J. Chem. Eng. Data **1999,** *44,* 959−964

Vapor−Liquid Equilibria and Excess Enthalpy Data for the Binary Systems 2-Methyltetrahydrofuran with 2,2,4-Trimethylpentane (Isooctane), Ethanol, Toluene, Cyclohexane, and Methylcyclohexane[§]

Sven Horstmann,[†] Hergen Gardeler,[†] Rainer Bölts,[†] David Zudkevitch,[‡] and Jürgen Gmehling*[,†]

Technische Chemie, Carl von Ossietzky Universitaet Oldenburg, Postfach 2503, D-26111 Oldenburg, Germany, and Department of Chemical Engineering, Columbia University, New York, New York 10027

Isothermal $P-x$ data (vapor−liquid equilibrium (VLE)) and excess enthalpy data (H^E) for the five binary systems 2-methyltetrahydrofuran with 2,2,4-trimethylpentane (isooctane), ethanol, toluene, cyclohexane, and methylcyclohexane are presented. The VLE data were obtained experimentally, in a computer-controlled static apparatus, and the heat of mixing data were measured in an isothermal flow calorimeter. Also presented are linear temperature-dependent interaction parameters for the NRTL and UNIQUAC models which were fitted simultaneously to the experimental VLE and H^E data. These data and the correlation parameters should be useful for predicting properties, e.g., volatility (Reid vapor pressure (RVP), etc.) of blends of alternative automotive fuels which contain ethanol, 2-methyltetrahydrofuran, and light hydrocarbons.

Background

Blends of ethanol, 2-methyltetrahydrofuran (MeTHF), and light naphthas, e.g., natural gas liquids (NGL), have been proposed as alternative P-series automotive fuels (Paul, 1997 and 1998). More than 70% of these fuels are made from renewable biomass, such as waste paper, wood, and agricultural waste. Both ethanol and MeTHF, to be produced from furfural, are derived from these renewable resources (Caruana, 1998). However, reliable predictions of the properties of such blends, as has been proposed by Zudkevitch et al. (1995), could not be made due to lack of phase equilibrium and heat of mixing data on mixtures of MeTHF with hydrocarbons and oxygenated additives such as ethanol and tertiary ethers. The study described herein is part of a larger undertaking to augment the parameter matrix for simulating the behavior of reformulated and alternative automotive fuels.

No experimental VLE or H^E data are available in the literature on binary systems of 2-methyltetrahydrofuran with 2,2,4-trimethylpentane (isooctane), ethanol, toluene, cyclohexane, and methylcyclohexane. Paul (1998) presented $P-x$ (Reid vapor pressure (RVP)) data on some mixtures of MeTHF with ethanol, light hydrocarbons, and NGL. Though those data provide an indirect description of the phase behavior, at 37.8 °C, of the system studied by Paul, it is apparent that more experimental data would be needed for supporting reliable predictions of fuel blends' behavior, e.g., volatility and emissions.

In this study, isothermal $P-x$ data were measured in a computer-operated static apparatus at temperatures between 310.93 K and 318.15 K. In addition, H^E data for these systems were measured at 323.15 K. For this purpose a commercial isothermal flow calorimeter was used.

Table 1. Suppliers, Purities and Water Contents of the Chemicals Used

component	supplier	purity[a]/%	water content[b] /(mass ppm)
2-methyltetrahydrofuran	Aldrich	99.80	100
2,2,4-trimethylpentane	Aldrich	>99.9	20
ethanol	Scharlau	>99.9	30
toluene	Scharlau	99.97	70
cyclohexane	Scharlau	99.95	10
methylcyclohexane	Merck	>99.9	10

[a] Determined by gas chromatography. [b] Determined by Karl Fischer titration.

The excess enthalpy (H^E) data are useful in interpolation and extrapolation of the temperature-dependent activity coefficient γ_i to the excess enthalpy with the Gibbs−Helmholtz equation

$$\left(\frac{\partial \ln \gamma_i}{\partial 1/T}\right)_{P,x} = \frac{H_i^E}{R} \qquad (1)$$

The experimental VLE and H^E data of this work are presented together with linear temperature-dependent NRTL and UNIQUAC parameters and the derived azeotropic conditions.

Experimental Section

Purity of Materials. For the VLE measurements all chemicals were dried over molecular sieves, degassed, and distilled as described by Fischer and Gmehling (1994). For the H^E measurements the compounds were used without degassing. The properties and final purities, as determined by gas chromatography and Karl Fischer titration, are listed in Table 1.

Apparatus and Procedure. The VLE measurements (isothermal $P-x$ data) were performed with a computer-driven static apparatus. The experimental procedure is based on that proposed by Gibbs and Van Ness (1972) in which the total pressure P of each of several mixtures of

---

* Corresponding author. E-mail: Gmehling@tech.chem.uni-oldenburg.de.
[†] Carl von Ossietzky Universitaet Oldenburg.
[‡] Columbia University.
[§] Dedicated to Dr. Henry V. Kehiaian, on the occasion of his 70th birthday.

10.1021/je990023x CCC: $18.00

Table 2. Experimental $P-x$ Data for the System 2-Methyltetrahydrofuran (1) + 2,2,4-Trimethylpentane (2) at 310.93 K

x_1	P/kPa	x_1	P/kPa	x_1	P/kPa
0.000 00	11.863	0.407 31	17.981	0.874 93	21.756
0.002 42	11.912	0.449 39	18.436	0.898 95	21.881
0.004 91	11.961	0.485 84	18.808	0.921 00	21.988
0.007 74	12.016	0.520 10	19.142	0.940 73	22.076
0.010 24	12.067	0.553 14	19.453	0.955 96	22.141
0.013 91	12.140	0.584 56	19.734	0.967 97	22.193
0.020 64	12.274	0.613 39	19.985	0.977 55	22.232
0.026 95	12.398	0.621 34	20.069	0.983 16	22.252
0.037 01	12.593	0.638 45	20.196	0.986 96	22.266
0.051 46	12.860	0.649 24	20.285	0.990 83	22.278
0.076 11	13.306	0.663 38	20.400	0.992 74	22.285
0.106 02	13.830	0.678 00	20.502	0.994 66	22.294
0.141 52	14.409	0.706 53	20.708	0.995 99	22.297
0.184 18	15.069	0.734 45	20.902	0.997 33	22.301
0.228 94	15.733	0.762 39	21.089	0.998 67	22.307
0.274 43	16.360	0.792 56	21.278	1.000 00	22.313
0.319 80	16.948	0.821 27	21.453		
0.364 51	17.493	0.849 36	21.616		

Table 3. Experimental H^E Data for the System 2-Methyltetrahydrofuran (1) + 2,2,4-Trimethylpentane (2) at 323.15 K and 1.48 MPa

x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}
0.0797	136.40	0.4420	483.98	0.8315	301.53
0.1546	242.34	0.5231	496.68	0.8681	251.38
0.2250	332.09	0.6220	481.41	0.9031	192.98
0.2914	395.56	0.7116	431.21	0.9367	133.89
0.3542	442.17	0.7736	371.63	0.9690	68.229

Table 4. Experimental $P-x$ Data for the System 2-Methyltetrahydrofuran (1) + Ethanol (2) at 318.15 K

x_1	P/kPa	x_1	P/kPa	x_1	P/kPa
0.000 00	23.007	0.16462	27.686	0.716 99	32.512
0.000 71	23.038	0.191 81	28.248	0.762 93	32.427
0.001 43	23.066	0.220 49	28.787	0.808 08	32.256
0.002 07	23.091	0.247 34	29.250	0.850 92	31.992
0.003 66	23.147	0.274 31	29.676	0.885 60	31.687
0.005 81	23.226	0.302 58	30.076	0.914 20	31.365
0.007 89	23.301	0.330 84	30.447	0.937 38	31.064
0.010 12	23.382	0.358 17	30.760	0.953 86	30.804
0.013 31	23.489	0.383 31	31.020	0.966 60	30.576
0.018 79	23.677	0.409 72	31.267	0.975 12	30.412
0.028 60	23.997	0.432 68	31.467	0.983 72	30.242
0.040 52	24.381	0.465 86	31.719	0.988 07	30.144
0.054 19	24.805	0.500 50	31.941	0.991 08	30.072
0.072 14	25.343	0.537 60	32.144	0.994 08	30.003
0.092 36	25.911	0.580 67	32.324	0.997 04	29.934
0.114 55	26.496	0.624 84	32.445	1.000 00	29.860
0.138 32	27.083	0.671 40	32.515		

Table 5. Experimental H^E Data for the System 2-Methyltetrahydrofuran (1) + Ethanol (2) at 323.15 K and 1.51 MPa

x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}
0.0297	54.567	0.2187	401.29	0.6356	714.74
0.0607	112.03	0.2793	493.71	0.6993	680.63
0.0931	174.18	0.3677	606.68	0.7672	608.90
0.1269	238.48	0.4659	690.01	0.8396	481.23
0.1623	303.38	0.5470	720.10	0.9170	291.21

Table 6. Experimental $P-x$ Data for the System 2-Methyltetrahydrofuran (1) + Toluene (2) at 313.15 K

x_1	P/kPa	x_1	P/kPa	x_1	P/kPa
0.000 00	7.908	0.353 52	13.418	0.791 95	20.780
0.002 57	7.949	0.387 35	13.970	0.825 55	21.361
0.005 46	7.994	0.420 02	14.508	0.857 75	21.918
0.007 25	8.024	0.452 36	15.045	0.887 88	22.441
0.010 85	8.080	0.467 83	15.248	0.915 21	22.915
0.014 52	8.138	0.483 90	15.572	0.936 36	23.282
0.018 20	8.195	0.495 51	15.709	0.953 03	23.571
0.022 29	8.259	0.513 14	16.060	0.966 14	23.798
0.028 46	8.352	0.522 59	16.164	0.974 80	23.946
0.037 64	8.497	0.539 30	16.503	0.98165	24.069
0.055 60	8.763	0.552 81	16.673	0.986 80	24.159
0.076 53	9.080	0.565 87	16.953	0.990 29	24.215
0.102 11	9.467	0.584 73	17.215	0.993 86	24.279
0.133 88	9.951	0.617 15	17.767	0.996 35	24.319
0.167 63	10.471	0.649 62	18.322	0.997 58	24.338
0.202 91	11.015	0.682 92	18.894	0.998 79	24.362
0.239 06	11.582	0.719 83	19.529	1.000 00	24.381
0.277 60	12.194	0.755 86	20.154		
0.315 14	12.795				

Table 7. Experimental H^E Data for the System 2-Methyltetrahydrofuran (1) + Toluene (2) at 323.15 K and 1.38 MPa

x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}
0.0528	−42.345	0.3377	−197.56	0.7606	−163.64
0.1053	−81.121	0.4138	−214.70	0.8090	−141.49
0.1574	−114.41	0.5143	−224.67	0.8572	−111.53
0.2093	−143.88	0.6137	−213.37	0.9050	−78.721
0.2609	−170.04	0.6874	−194.58	0.9527	−42.080

Table 8. Experimental $P-x$ Data for the System Cyclohexane (1) + 2-Methyltetrahydrofuran (2) at 310.95 K

x_1	P/kPa	x_1	P/kPa	x_1	P/kPa
0.000 00	22.331	0.242 00	24.195	0.811 76	24.202
0.001 46	22.353	0.277 88	24.358	0.846 62	24.003
0.002 95	22.366	0.314 65	24.498	0.879 42	23.778
0.004 44	22.381	0.347 82	24.605	0.909 42	23.542
0.005 95	22.395	0.380 19	24.691	0.932 68	23.338
0.008 06	22.419	0.412 53	24.761	0.951 15	23.157
0.012 39	22.465	0.444 36	24.813	0.966 90	22.991
0.016 66	22.510	0.474 53	24.846	0.976 16	22.885
0.023 14	22.578	0.501 57	24.863	0.98284	22.807
0.031 71	22.667	0.529 22	24.870	0.987 90	22.746
0.045 06	22.797	0.558 32	24.858	0.991 25	22.705
0.061 92	22.957	0.591 63	24.838	0.994 65	22.665
0.083 14	23.143	0.625 23	24.801	0.996 81	22.638
0.110 45	23.370	0.659 93	24.739	0.997 85	22.626
0.140 49	23.594	0.698 68	24.645	0.998 92	22.617
0.172 59	23.807	0.736 90	24.525	1.000 00	22.599
0.206 08	24.007	0.775 51	24.371		

different overall compositions is measured at the same constant temperature T. The apparatus and measurement procedure have been described previously (Rarey and Gmehling, 1993, Rarey et al., 1999). They have been found applicable at temperatures between 278 K and 368 K and pressures from 0 MPa to 0.3 MPa.

The thermostated, purified, and degassed compounds are charged into the VLE cell which is evacuated and kept in a thermostatic oil bath. The pressure inside the cell is monitored with a Digiquartz pressure sensor (Model 245A, Paroscientific), and the temperature is measured with a Pt100 resistance thermometer (Model 1506, Hart Scientific, Provo, UT). The total compositions are determined from the known quantities of liquids which are injected into the equilibrium cell by stepping-motor-driven injection pumps and valves. The liquid-phase compositions are established from the injected quantity by solving mass and volume balance equations which also account for the vapor−liquid equilibrium. At the low system pressures of this investigation, the calculated liquid-phase compositions are nearly identical to the feed compositions. The experimental uncertainties of this apparatus are as follows: $\sigma(T) = 0.03$ K, $\sigma(P) = (20\ \text{Pa}) + 0.0001(P/\text{Pa})$, $\sigma(x_i) = 0.0001$.

A commercial isothermal flow calorimeter (Model 7501, Hart Scientific), described by Gmehling (1993), was used for determining the excess enthalpy data. In this experimental setup, two syringe pumps (Model LC-2600, ISCO)

Table 9. Experimental H^E Data for the System Cyclohexane (1) + 2-Methyltetrahydrofuran (1) at 323.15 K and 1.48 MPa

x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}
0.0466	86.136	0.3089	427.38	0.7358	419.61
0.0935	164.83	0.3823	477.70	0.7878	366.53
0.1408	235.96	0.4814	514.45	0.8403	299.51
0.1884	300.63	0.5820	508.99	0.8931	216.07
0.2363	355.76	0.6585	479.14	0.9463	111.96

Table 10. Experimental $P-x$ Data for the System 2-Methyltetrahydrofuran (1) + Methylcyclohexane (2) at 310.95 K

x_1	P/kPa	x_1	P/kPa	x_1	P/kPa
0.000 00	11.387	0.388 18	17.328	0.823 23	21.152
0.007 30	11.540	0.460 45	18.092	0.874 02	21.501
0.014 37	11.685	0.497 65	18.444	0.914 89	21.776
0.022 00	11.851	0.526 30	18.724	0.945 54	21.972
0.035 54	12.145	0.558 05	19.016	0.971 05	22.130
0.056 52	12.578	0.587 30	19.272	0.984 46	22.212
0.107 26	13.486	0.623 60	19.596	0.990 78	22.257
0.163 02	14.387	0.641 05	19.732	0.993 85	22.282
0.248 19	15.631	0.692 20	20.165	0.996 91	22.309
0.314 43	16.476	0.760 41	20.693	1.000 00	22.315

Table 11. Experimental H^E Data for the System 2-Methyltetrahydrofuran (1) + Methylcyclohexane (2) at 323.15 K and 1.48 MPa

x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}
0.0627	100.15	0.3797	396.65	0.7923	279.93
0.1238	186.09	0.4587	419.09	0.8357	234.42
0.1832	257.39	0.5597	419.42	0.8781	183.76
0.2412	311.93	0.6560	380.31	0.9196	127.32
0.2976	354.39	0.7253	338.20	0.9602	65.392

provide a flow of constant composition through a calorimeter cell (in a thermostat) that is equipped with a pulsed heater and a Peltier cooler. The use of a Peltier cooler allows the measurement of endothermal as well as exothermal heat effects. A back-pressure regulator serves to keep the pressure at a level at which evaporation effects can be prevented. The experimental uncertainties of this device are as follows: $\sigma(T) = 0.03$ K, $\sigma(H^E) = 0.01(H^E/(\text{J}\cdot\text{mol}^{-1}))$, and $\sigma(x_i) = 0.0001$.

Results

The experimental $P-x$ and H^E data for the investigated systems are listed in Tables 2−11. All the experimental VLE and heat of mixing data on each of the systems were correlated simultaneously to obtain linear temperature-dependent G^E model parameters for the NRTL (Renon and Prausnitz, 1968) and UNIQUAC (Abrams and Prausnitz, 1975) models. The following expression was used to describe the temperature dependence of the interaction parameters:

$$A_{ij}/(\text{J}\cdot\text{mol}^{-1}) = a_{ij} + b_{ij}(T/\text{K}) \qquad (2)$$

where A_{ij} is either $(g_{ij} - g_{jj})$ of the NRTL or $(u_{ij} - u_{jj})$ of the UNIQUAC correlation. The parameters of eq 2 are presented in Tables 12 and 13.

The van der Waals properties r_i and q_i and the three coefficients A_i, B_i, and C_i of the Antoine equation for vapor pressures,

$$\log(P_i^s/\text{kPa}) = A_i - \frac{B_i}{C_i + (T/\text{K})} \qquad (3)$$

which were used in the calculations, are listed in Table 14. The coefficients A_i of the Antoine equation were adjusted to the experimental vapor pressures of the pure components in order to account only for the excess Gibbs energy during the fitting procedure. The deviations between experimental pure component vapor pressures and values calculated with the Antoine coefficients taken from the Dortmund Data Bank (Gmehling et al., 1999) are smaller than 1.0% for all components except methylcyclohexane,

Table 12. Linear Temperature-Dependent NRTL Interaction Parameters Fitted Simultaneously to Isothermal $P-x$ and H^E Data

component 1	component 2	i	j	a_{ij} /J·mol^{-1}	b_{ij} /J·mol^{-1}·K^{-1}
2-methyltetrahydrofuran	2,2,4-trimethylpentane	1	2	838.02	1.7219
		2	1	1308.79	−4.7525
				$\alpha_{12} = 0.4700$	
2-methyltetrahydrofuran	ethanol	1	2	4920.87	−9.4221
		2	1	−996.64	4.0568
				$\alpha_{12} = 0.3325$	
2-methyltetrahydrofuran	toluene	1	2	−2647.24	0.9114
		2	1	3391.07	−1.5125
				$\alpha_{12} = 0.2788$	
cyclohexane	2-methyltetrahydrofuran	1	2	1434.92	−1.4502
		2	1	896.88	−2.3672
				$\alpha_{12} = 0.4700$	
2-methyltetrahydrofuran	methylcyclohexane	1	2	1526.43	−4.3451
		2	1	241.12	2.0139
				$\alpha_{12} = 0.4700$	

Table 13. Linear Temperature-Dependent UNIQUAC Interaction Parameters Fitted Simultaneously to Isothermal $P-x$ and H^E Data

component 1	component 2	i	j	a_{ij}/J·mol^{-1}	b_{ij}/J·mol^{-1}·K^{-1}
2-methyltetrahydrofuran	2,2,4-trimethylpentane	1	2	−19.97	−0.5731
		2	1	573.84	−0.0900
2-methyltetrahydrofuran	ethanol	1	2	2915.02	−2.1221
		2	1	−670.16	−0.5069
2-methyltetrahydrofuran	toluene	1	2	−832.16	4.6593
		2	1	383.70	−3.7343
cyclohexane	2-methyltetrahydrofuran	1	2	152.89	1.7373
		2	1	468.23	−2.7657
2-methyltetrahydrofuran	methylcyclohexane	1	2	800.86	−4.6939
		2	1	−526.62	4.9370

Table 14. Pure Component Parameters:[a] Relative van der Waals Volumes r_i, Surfaces q_i, and Antoine Coefficients A_i, B_i, and C_i

component	r_i	q_i	A_i	B_i/K	C_i/K
2-methyltetrahydrofuran	3.6151	3.256	6.19376	1298.63	−43.150
2,2,4-trimethylpentane	5.8463	5.008	6.09454^b	1339.49	−44.117
ethanol	2.1055	1.972	7.32860^b	1642.89	−42.809
toluene	3.9228	2.968	6.07700^b	1342.31	−53.963
cyclohexane	4.0464	3.240	5.97772^b	1206.47	−50.014
methylcyclohexane	4.7200	3.776	5.97458^b	1278.57	−50.982

[a] Dortmund Data Bank (Gmehling et al., 1999). [b] Adjusted to the experimental data.

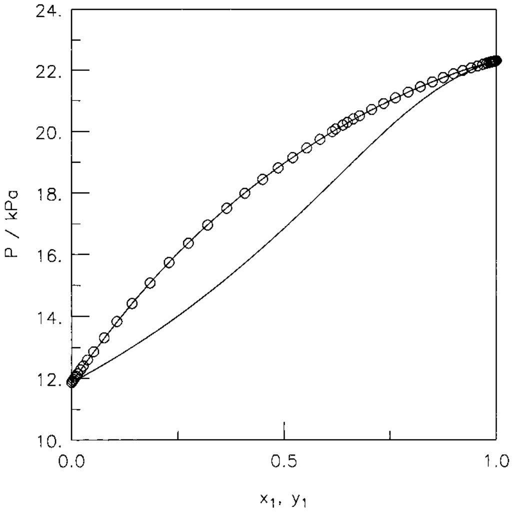

Figure 1. Experimental and predicted $P-x(y)$ behavior of the system 2-methyltetrahydrofuran (1) + 2,2,4-trimethylpentane (2) at 310.93 K: experimental (○) and UNIQUAC (—).

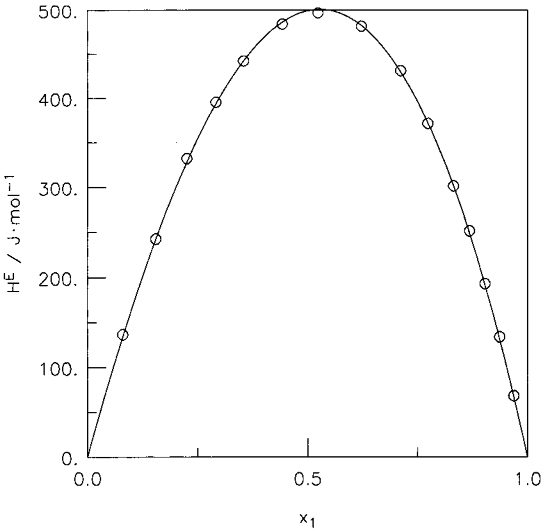

Figure 2. Experimental and predicted excess enthalpy data for the system 2-methyltetrahydrofuran (1) + 2,2,4-trimethylpentane (2) at 323.15 K: experimental (○) and UNIQUAC (—).

where the experimental value is 2% higher than the calculated one at the temperature of interest.

The experimental $P-x$ and H^E data are graphically presented in Figures 1−10 together with values predicted by the UNIQUAC model with the parameters from Table 13. As illustrated in the diagrams, the predicted values are in good agreement with the experimental data.

The azeotropic conditions for the systems 2-methyltetrahydrofuran + ethanol and cyclohexane + 2-methyltet-

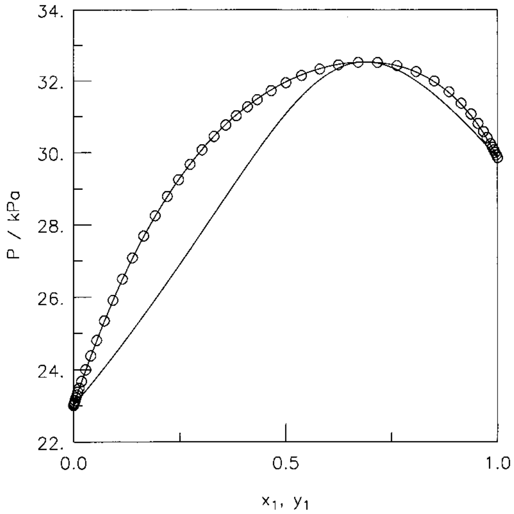

Figure 3. Experimental and predicted $P-x(y)$ behavior of the system 2-methyltetrahydrofuran (1) + ethanol (2) at 318.15 K: experimental (○) and UNIQUAC (—).

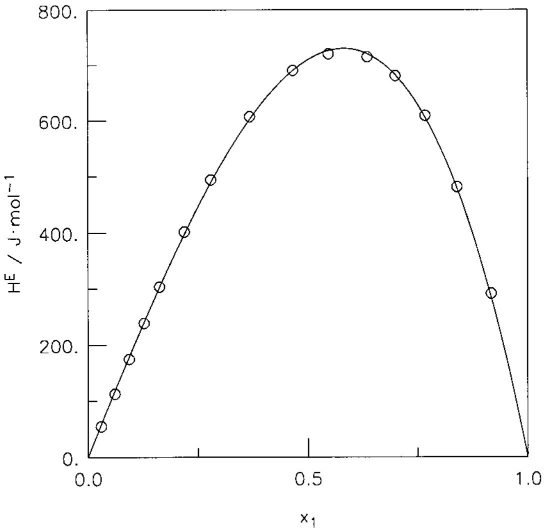

Figure 4. Experimental and predicted excess enthalpy data for the system 2-methyltetrahydrofuran (1) + ethanol (2) at 323.15 K: experimental (○) and UNIQUAC (—).

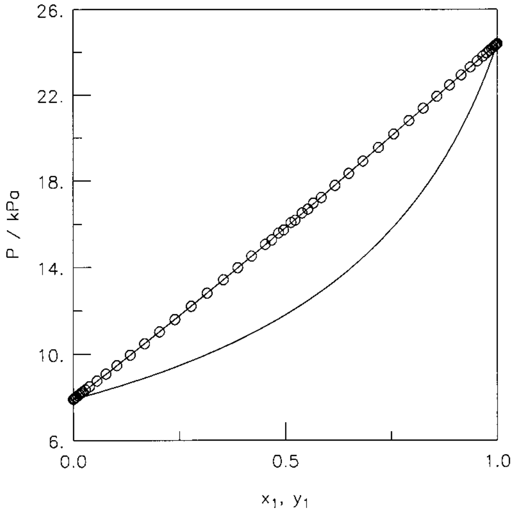

Figure 5. Experimental and predicted $P-x(y)$ behavior of the system 2-methyltetrahydrofuran (1) + toluene (2) at 313.15 K: experimental (○) and UNIQUAC (—).

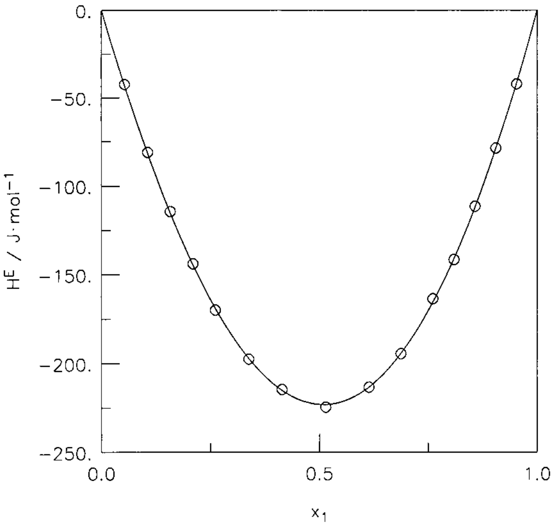

Figure 6. Experimental and predicted excess enthalpy data for the system 2-methyltetrahydrofuran (1) + toluene (2) at 323.15 K: experimental (○) and UNIQUAC (—).

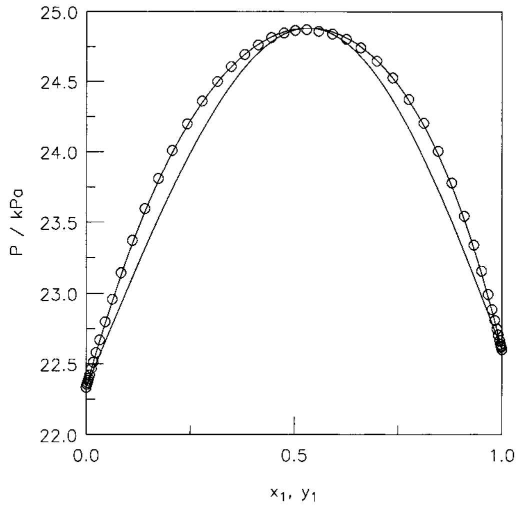

Figure 7. Experimental and predicted $P-x(y)$ behavior of the system cyclohexane (1) + 2-methyltetrahydrofuran (2) at 310.95 K: experimental (○) and UNIQUAC (—).

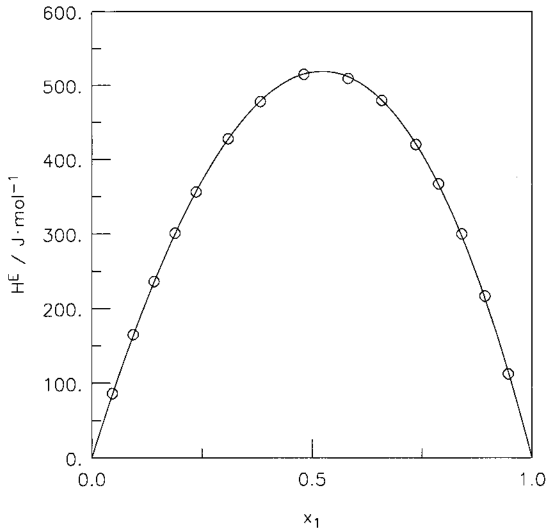

Figure 8. Experimental and predicted excess enthalpy data for the system cyclohexane (1) + 2-methyltetrahydrofuran (2) at 323.15 K: experimental (○) and UNIQUAC (—).

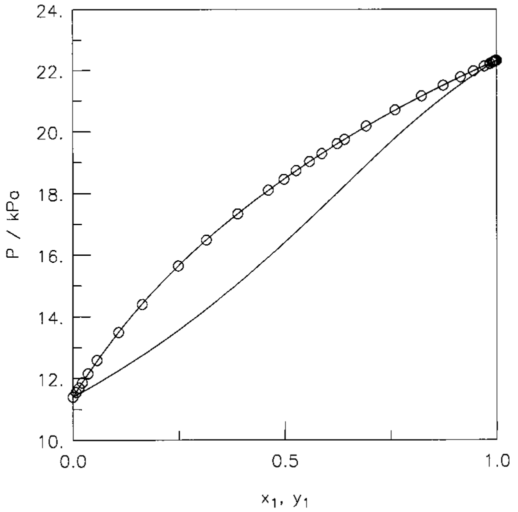

Figure 9. Experimental and predicted $P-x(y)$ behavior of the system 2-methyltetrahydrofuran (1) + methylcyclohexane (2) at 310.95 K: experimental (○) and UNIQUAC (—).

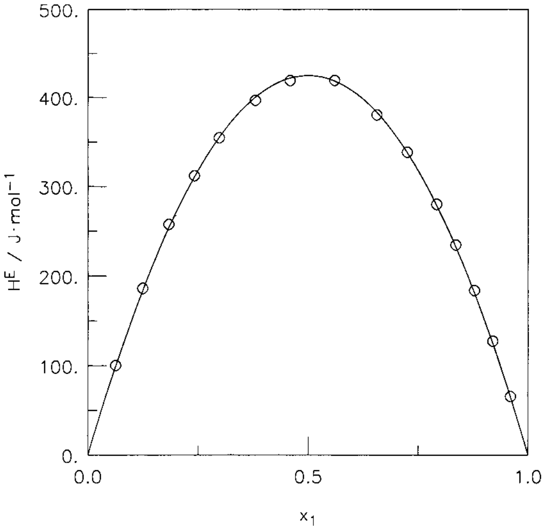

Figure 10. Experimental and predicted excess enthalpy data for the system 2-methyltetrahydrofuran (1) + methylcyclohexane (2) at 323.15 K: experimental (○) and UNIQUAC (—).

Table 15. Derived Azeotropic Condition

component 1	component 2	T/K	$y_{az,1}$	P_{az}/kPa
2-methyltetrahydrofuran	ethanol	318.15	0.686	32.522
cyclohexane	2-methyltetrahydrofuran	310.95	0.533	24.870

rahydrofuran, at the temperatures of this study, were derived by graphical interpolation of the experimental $P-x$ data. They are given in Table 15. The same azeotropic values have been reproduced by computations with the G^E models and the parameters from Tables 12 and 13.

Conclusions

$P-x$ and H^E data were measured for the binary systems of 2-methyltetrahydrofuran with 2,2,4-trimethylpentane (isooctane), ethanol, toluene, cyclohexane, and methylcyclohexane. The data were obtained with a static VLE apparatus and an isothermal flow calorimeter. From these data, linear temperature-dependent G^E model interaction parameters (NRTL, UNIQUAC) were established. Values predicted with the correlation models and the derived coefficients are in agreement (practically identical) with the experimental values. All relative deviations between experimental and calculated pressures, $\Delta P/P$, are smaller than 0.2%. Similarly, deviations between predicted values of molar excess enthalpy and the experimental data are within the margin of experimental error. The azeotropic compositions and pressures of the binaries 2-methyltetrahydrofuran + ethanol and cyclohexane + 2-methyltetrahydrofuran were established by interpolations of the experimental $P-x$ data. They can be accurately calculated with the G^E model parameters reported herein. Due to the excellent agreement between all experimental and calculated values, these parameters can be recommended for the investigated systems in a temperature range from 293 K to 343 K.

The data and the correlation parameters were deemed necessary and, hence, obtained as part of an undertaking to augment the capability to predict/simulate the volatilities of reformulated and alternative automotive fuels (Zudkevitch et al., 1995).

Acknowledgment

The authors thank J. Schröder for the technical assistance.

Literature Cited

Abrams, D. S.; Prausnitz, J. M. Statistical Thermodynamics of Liquid Mixtures: A New Expression for the Excess Gibbs Energy of Partly or Completely Miscible Systems. *AIChE J.* **1975**, *21*, 116−128.

Caruana, C. M. New Fuels Aim to Put AFVs into High Gear. *Chem. Eng. Prog.* **1998**, *94* (12), 11−14.

Fischer, K.; Gmehling, J. $P-x$ and γ^∞ Data for the Different Binary Butanol−Water Systems at 50 °C. *J. Chem. Eng. Data* **1994**, *39*, 309−315.

Gibbs, R. E.; Van Ness, H. C. Vapor−Liquid Equilibria from Total-Pressure Measurements. A New Apparatus. *Ind. Eng. Chem. Fundam.* **1972**, *11*, 410−413.

Gmehling, J.; Excess Enthalpies for 1,1,1-Trichloroethane with Alkanes, Ketones, and Esters. *J. Chem. Eng. Data* **1993**, *38*, 143−146.

Gmehling, J.; et al. *Ind. Eng. Chem. Res.* **1999**, in preparation.

Paul, S. F. U.S. Patent No. 5,697,987, Dec 16, 1997.

Paul, S. F. An Optimized Alternative Motor Fuel Formulation: Natural Gas Liquids, Ethanol and Biomass-Derived Ether, Presented at the 216th American Chemical Society National Meeting, Boston, August, 1998, Division of Fuel Chemistry, Preprint Vol. 43, No. 3, p 373.

Rarey, J.; Gmehling, J. Computer-Operated Differential Static Apparatus for the Measurement of Vapor-Liquid Equilibrium Data. *Fluid Phase Equilib.* **1993**, *83*, 279−287.

Rarey, J.; Horstmann, S.; Gmehling J. Vapor−Liquid Equilibria and Vapor Pressure Data for the Systems Ethyl *tert*-Butyl Ether + Ethanol and Ethyl *tert*-Butyl Ether + Water. *J. Chem. Eng. Data* **1999**, *44*, 532−538.

Renon, H.; Prausnitz, J. M. Local Compositions in Thermodynamic Excess Functions for Liquid Mixtures. *AIChE J.* **1968**, *14*, 135−144.

Zudkevitch, D.; Murthy, A. K. S.; Gmehling, J. Thermodynamics of Reformulated Automotive Fuels. *Hydrocarbon Process.* **1995**, *74*, 93−100.

Received for review January 18, 1999. Accepted May 26, 1999.

JE990023X