each point across the composition range. The calculated pressures are compared

Table 6. Results of Vapor−Liquid Equilibrium Measurements by the *PTx* Method for the 2-Butoxyethanol (A)/Acetic Acid (B) System at 50 °C[a]

	mol % A			pressure/kPa		activity coefficient		fugacity coefficient		relative volatility
run no.	charge	liquid	vapor	meas	calc	*A*	*B*	*A*	*B*	*B*/*A*
2	100.00	100.00	100.00	0.631	0.631	1.000	0.468	0.999	1.000	1.500
3	100.00	100.00	100.00	0.633	0.631	1.000	0.468	0.999	1.000	1.500
2	95.29	95.29	91.86	0.652	0.651	0.999	0.494	0.999	1.000	1.792
2	89.60	89.60	79.48	0.713	0.689	0.993	0.527	0.999	1.000	2.223
2	81.16	81.17	58.47	0.807	0.788	0.977	0.580	0.999	1.000	3.061
3	79.47	79.47	54.26	0.855	0.816	0.973	0.591	0.999	1.000	3.264
3	69.16	69.16	31.76	1.032	1.053	0.936	0.659	0.999	1.000	4.820
3	60.26	60.27	18.38	1.340	1.383	0.892	0.721	0.999	1.000	6.737
3	49.02	49.02	8.59	1.962	2.013	0.819	0.799	0.999	1.000	10.238
3	40.29	40.29	4.57	2.597	2.702	0.751	0.857	0.999	1.000	14.090
1	40.12	40.12	4.51	2.732	2.717	0.750	0.858	0.999	1.000	14.177
1	29.94	29.94	2.06	3.982	3.756	0.662	0.917	0.999	1.000	20.366
1	21.21	21.21	0.97	4.945	4.820	0.583	0.958	0.999	1.000	27.420
1	10.36	10.36	0.30	6.325	6.277	0.488	0.990	0.999	0.999	38.684
1	5.22	5.22	0.12	7.033	6.977	0.447	0.998	0.999	0.999	44.881
1	2.62	2.62	0.06	7.347	7.327	0.428	0.999	0.999	0.999	48.183
1	0.00	0.00	0.00	7.673	7.673	0.409	1.000	0.999	0.999	51.556

[a] NRTL parameters: $\tau_{AB} = -2.407$, $\tau_{BA} = 3.001$, and $\alpha = 0.2$.

Table 7. Results of Vapor−Liquid Equilibrium Measurements by the PTx Method for the 2-Butoxyethanol (A)/Acetic Acid (B) System at 100 °C[a]

	mol % A			pressure/kPa		activity coefficient		fugacity coefficient		relative volatility
run no.	charge	liquid	vapor	meas	calc	*A*	*B*	*A*	*B*	*B*/*A*
3	100.00	100.00	100.00	8.60	8.53	1.000	0.859	0.995	1.000	2.159
4	100.00	100.00	100.00	8.53	8.53	1.000	0.859	0.995	1.000	2.159
3	97.14	97.14	93.53	8.82	8.83	1.000	0.866	0.995	1.000	2.351
3	95.18	95.18	88.82	9.01	9.08	1.000	0.870	0.995	1.000	2.486
3	92.73	92.74	82.77	9.26	9.41	0.999	0.876	0.995	1.000	2.658
3	90.28	90.28	76.62	9.57	9.78	0.999	0.881	0.994	1.000	2.835
3	84.86	84.87	63.37	10.44	10.76	0.997	0.893	0.994	0.999	3.241
3	80.63	80.64	53.82	11.21	11.66	0.995	0.902	0.994	0.999	3.574
4	70.03	70.04	34.36	14.11	14.52	0.987	0.924	0.993	0.998	4.468
3	69.64	69.66	33.77	14.22	14.65	0.987	0.925	0.993	0.998	4.502
4	58.65	58.66	20.43	18.13	18.61	0.975	0.945	0.992	0.997	5.527
3	58.48	58.50	20.27	19.18	18.68	0.975	0.945	0.992	0.997	5.544
4	49.80	49.81	13.38	22.19	22.56	0.963	0.959	0.992	0.997	6.425
3	48.20	48.21	12.37	23.97	23.35	0.960	0.962	0.992	0.997	6.594
1	43.21	43.21	9.64	27.74	25.94	0.952	0.969	0.992	0.997	7.135
4	39.40	39.40	7.92	29.08	28.07	0.945	0.974	0.991	0.997	7.562
1	34.97	34.97	6.25	32.31	30.70	0.936	0.979	0.991	0.996	8.073
4	29.48	29.48	4.57	35.26	34.19	0.924	0.985	0.991	0.996	8.729
1	24.89	24.90	3.44	37.70	37.29	0.914	0.989	0.991	0.996	9.295
1	18.86	18.86	2.26	41.82	41.61	0.899	0.994	0.991	0.996	10.067
1	12.30	12.30	1.27	46.69	46.61	0.881	0.997	0.991	0.996	10.938
1	5.82	5.82	0.52	52.09	51.81	0.863	0.999	0.991	0.996	11.830
1	2.52	2.53	0.21	54.74	54.54	0.853	1.000	0.990	0.996	12.295
1	0.00	0.00	0.00	56.67	56.67	0.845	1.000	0.990	0.996	12.657

[a] NRTL parameters: $\tau_{AB} = -0.3440$, $\tau_{BA} = 0.2000$, and $\alpha = 0.2$.

to the measured pressures, and the activity coefficient parameters are adjusted to find the best fit of the total pressure data.

Results and Discussion

The *PTx* measurements include pure-component vapor pressures. Table 3 compares these measured vapor pressures with values calculated from the vapor pressure correlations given in the DIPPR 801 database[3] for each component at each isotherm. The agreement is generally good, with the exception of a few of the low-pressure points where the percent error magnifies a small absolute error in pressure and where there are only sparse data incorporated into the DIPPR 801 correlations.

Allyl Alcohol/Acetonitrile. Tables 4 and 5 give the results of the *PTx* measurements on the allyl alcohol/acetonitrile system at 40 °C and 80 °C. Moderate positive deviation from Raoult's law exists at both temperatures. The NRTL equation parameters used to correlate the data are given at the bottom of each table. The activity coefficients are nearly symmetric, as evidenced by the infinite dilution activity coefficients which are nearly equal for the two compounds. Figure 2 shows the measured data and the total-pressure correlation at 40 °C, and Figures 3 and 4 show the derived *y*−*x* and activity coefficient plots, respectively. Figure 5 is the total-pressure plot for the measurements at 80 °C, and Figures 6 and 7 show the derived *y*−*x* and activity coefficient plots for these data.

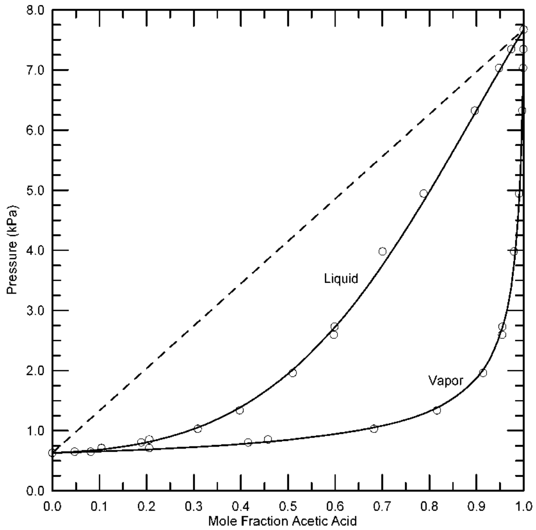

Figure 8. *PTx* results for the 2-butoxyethanol/acetic acid system at 50 °C.

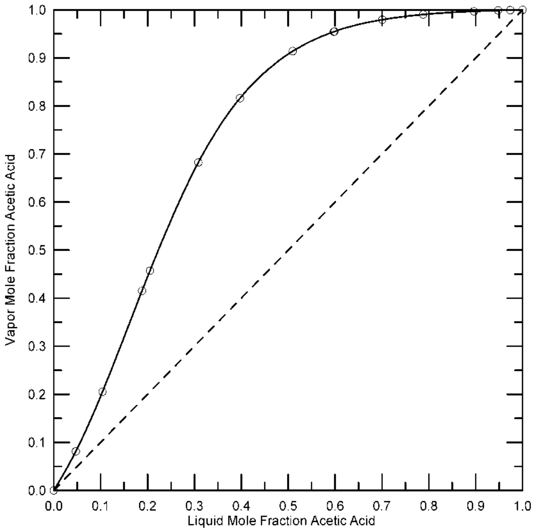

Figure 9. $y-x$ plot for the 2-butoxyethanol/acetic acid system at 50 °C.

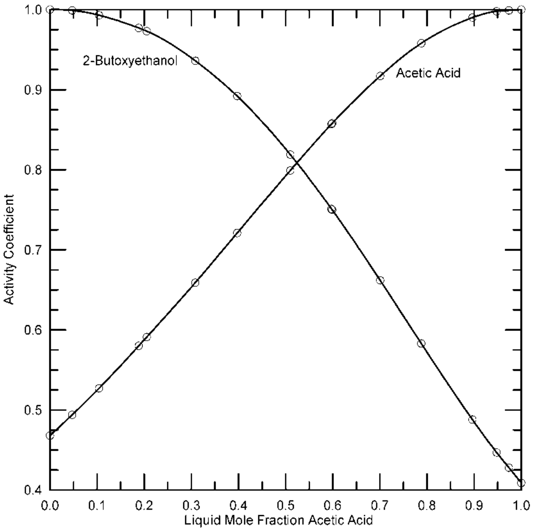

Figure 10. Activity coefficients for the 2-butoxyethanol/acetic acid system at 50 °C.

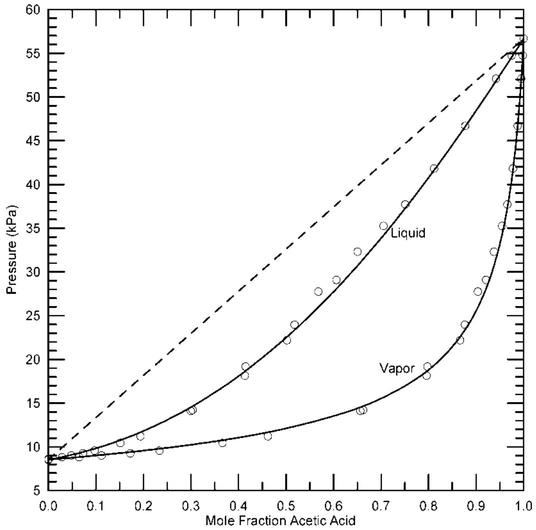

Figure 11. *PTx* results for the 2-butoxyethanol/acetic acid system at 100 °C.

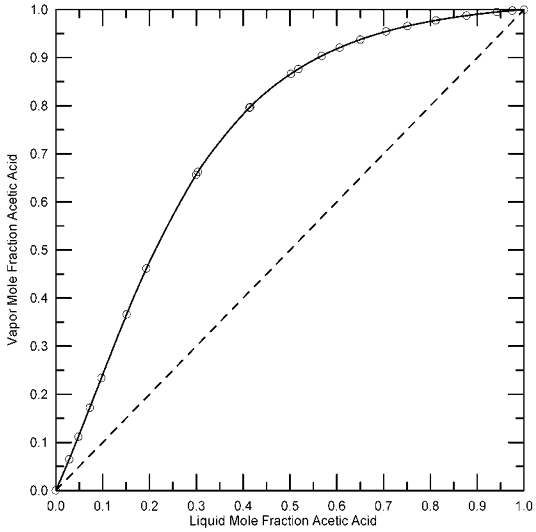

Figure 12. $y-x$ plot for the 2-butoxyethanol/acetic acid system at 100 °C.

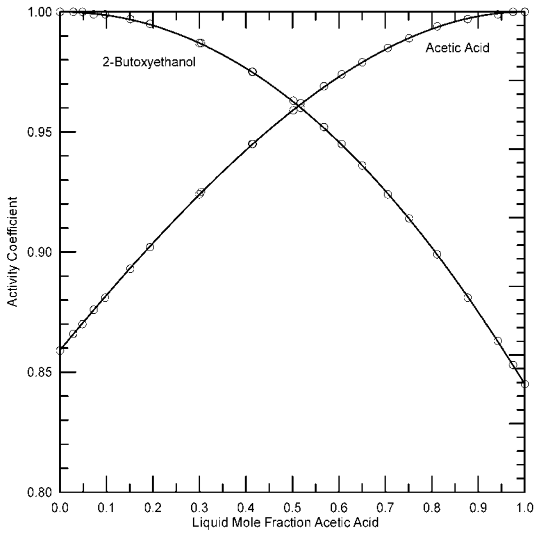

Figure 13. Activity coefficients for the 2-butoxyethanol/acetic acid system at 100 °C.

2-Butoxyethanol/Acetic Acid. Tables 6 and 7 present the results for the 2-butoxyethanol/acetic acid system at 50 °C and 100 °C. Negative deviations from Raoult's law exist at both temperatures. Vapor-phase dimerization of

Table 8. Results of Vapor−Liquid Equilibrium Measurements by the PTx Method for the 2,3-Epoxy-1-propanol (A)/ 1-Methoxy-2-propanol (B) System at 70 °C[a]

	mol % A			pressure/kPa		activity coefficient		fugacity coefficient		relative volatility
run no.	charge	liquid	vapor	meas	calc	*A*	*B*	*A*	*B*	*B*/*A*
1	100.00	100.00	100.00	2.98	2.98	1.000	1.206	0.999	0.999	6.417
1	98.19	98.19	89.48	3.20	3.27	1.000	1.201	0.999	0.999	6.392
1	94.30	94.31	72.34	3.85	3.89	1.000	1.192	0.998	0.998	6.337
1	89.17	89.19	56.87	4.67	4.68	1.001	1.178	0.998	0.998	6.260
1	79.63	79.66	39.09	6.20	6.11	1.005	1.153	0.997	0.997	6.100
1	79.42	79.45	38.81	6.20	6.14	1.006	1.152	0.997	0.997	6.096
1	68.55	68.57	27.04	7.74	7.68	1.015	1.123	0.997	0.997	5.888
1	58.17	58.19	19.73	9.12	9.07	1.029	1.096	0.996	0.996	5.664
2	53.30	53.32	17.07	9.74	9.70	1.039	1.083	0.996	0.996	5.549
1	48.74	48.76	14.89	10.28	10.27	1.049	1.072	0.996	0.996	5.437
2	41.99	42.01	12.10	10.92	11.09	1.068	1.056	0.995	0.995	5.262
1	40.60	40.61	11.57	11.19	11.26	1.073	1.053	0.995	0.995	5.224
2	31.52	31.54	8.48	12.27	12.32	1.108	1.034	0.995	0.995	4.969
2	21.40	21.42	5.52	13.53	13.48	1.161	1.017	0.994	0.994	4.662
2	11.20	11.21	2.83	14.66	14.64	1.235	1.005	0.994	0.994	4.331
2	5.32	5.33	1.34	15.38	15.32	1.289	1.001	0.993	0.994	4.131
2	2.95	2.95	0.75	15.60	15.60	1.315	1.000	0.993	0.994	4.049
2	0.00	0.00	0.00	15.95	15.95	1.349	1.000	0.993	0.993	3.945

[a] NRTL parameters: $\tau_{AB} = -0.6893$, $\tau_{BA} = 1.090$, and $\alpha = 0.2$.

Table 9. Results of Vapor−Liquid Equilibrium Measurements by the *PTx* Method for the 2,3-Epoxy-1-propanol (A)/ 1-Methoxy-2-propanol (B) System at 120 °C[a]

	mol % A			pressure/kPa		activity coefficient		fugacity coefficient		relative volatility
run no.	charge	liquid	vapor	meas	calc	*A*	*B*	*A*	*B*	*B*/*A*
2	100.00	100.00	100.00	25.21	25.21	1.000	1.183	0.993	0.993	4.629
2	97.02	97.06	87.71	27.34	27.92	1.000	1.183	0.992	0.992	4.628
2	94.26	94.33	78.24	29.91	30.44	1.000	1.182	0.991	0.992	4.625
2	89.31	89.42	64.68	34.67	34.97	1.000	1.179	0.990	0.991	4.614
2	83.14	83.29	52.07	40.78	40.56	1.001	1.174	0.988	0.989	4.589
2	67.88	68.06	32.30	54.96	54.03	1.008	1.151	0.984	0.985	4.466
1	67.34	67.45	31.72	54.63	54.55	1.008	1.149	0.984	0.985	4.459
2	60.14	60.31	25.82	61.18	60.51	1.016	1.134	0.982	0.984	4.365
1	57.53	57.69	23.97	62.04	62.63	1.020	1.128	0.982	0.983	4.324
2	49.61	49.73	19.14	71.32	68.82	1.036	1.107	0.980	0.981	4.179
1	47.01	47.20	17.81	69.46	70.72	1.043	1.100	0.979	0.981	4.125
2	39.03	39.11	14.04	76.23	76.52	1.072	1.078	0.978	0.979	3.931
1	35.50	35.70	12.64	77.37	78.85	1.089	1.068	0.977	0.979	3.838
1	24.11	24.29	8.45	85.04	86.23	1.167	1.037	0.975	0.977	3.477
1	12.24	12.35	4.45	93.19	93.49	1.308	1.011	0.973	0.975	3.023
1	6.16	6.22	2.34	97.33	97.18	1.419	1.003	0.972	0.974	2.764
1	3.18	3.21	1.24	99.48	99.01	1.487	1.001	0.971	0.973	2.632
1	0.00	0.00	0.00	100.99	100.99	1.572	1.000	0.971	0.973	2.488

[a] NRTL parameters: $\tau_{1AB2} = -1.094$, $\tau_{BA} = 1.813$, and $\alpha = 0.2$.

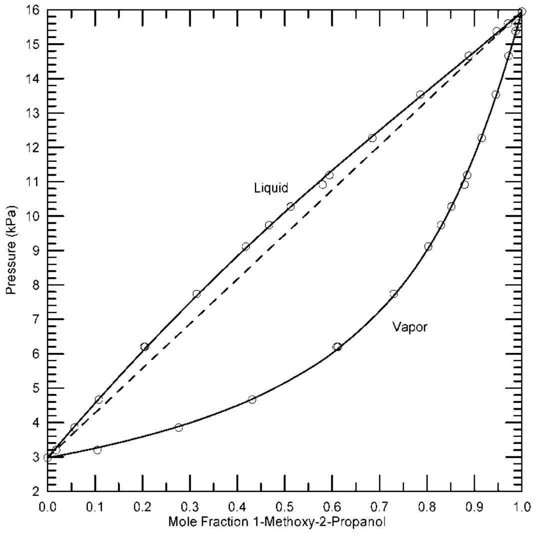

Figure 14. *PTx* results for the 2,3-epoxy-1-propanol/1-methoxy-2-propanol system at 70 °C.

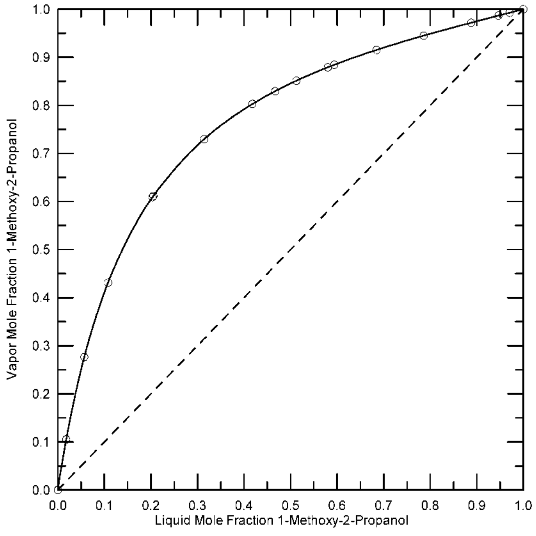

Figure 15. *y*−*x* plot for the 2,3-epoxy-1-propanol/1-methoxy-2-propanol system at 70 °C.

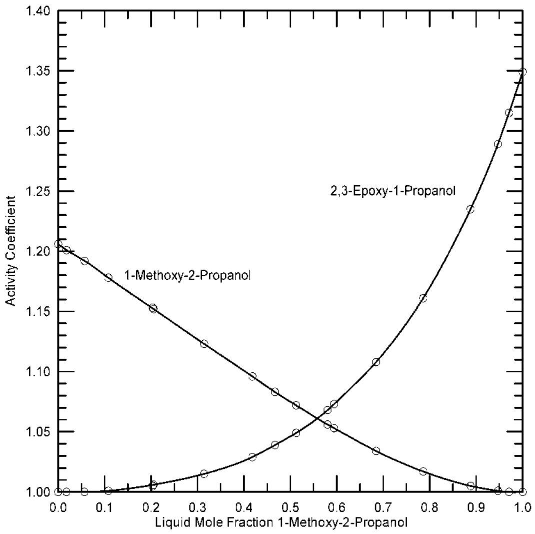

Figure 16. Activity coefficients for the 2,3-epoxy-1-propanol/1-methoxy-2-propanol system at 70 °C.

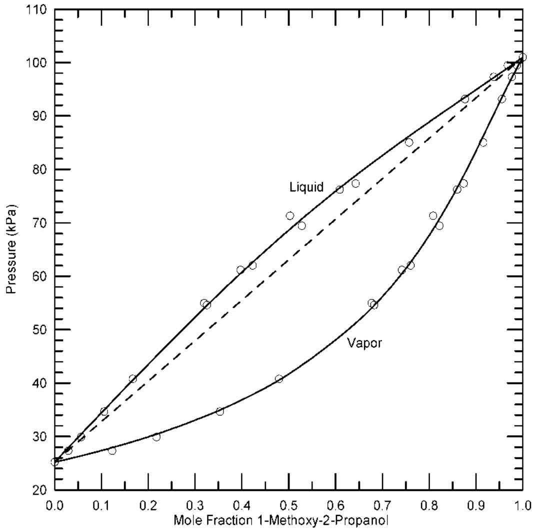

Figure 17. *PTx* results for the 2,3-epoxy-1-propanol/1-methoxy-2-propanol system at 120 °C.

acetic acid was accounted for by incorporating chemical equilibrium between monomer and dimer into the data reduction procedure and treating the vapor as a mixture of acetic acid monomer, acetic acid dimer, and 2-butoxyethanol. The 50 °C results are shown in Figures 8−10, and the 100 °C results are shown in Figures 11−13.

1-Methoxy-2-propanol/2,3-Epoxy-1-propanol. Tables 8 and 9 present the results for the 1-methoxy-2-propanol/2,3-epoxy-1-propanol system at 70 °C and 120 °C. Positive deviations from Raoult's law exist at both temperatures. The results at 70 °C are shown in Figures 14−16, and the 120 °C results are shown in Figures 17−19.

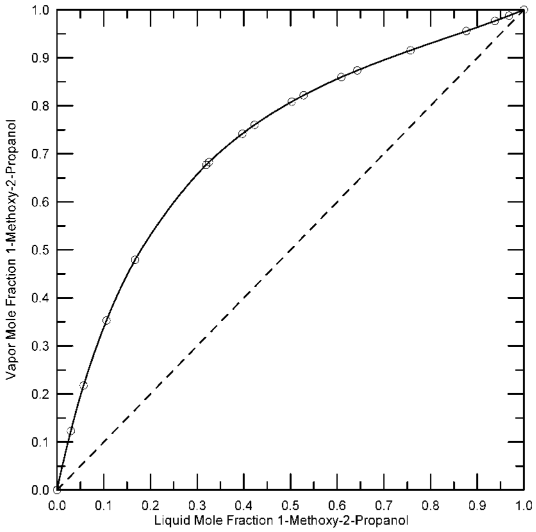

Figure 18. *y*−*x* plot for the 2,3-epoxy-1-propanol/1-methoxy-2-propanol system at 120 °C.

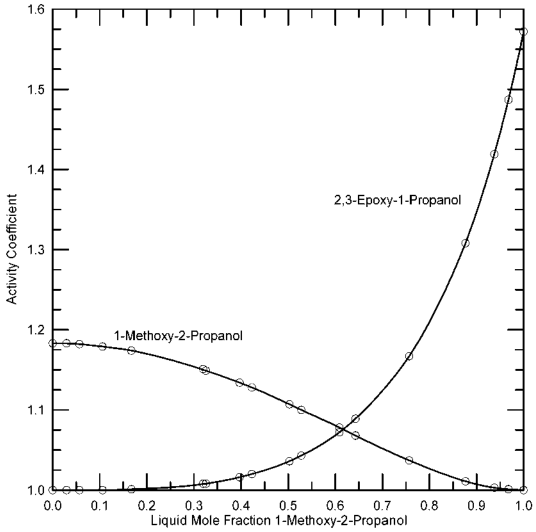

Figure 19. Activity coefficients for the 2,3-epoxy-1-propanol/1-methoxy-2-propanol system at 120 °C.

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Received for review September 17, 2001. Accepted January 19, 2002.

JE0155204