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Articles

Liquid−Liquid Equilibria for Mixtures of (Furfural + a Chlorinated Aromatic Compound + an Alkane) at $T = 298.15$ K

Piotr Morawski,[†] Trevor M. Letcher,* and Pavan K. Naicker[‡]

School of Pure and Applied Chemistry, University of Natal, Durban, South Africa 4041

Urszula Domańska

Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00664 Warsaw, Poland

Liquid−liquid equilibrium results for mixtures of furfural + a chlorinated aromatic compound + an alkane at $T = 298.15$ K are reported, where a chlorinated aromatic compound refers to chlorobenzene, 1,2-dichlorobenzene, 1,3-dichlorobenzene, or 1,2,4-trichlorobenzene and an alkane refers to *n*-hexane, *n*-dodecane, or *n*-hexadecane. The compositions of the conjugated phases were correlated with the UNIQUAC equation and the NRTL equation.

Introduction

Chlorinated aromatic compounds and aliphatic compounds are of great interest to the chemical industry as they appear in the manufacture of pesticides, paint, plasticizers, printing ink, adhesives, flame retardants, hydraulic, and heat transfer fluids.[1] They are also the subject of environmental impact studies.[2,3] In this work, liquid−liquid equilibrium results for mixtures of furfural + a chlorinated aromatic compound + an alkane at $T = 298.15$ K are reported, where a chlorinated aromatic compound refers to chlorobenzene, 1,2-dichlorobenzene, 1,3-dichlorobenzene, or 1,2,4-trichlorobenzene and an alkane refers to *n*-hexane, *n*-dodecane, or *n*-hexadecane.

A search of the literature has indicated that data for mixtures presented here have not been reported previously.

The NRTL model[4] and the UNIQUAC model[5] were used to correlate the tie line data.

Experimental Section

Procedure. The binodal curves were determined at 298.15 K using the cloud point method, described in detail by Letcher et al.[6,7] The tie lines were determined using a method described in detail by Letcher et al.[6,7] based on the refractive index method of Briggs and Comings.[8] The accuracy of this technique was established in a previous paper[9] by comparing results obtained in our laboratory with literature values for a test system. The results from the method used in this work agreed to within 0.005 mole fraction of the results of the test system, which were measured using gas−liquid chromatography. The method was further verified by comparing the results of the tie lines with tie line data obtained using gas−liquid chromatography, and the results were in excellent agreement. The GLC results for furfural suffered from very long retention times, as a result of it's low vapor pressure. This reduced the precision of the GLC results considerably. The results obtained from the binodal curve determination followed by the refractive index method to define the tie-line concentrations on the binodal curve were thus considered superior and are recorded here. The temperature was controlled to within 0.01 K using a Tronac temperature controller used in conjunction with a calibrated Hewlett-Packard Quartz Thermometer.

Table 1. Details of the Chemicals: Percentage Mole Fraction Purities, UNIQUAC Structural Parameters, and Refractive Indicies

compound	purity percent mole fraction	UNIQUAC structural parameters[14] r	q^a	n_D^{25} expt	lit.[15,16]
$C_5H_4O_2$	>99.5	3.17	2.48	1.4001	1.4001
C_6H_5Cl	>99.0	3.81	2.84	1.5218	1.5219
1,2-$C_6H_4Cl_2$	>99.0	4.44	3.29	1.5491	1.5491
1,3-$C_6H_4Cl_2$	>99.0	4.44	3.29	1.5432	1.5434
1,2,4-$C_6H_3Cl_3$	>99.0	5.06	3.73	1.5220	1.524
$CH_3(CH_2)_4CH_3$	>99.0	4.50	3.86	1.3728	1.3723
$CH_3(CH_2)_{10}CH_3$	>99.0	8.55	7.10	1.4275	1.4269
$CH_3(CH_2)_{12}CH_3$	>99.0	11.24	8.26	1.4325	1.4325

[a] $q' = q$ for the compounds used in this work.

Chemicals. The suppliers of all chemicals used in this work are given in Table 1. The purities of the chemicals were determined by gas chromatography and the results are recorded in Table 1. Furfural was distilled under vacuum and kept sealed in a bottle until use. Furfural was tested for moisture using the Karl Fischer method. The moisture was found to be less than 0.1% percentage mole fraction. All other chemicals were not treated further.

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* To whom correspondence should be addressed. E-mail: letcher@nu.ac.za. Fax: +27 31 260 3091.

[†] Visiting researcher from Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, 00664 Warsaw, Poland.

[‡] Presently on a Postdoctoral Grant to the Department of Chemical Engineering, The University of Tennessee, Knoxville, Tennessee 37996.

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Table 2. Composition of Points on the Binodal Curve for the Mixtures {$x_1C_5H_6O_2 + x_2C_6H_{6-m}HCl_m + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_nCH_3$} at $T = 298.15$ K

x_1	x_2	x_1	x_2	x_1	x_2
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_4CH_3$		$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2$+ $CH_3(CH_2)_4CH_3$		$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2$+ $CH_3(CH_2)_4CH_3$	
0.021	0.000	0.021	0.000	0.021	0.000
0.053	0.122	0.053	0.060	0.063	0.111
0.104	0.220	0.101	0.128	0.094	0.144
0.151	0.264	0.155	0.176	0.124	0.195
0.204	0.283	0.206	0.212	0.224	0.225
0.272	0.308	0.293	0.238	0.301	0.249
0.366	0.287	0.394	0.242	0.381	0.254
0.436	0.277	0.459	0.237	0.462	0.243
0.509	0.260	0.554	0.217	0.548	0.223
0.622	0.212	0.629	0.181	0.674	0.168
0.774	0.118	0.764	0.115	0.771	0.107
0.934	0.000	0.863	0.052	0.870	0.046
		0.934	0.000	0.934	0.000
$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3$ + $CH_3(CH_2)_4CH_3$		$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{10}CH_3$		$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{14}CH_3$	
0.021	0.000	0.040	0.000	0.028	0.000
0.049	0.041	0.072	0.143	0.066	0.203
0.095	0.122	0.084	0.252	0.098	0.345
0.145	0.170	0.111	0.320	0.122	0.408
0.192	0.215	0.146	0.380	0.140	0.460
0.253	0.235	0.226	0.434	0.228	0.514
0.303	0.241	0.305	0.439	0.300	0.509
0.394	0.245	0.371	0.427	0.354	0.497
0.460	0.236	0.424	0.415	0.411	0.475
0.549	0.216	0.471	0.415	0.457	0.457
0.669	0.168	0.541	0.372	0.511	0.426
0.769	0.105	0.652	0.299	0.599	0.364
0.874	0.042	0.838	0.132	0.702	0.278
0.934	0.000	0.966	0.000	0.995	0.000
$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2$ + $CH_3(CH_2)_{14}CH_3$		$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2$ + $CH_3(CH_2)_{14}CH_3$		$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3$ + $CH_3(CH_2)_{14}CH_3$	
0.028	0.000	0.028	0.000	0.028	0.000
0.046	0.149	0.046	0.175	0.045	0.132
0.082	0.283	0.075	0.261	0.088	0.285
0.123	0.355	0.100	0.342	0.125	0.345
0.166	0.396	0.147	0.403	0.157	0.397
0.207	0.430	0.191	0.444	0.217	0.417
0.259	0.449	0.246	0.474	0.269	0.433
0.330	0.455	0.317	0.469	0.390	0.433
0.403	0.441	0.386	0.454	0.494	0.408
0.497	0.409	0.496	0.410	0.563	0.367
0.558	0.377	0.559	0.377	0.628	0.328
0.615	0.340	0.621	0.338	0.762	0.219
0.754	0.227	0.725	0.254	0.995	0.000
0.995	0.000	0.995	0.000		

Results

The composition of points on the binodal curve for the mixtures ($C_5H_6O_2 + C_6H_{6-m}Cl_m + CH_3(CH_2)_nCH_3$) at $T = 298.15$ K are reported in Table 2 where m is the number of chlorine atoms on the benzene ring and n is number of CH_2 units in the alkane compound. The compositions of conjugate phases for these mixtures (tie lines) are given in Table 3. The composition of the plait points or critical points, which were determined following the method of Treybal,[10] are given in Table 4. The ternary phase diagrams showing the binodal curve together with tie lines and plait points are given in Figure 1. The ability of furfural to separate aromatic and aliphatic hydrocarbon mixtures is indicated by the selectivity, S, defined as[11,12]

$$S = (x_{21}/x_{31})/(x_{23}/x_{33})$$

where x_{ij} represents the molefraction of component "i" in the phase rich in component "j". The selectivities are presented in Table 3. A good solvent for separating two components is characterized by a value of the separation factor which is significantly different from one.

Tie Line Correlation. The nonrandom two liquid (NRTL) model[4] and the universal quasichemical (UNIQUAC) model[5] are used to correlate the tie line data. The parameters for these models were determined using a computer program that minimized the following objective function using a simplex optimization routine.[13]

$$OF = \sum_{k=1}^{n}\sum_{l=1}^{2}\sum_{i=1}^{3}(x_{kli} - \bar{x}_{kli})^2$$

where x_{kli} is the experimental composition of component i in phase l for kth tie line and $\bar{x}_{kli}$ is the calculated composition of component i in phase l for kth tie line. In fitting the NRTL equation, the nonrandomness parameter α of 0.30 was found to yield the best results. The pure component structural parameters (r, q, and q') from the UNIQUAC model were defined in the original paper[5] and are given in Table 1. The resulting binary interaction parameters and the root-mean-square (rms) deviations are reported in Tables 5 and 6. The symbols and notation used in these tables are consistent with the original work by Renon and Prausnitz[4] and Abrams and Prausnitz.[5]

Table 3. Composition of Conjugate Phases for the Mixtures $\{x_1C_5H_6O_2 + x_2C_6H_{6-m}HCl_m + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_nCH_3\}$ at T = 298.15 K and the Selectivity, S

x_{11}	x_{21}	x_{13}	x_{23}	S
		$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_4CH_3$		
0.038	0.069	0.87	0.051	8.4
0.059	0.147	0.798	0.104	5.7
0.136	0.253	0.656	0.188	2.9
0.268	0.302	0.475	0.268	1.5
		$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2 + CH_3(CH_2)_4CH_3$		
0.042	0.056	0.873	0.050	10.5
0.083	0.110	0.816	0.086	6.4
0.149	0.172	0.700	0.152	4.1
0.22	0.218	0.585	0.202	2.4
		$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2 + CH_3(CH_2)_4CH_3$		
0.038	0.061	0.911	0.020	4.3
0.052	0.104	0.870	0.051	5.2
0.120	0.171	0.751	0.125	4.2
0.241	0.240	0.552	0.229	2.3
		$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3 + CH_3(CH_2)_4CH_3$		
0.055	0.059	0.891	0.032	6.2
0.103	0.123	0.799	0.087	4.8
0.155	0.176	0.730	0.139	4.0
0.234	0.232	0.595	0.197	2.2
		$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{10}CH_3$		
0.06	0.101	0.914	0.040	7.2
0.072	0.173	0.842	0.111	10.3
0.103	0.300	0.751	0.200	8.1
0.141	0.392	0.661	0.289	6.9
		$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{14}CH_3$		
0.050	0.116	0.932	0.058	41.7
0.069	0.210	0.859	0.127	31.1
0.098	0.347	0.768	0.213	17.9
0.136	0.447	0.693	0.284	11.5
		$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2 + CH_3(CH_2)_{14}CH_3$		
0.045	0.104	0.932	0.059	53.6
0.060	0.191	0.888	0.102	40.0
0.102	0.332	0.768	0.213	19.1
0.169	0.410	0.680	0.289	9.6
		$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2 + CH_3(CH_2)_{14}CH_3$		
0.041	0.119	0.944	0.047	36.9
0.056	0.219	0.902	0.087	26.2
0.104	0.35	0.811	0.173	16.9
0.160	0.431	0.757	0.222	10.0
		$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3 + CH_3(CH_2)_{14}CH_3$		
0.053	0.112	0.935	0.052	29.8
0.068	0.197	0.878	0.105	23.0
0.104	0.32	0.8	0.179	15.3
0.144	0.383	0.742	0.231	10.6

Table 4. Composition of Plait Points for the Mixtures $\{x_1C_5H_4O_2 + x_2C_6H_{6-m}Cl_m + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_nCH_3\}$ at T = 298.15 K

	x_1	x_2
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_4CH_3$	0.395	0.286
$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2 + CH_3(CH_2)_4CH_3$	0.400	0.242
$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2 + CH_3(CH_2)_4CH_3$	0.387	0.251
$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3 + CH_3(CH_2)_4CH_3$	0.408	0.248
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{10}CH_3$	0.380	0.429
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{14}CH_3$	0.370	0.492
$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2 + CH_3(CH_2)_{14}CH_3$	0.376	0.452
$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2 + CH_3(CH_2)_{14}CH_3$	0.438	0.434
$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3 + CH_3(CH_2)_{14}CH_3$	0.403	0.435

Discussion

All of the data reported here contributes new information to the literature. The mixtures (furfural + a chlorinated aromatic compound + an alkane) were studied in order to determine the suitability of furfural for separating halogenated aromatic compound−aliphatic hydrocarbon mixtures. Aromatic compounds with increasing numbers of chlorine atoms (1, 2, and 3) on the benzene ring were investigated to establish the effect of substitution on the benzene ring on the phase equilibrium. Alkanes of three different chain lengths (6, 12, and 16) were investigated to establish the effect of chain length on the phase equilibrium.

The area of the two-phase region for the mixtures (furfural + a chlorinated aromatic hydrocarbon + an alkane) is appreciably large, indicating the mutual immiscibility of the components of the mixture. An increase in the number of carbon atoms in the alkane results in an increase in the area of the two-phase region. This indicates a decrease in the mutual solubility of the components as the alkane chain length increases. There is a slight decrease in the area of the two-phase region as the number of chlorine atoms on the benzene rings increases. This indicates that as the number of chlorine atoms in the benzene ring increases there is an increase in the mutual solubility of the components of the mixture.

The solubility of the chlorinated aromatic compound in the aliphatic rich phase increases as the carbon chain

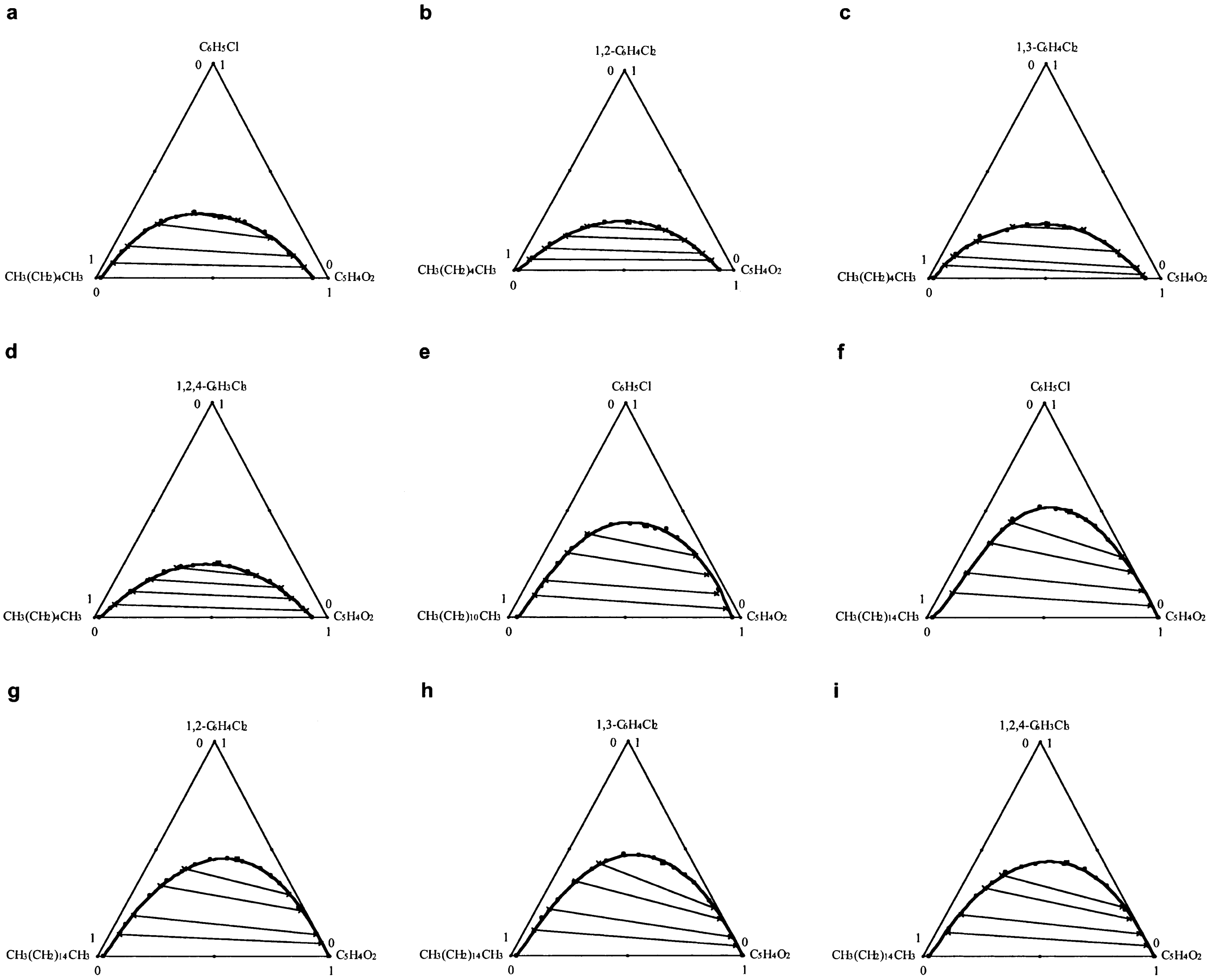

Figure 1. Liquid−liquid equilibrium results for the mixture a, $\{x_1C_5H_4O_2 + x_2C_6H_5Cl + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_4CH_3\}$; b, $\{x_1C_5H_4O_2 + x_21,2\text{-}C_6H_4Cl_2 + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_4CH_3\}$; c, $\{x_1C_5H_4O_2 + x_21,3\text{-}C_6H_4Cl_2 + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_4CH_3\}$; d, $\{x_1C_5H_4O_2 + x_21,2,4\text{-}C_6H_3Cl_3 + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_4CH_3\}$; e, $\{x_1C_5H_4O_2 + x_2C_6H_5Cl + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_{10}CH_3\}$; f, $\{x_1C_5H_4O_2 + x_2C_6H_5Cl + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_{14}CH_3\}$; g, $\{x_1C_5H_4O_2 + x_21,2\text{-}C_6H_5Cl_2 + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_{14}CH_3\}$; h, $\{x_1C_5H_4O_2 + x_21,3\text{-}C_6H_5Cl_2 + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_{14}CH_3\}$; i, $\{x_1C_5H_4O_2 + x_21,2,4\text{-}C_6H_5Cl_3 + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_{14}CH_3\}$; at $T = 298.15$ K. ●, points on the binodal curve; ×, points connecting conjugate phases; ■, critical or plait point.

Table 5. NRTL Binary Interaction Parameters and the Root-Mean-Square-Deviations (rms) for the Mixtures[a] $\{x_1C_5H_4O_2 + x_2C_6H_{6-m}Cl_m + (1\text{-}x_1\text{-}x_2)CH_3(CH_2)_nCH_3\}$ **at** $T = 298.15$ **K**

	g_{12}-g_{22} / J mol^{-1}	g_{21}-g_{11} / J mol^{-1}	g_{13}-g_{33} / J mol^{-1}	g_{31}-g_{11} / J mol^{-1}	g_{23}-g_{33} / J mol^{-1}	g_{32}-g_{22} / J mol^{-1}	rms
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_4CH_3$	44.3	−3794.2	−3938.9	−2947.5	−2382.6	−1138.0	0.007
$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2 + CH_3(CH_2)_4CH_3$	−20.9	−2947.6	−3379.8	−3226.3	−4179.3	2402.6	0.009
$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2 + CH_3(CH_2)_4CH_3$	−63.4	−3748.3	−3924.3	−2776.8	−3209.9	−134.9	0.009
$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3 + CH_3(CH_2)_4CH_3$	−124.7	−3700.0	−3900.0	−2770.0	−3520.0	−130.0	0.009
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{10}CH_3$	100.4	580.5	−2850.5	−3809.4	1614.0	1924.2	0.007
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{14}CH_3$	−38.8	−1802.6	−3450.3	−4885.3	−2477.3	2986.7	0.009
$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2 + CH_3(CH_2)_{14}CH_3$	−43.0	−1801.9	−3407.1	−4676.5	−2775.6	2873.0	0.006
$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2 + CH_3(CH_2)_{14}CH_3$	106.2	−2454.4	−3631.9	−4581.9	−1936.3	1612.0	0.005
$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3 + CH_3(CH_2)_{14}CH_3$	7.37	−2098.7	−3421.7	−4465.9	−2745.7	3228.1	0.006

[a] $\alpha = 0.30$.

length of the alkane increases from 6 to 16. Further evidence of this is the slope of the tie lines (Figure 1) and the solubility graph (Figure 2) which shows the distribution of the chlorinated aromatic compound in the aliphatic rich phase and in the furfural rich phase. The solubility graph (Figure 2) also shows that, as the number of chlorine atoms on the benzene ring increases, the chlorinated aromatic compound becomes more soluble in the alkane-rich phase.

The significant two-phase region as well as the *S* values (ranging from 1.5 to 53) indicate that furfural is a suitable solvent in the liquid−liquid extraction processes for separating chlorinated aromatic compound−aliphatic mixtures.

Table 6. UNIQUAC Binary Interaction Parameters and the Root-Mean-Square-Deviations (rms) for the Mixtures $\{x_1C_5H_4O_2 + x_2C_6H_{6-m}Cl_m + (1-x_1-x_2)CH_3(CH_2)_nCH_3\}$ at $T = 298.15$ K

	$u_{12}-u_{22}$ J mol^{-1}	$u_{21}-u_{11}$ J mol^{-1}	$u_{13}-u_{33}$ J mol^{-1}	$u_{31}-u_{11}$ J mol^{-1}	$u_{23}-u_{33}$ J mol^{-1}	$u_{32}-u_{22}$ J mol^{-1}	rms
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_4CH_3$	−71.96	−228.0	−261.4	−9.64	−262.3	37.37	0.011
$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2 + CH_3(CH_2)_4CH_3$	−71.11	−209.7	−245.8	−19.16	−274.9	72.96	0.010
$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2 + CH_3(CH_2)_4CH_3$	−47.35	−206.5	−250.7	−18.52	−256.8	69.06	0.012
$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3 + CH_3(CH_2)_4CH_3$	−55.98	−178.4	−236.2	−37.57	−270.9	112.2	0.016
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{10}CH_3$	−168.6	−62.20	−318.1	256.2	−133.4	9.45	0.011
$C_5H_4O_2 + C_6H_5Cl + CH_3(CH_2)_{14}CH_3$	−208.3	−61.49	−311.6	259.7	−142.9	12.97	0.012
$C_5H_4O_2$ + 1,2-$C_6H_4Cl_2 + CH_3(CH_2)_{14}CH_3$	21.05	−52.91	−292.2	184.9	−158.0	274.2	0.013
$C_5H_4O_2$ + 1,3-$C_6H_4Cl_2 + CH_3(CH_2)_{14}CH_3$	46.46	−76.06	−269.9	122.6	−107.0	229.0	0.013
$C_5H_4O_2$ + 1,2,4-$C_6H_3Cl_3 + CH_3(CH_2)_{14}CH_3$	58.29	−82.00	−270.7	129.1	−135.7	229.0	0.011

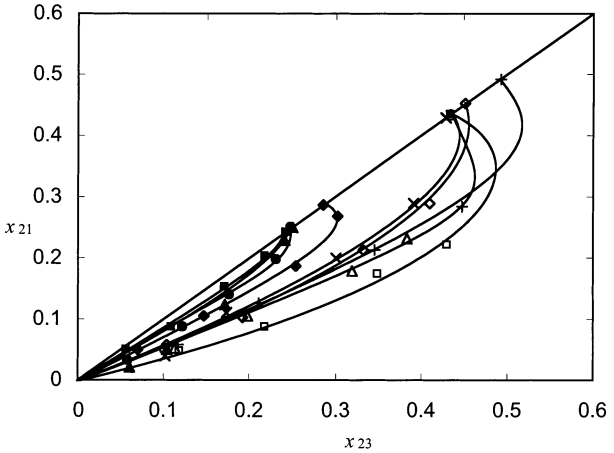

Figure 2. Distribution of the halogenated aromatic compound between the furfural rich phase and the alkane rich phase at $T = 298.15$ K. x_{21} and x_{23} are the concentration of the halogenated aromatic compound in the furfural rich phase and the concentration of the halogenated aromatic compound in the alkane rich phase, respectively. ◆, $\{x_1C_5H_4O_2 + x_2C_6H_5Cl + (1-x_1-x_2)CH_3(CH_2)_4CH_3\}$; ■, $\{x_1C_5H_4O_2 + x_2$1,2-$C_6H_4Cl_2 + (1-x_1-x_2)CH_3(CH_2)_4CH_3\}$; ▲, $\{x_1C_5H_4O_2 + x_2$1,3-$C_6H_4Cl_2 + (1-x_1-x_2)CH_3(CH_2)_4CH_3\}$; ●, $\{x_1C_5H_4O_2 + x_2$1,2,4-$C_6H_3Cl_3 + (1-x_1-x_2)CH_3(CH_2)_4CH_3\}$; ×, $\{x_1C_5H_4O_2 + x_2C_6H_5Cl + (1-x_1-x_2)CH_3(CH_2)_{10}CH_3\}$; +, $\{x_1C_5H_4O_2 + x_2C_6H_5Cl + (1-x_1-x_2)CH_3(CH_2)_{14}CH_3\}$; ◇, $\{x_1C_5H_4O_2 + x_2$1,2-$C_6H_4Cl_2 + (1-x_1-x_2)CH_3(CH_2)_{14}CH_3\}$; □, $\{x_1C_5H_4O_2 + x_2$1,3-$C_6H_4Cl_2 + (1-x_1-x_2)CH_3(CH_2)_{14}CH_3\}$; △, $\{x_1C_5H_4O_2 + x_2$1,2,4-$C_6H_3Cl_3 + (1-x_1-x_2)CH_3(CH_2)_{14}CH_3\}$.

The selectivities for mixtures containing hexadecane are higher than those for the corresponding mixtures with hexane and dodecane which indicates that furfural is more effective at separating chlorinated aromatic compounds−hexadecane mixtures.

Both the NRTL and UNIQUAC models are able to model the tie-line data; however, the NRTL performs slightly better at correlating the data. This is not entirely unexpected as the additional parameter in the NRTL model compared to the UNIQUAC model makes it more flexible and it is able to correlate the data better.

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