Liquid−Liquid Equilibria for Phenolic Compounds, Neutral Oils, and Nitrogen Bases at 313.15 K

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Liquid−liquid extraction with triethylene glycol as solvent, water as cosolvent, and hexane as countersolvent is being investigated as a process for the separation of phenolic compounds from neutral oils and nitrogen bases. To this end, liquid−liquid equilibria at 313.15 K and atmospheric pressure have been determined for the systems triethylene glycol + hexane + water + (phenol + aniline + benzonitrile + 5-ethyl-2-methyl pyridine + mesitylene) or (*m*-cresol + *o*-tolunitrile + *o*-toluidine + indene + pseudocumene + undecane) or (2,4-xylenol + 3,4-xylenol + 3,5-xylenol + indane + naphthalene + dodecane). From the experimental results it is concluded that triethylene glycol, hexane, and water are effective solvents for the separation of phenolic compounds from neutral oils and nitrogen bases by means of liquid−liquid extraction. LLE binary parameters for the NRTL equation were obtained for each of the three systems by regression of the equilibrium data. The NRTL equation fit the experimental data with a root-mean-square-deviation (RMSD) of 0.0037, 0.0100, and 0.0058 for the systems containing phenol, *m*-cresol, and the xylenol isomers, respectively.

Introduction

Coal pyrolysis liquors are rich in valuable phenolic compounds−cresols typically account for 25%−45% of light and middle coal liquor distillates.[1] The separation of the phenolic compounds from the neutral oils and nitrogen bases also present in the pyrolysis liquors is however difficult due to low relative volatilities and the formation of azeotropes and eutectics. The desired phenolic recovery and phenolic product purity can therefore not be achieved by means of conventional distillation processes.

Numerous liquid−liquid extraction processes using only a single selective solvent were therefore proposed as alternative separation processes. The solvents investigated include aqueous solutions of glycols,[2] ethanol amine, acetic acid, ethylamine, sodium salicylate, methanol,[4] and isobutyl acetate.[6] Unfortunately, all of these processes were incapable of achieving adequate phenolic product purity. Significant amounts of residual neutral oils and nitrogen bases remained, especially when phenolic recovery was high.

Dual solvent processes, which incorporated a polar solvent to dissolve the phenolic compounds and a nonpolar solvent to dissolve the neutral oil and nitrogen bases, were therefore investigated. Polar solvents include methanol, ammonia, acetamide, acetic acid, ethanol, monoethylamine, sodium salts of sulfonic acids,[4] and so forth. The nonpolar solvents most commonly used are hexane, heptane, petroleum ether, diesel, and various nonaromatic naphthas.[4] An alternative process in which aqueous ethylene, diethylene, and triethylene glycol are contacted with a distilled tar fraction before washing with a light petroleum ether has also been investigated.[8] In this investigation it was concluded that 80% aqueous ethylene glycol was the optimum solvent with respect to phenolic recovery and product purity. The product purities obtained were however very low, with values ranging from 82 to 93%.

Typical disadvantages of all the above-mentioned solvent extraction processes for the recovery of phenolic compounds from coal tars are the high solvent ratios required, high solvent losses, the complex postpurification required to achieve the desired phenolic product purity, the poor recovery of higher substituted phenols, and the toxicity of the reagents used.

No published liquid−liquid equilibrium data sets that are comprehensive enough to fit thermodynamic models are available for any of the above-mentioned processes.

Solvent extraction using a high-boiling solvent in conjunction with water as a cosolvent and hexane as a countersolvent has been proposed as an alternative separation process. High-boiling solvents such as glycerol, triethylene glycol,[10] and tetraethylene glycol[11] have been previously evaluated using a simplified feed stream composed solely of *m*-cresol and *o*-tolunitrile. A thermodynamic model based on the generated liquid−liquid equilibrium data was used in simulations to assess the performance of a commercial separation unit.[9,11] Both the experimental and simulated results obtained in these preliminary studies indicated that both tri- and tetraethylene glycol are effective solvents for the separation of *m*-cresol from *o*-tolunitrile. It was however imperative that additional data be generated in order to verify that the proposed separation system is effective for a more comprehensive range of the phenolic compounds and neutral oils commonly present in pyrolysis liquors.

Liquid−liquid equilibrium data for a wider range of phenolic compounds, neutral oils, and nitrogen bases is also required in order to determine a thermodynamic model with which the proposed process can be explored and optimized.

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10.1021/je0003389 CCC: $20.00

Table 1. Extract Phase Molar Percentages, x^{I}_{i}, Raffinate Phase Molar Percentages, x^{II}_{i}, and Selectivities, β_{12}, β_{13}, β_{14}, and β_{15}, for Phenol (1) + Benzonitrile (2) + Aniline (3) + 5-Ethyl-2-methylpyridine (4) + Mesitylene (5) + Triethylene Glycol (6) + Water (7) + Hexane (8) at 313.15 K and 101.3 kPa

x^{I}_{1}	x^{I}_{2}	x^{I}_{3}	x^{I}_{4}	x^{I}_{5}	x^{I}_{6}	x^{I}_{7}	x^{II}_{1}	x^{II}_{2}	x^{II}_{3}	x^{II}_{4}	x^{II}_{5}	x^{II}_{6}	x^{II}_{7}	β_{12}	β_{13}	β_{14}	β_{15}
20.90	1.27	1.84	0.79	0.10	19.91	54.37	1.33	0.75	0.31	0.89	2.08	0.19	0.21	9.2	2.6	17.5	341.0
21.43	1.62	1.98	1.15	0.29	19.15	53.28	1.90	1.02	0.38	1.32	5.34	0.07	0.26	7.1	2.2	13.0	209.0
21.03	1.71	1.95	1.24	0.48	19.59	52.85	2.53	1.26	0.47	1.77	8.66	0.06	0.19	6.1	2.0	11.9	149.9
8.90	0.39	0.80	0.21	0.01	12.91	76.55	1.15	0.65	0.30	0.68	1.20	0.08	0.08	12.9	2.9	25.4	726.8
20.51	1.06	1.74	0.56	0.06	19.90	55.27	0.97	0.50	0.24	0.62	1.25	0.00	0.16	10.1	2.9	23.2	413.2
13.33	0.95	1.21	0.64	0.12	12.12	71.24	2.49	1.28	0.43	1.58	5.68	0.01	0.22	7.2	1.9	13.3	264.4
13.81	1.05	1.26	0.73	0.23	12.71	69.73	3.56	1.66	0.70	2.39	9.84	0.01	0.32	6.2	2.2	12.6	169.1
13.38	0.72	1.14	0.42	0.05	12.81	71.12	1.61	0.80	0.34	0.95	2.11	0.11	0.29	9.3	2.5	18.7	371.4
23.78	1.80	2.05	1.29	0.57	10.25	59.28	4.62	1.55	0.86	2.40	9.53	0.02	0.43	4.4	2.2	9.6	85.8
9.77	0.71	0.88	0.52	0.12	13.24	74.57	3.44	1.87	0.70	2.55	9.92	0.03	0.32	7.5	2.2	14.0	235.8
7.73	0.61	0.71	0.39	0.08	14.04	76.32	3.08	2.07	0.48	2.71	10.58	0.03	0.26	8.5	1.7	17.3	333.0
5.31	0.40	0.49	0.29	0.05	13.95	79.46	2.35	1.63	0.34	2.45	11.01	0.04	0.30	9.3	1.6	18.9	477.6
22.33	1.29	1.96	0.73	0.10	10.97	61.98	2.24	0.80	0.37	0.99	2.03	0.03	0.25	6.2	1.9	13.6	211.4
9.20	0.52	0.80	0.27	0.02	13.26	75.76	1.40	0.78	0.29	0.99	1.98	0.02	0.17	9.8	2.4	24.0	587.1
7.24	0.42	0.67	0.21	0.02	13.57	77.77	1.39	0.83	0.30	1.09	2.13	0.06	0.17	10.2	2.3	27.1	679.0
5.10	0.30	0.47	0.15	0.01	13.88	79.92	1.07	0.84	0.25	1.01	2.21	0.02	0.14	13.3	2.6	33.1	723.4
33.12	2.52	3.07	1.83	0.71	29.46	28.63	1.81	0.92	0.36	1.14	5.46	0.05	0.20	6.7	2.1	11.3	139.6
32.73	2.70	3.18	2.14	1.14	28.53	29.02	2.20	1.04	0.39	1.35	9.00	0.07	0.47	5.7	1.8	9.4	117.2
25.17	1.62	2.18	1.07	0.21	35.38	33.23	0.96	0.58	0.22	0.74	1.88	0.04	0.15	9.3	2.6	18.1	240.3
32.82	1.78	2.73	1.01	0.14	30.60	28.83	1.08	0.51	0.26	0.55	1.21	0.04	0.10	8.7	2.9	16.7	258.2
45.36	2.68	3.65	1.75	0.33	21.33	20.76	2.00	0.65	0.33	0.71	1.82	0.04	0.11	5.5	2.0	9.2	123.8
32.64	2.09	2.93	1.38	0.27	30.13	28.48	1.13	0.59	0.26	0.70	1.89	0.03	0.08	8.2	2.6	14.5	202.6
21.67	1.30	1.89	0.90	0.21	37.80	35.13	0.91	0.60	0.24	0.73	1.90	0.03	0.07	10.9	3.0	19.5	217.0
15.57	1.01	1.41	0.74	0.19	41.44	38.66	0.48	0.44	0.14	0.60	1.89	0.00	0.09	14.2	3.3	26.3	331.0
21.37	1.09	1.73	0.59	0.06	10.86	62.98	1.73	0.63	0.35	0.64	1.24	0.03	0.12	7.1	2.5	13.5	238.0
13.10	0.56	1.06	0.29	0.03	12.84	71.60	1.25	0.60	0.29	0.67	1.24	0.01	0.11	11.4	2.9	24.1	485.8
7.17	0.31	0.61	0.16	0.01	13.82	77.59	1.06	0.62	0.27	0.66	1.25	0.01	0.09	13.6	3.0	27.5	735.3
4.94	0.23	0.44	0.13	0.01	14.25	79.82	0.74	0.55	0.21	0.64	1.16	0.02	0.06	16.2	3.1	33.8	624.5
22.54	1.60	2.06	1.20	0.31	10.59	60.47	3.19	1.09	0.47	1.36	5.12	0.02	0.33	4.8	1.6	8.1	118.2
9.90	0.68	0.96	0.46	0.07	13.39	74.24	2.34	1.23	0.43	1.75	5.22	0.03	0.19	7.7	1.9	16.1	314.6
6.89	0.47	0.64	0.30	0.04	12.53	78.91	2.10	1.25	0.37	1.70	5.16	0.03	0.13	8.8	1.9	18.4	464.4
5.03	0.37	0.49	0.25	0.03	13.90	79.80	1.60	1.18	0.30	1.72	5.54	0.40	0.15	10.1	1.9	21.6	635.1
31.89	2.01	3.00	1.28	0.20	15.17	43.93	1.96	0.69	0.35	0.75	1.99	0.04	0.15	5.6	1.9	9.6	162.9
14.68	0.91	1.40	0.57	0.07	20.69	61.03	1.09	0.68	0.27	0.80	2.08	0.02	0.10	10.1	2.6	18.9	385.6
11.84	0.72	1.09	0.46	0.04	22.16	63.25	0.92	0.64	0.24	0.82	2.13	0.01	0.08	11.3	2.9	22.8	672.0
8.60	0.56	0.81	0.36	0.04	23.42	65.66	0.61	0.58	0.18	0.76	2.08	0.17	0.05	14.5	3.1	29.6	716.4
15.13	1.19	1.45	0.82	0.19	20.56	59.97	1.62	1.01	0.34	1.33	5.37	0.06	0.12	7.9	2.2	15.1	268.6
31.34	2.51	3.10	1.97	0.60	15.01	43.78	2.76	1.01	0.51	1.31	5.10	0.07	0.19	4.6	1.9	7.6	96.7
11.90	0.90	1.11	0.69	0.13	22.27	62.35	1.25	0.86	0.26	1.30	5.50	0.05	0.12	9.1	2.2	17.8	389.1
8.90	0.65	0.85	0.52	0.11	23.54	65.13	1.00	0.82	0.21	1.25	6.10	0.04	0.10	11.1	2.2	21.5	480.7
15.31	1.27	1.50	0.99	0.34	20.26	59.53	1.94	1.16	0.37	1.64	10.16	0.02	0.15	7.3	1.9	13.1	235.5
32.24	2.73	3.14	2.07	1.02	15.17	42.33	3.21	1.08	0.51	1.32	8.25	0.02	0.23	4.0	1.6	6.4	81.4
12.14	0.99	1.20	0.75	0.24	21.88	62.06	1.64	1.12	0.32	1.54	9.67	0.00	0.13	8.3	1.9	15.3	298.1
8.71	0.70	0.84	0.55	0.17	22.66	65.84	1.34	0.98	0.25	1.47	11.71	0.04	0.11	9.1	2.0	17.5	436.3
25.36	1.95	2.48	1.51	0.53	33.55	32.41	1.14	0.76	0.27	1.02	4.90	0.04	0.07	8.7	2.4	15.0	205.0
20.37	1.84	2.07	1.26	0.44	37.06	35.77	0.90	0.71	0.22	0.97	4.93	0.02	0.08	8.8	2.4	17.6	253.3
42.84	3.40	4.04	2.61	0.94	20.34	20.84	2.63	0.93	0.46	1.04	5.00	0.04	0.15	4.4	1.9	6.5	86.7
15.35	1.22	1.44	0.98	0.37	40.68	39.00	0.66	0.58	0.15	0.90	4.93	0.03	0.07	10.9	2.4	21.2	311.5
29.23	1.71	2.68	0.91	0.10	16.70	46.94	1.58	0.59	0.28	0.55	1.14	0.03	0.07	6.3	1.9	11.1	204.9
15.08	0.78	1.32	0.46	0.04	21.23	60.34	0.81	0.54	0.23	0.58	1.22	0.22	0.05	13.0	3.3	23.7	616.3
12.05	0.60	1.07	0.37	0.03	22.44	62.87	0.64	0.49	0.19	0.54	1.24	0.30	0.06	15.2	3.4	27.7	688.6
8.43	0.45	0.77	0.30	0.03	23.84	65.80	0.47	0.47	0.16	0.54	1.22	0.06	0.05	18.3	3.6	32.7	842.6
42.53	2.29	3.51	1.44	0.18	22.09	23.73	1.63	0.54	0.32	0.56	1.21	0.06	0.09	6.1	2.4	10.2	173.9
25.19	1.48	2.12	0.89	0.13	35.32	32.82	0.68	0.48	0.19	0.54	1.19	0.06	0.06	11.8	3.3	22.4	342.7
21.14	1.23	1.85	0.77	0.15	38.43	35.22	0.53	0.45	0.16	0.50	1.21	0.06	0.04	14.4	3.4	26.1	309.9
15.45	0.95	1.42	0.61	0.15	42.19	38.15	0.36	0.37	0.12	0.43	1.12	0.05	0.04	17.0	3.7	30.3	329.6
43.67	2.46	3.92	1.76	0.50	43.10	0.00	1.01	0.47	0.21	0.50	1.24	0.05	0.00	8.3	2.3	12.2	108.0
36.90	2.28	3.27	1.52	0.50	51.76	0.00	0.66	0.42	0.16	0.49	1.11	0.06	0.00	10.4	2.8	18.3	123.5
32.25	1.98	2.90	1.37	0.49	57.70	0.00	0.53	0.39	0.14	0.45	1.08	0.04	0.00	12.1	2.9	19.9	133.2
24.36	1.58	2.23	1.11	0.48	67.43	0.00	0.41	0.30	0.10	0.39	1.06	0.07	0.00	11.2	2.6	21.0	131.6
36.34	2.47	3.35	1.83	0.51	50.58	0.00	0.81	0.50	0.17	0.67	1.84	0.06	0.00	9.0	2.3	16.5	163.3
31.40	2.19	3.05	1.53	0.48	57.70	0.00	0.58	0.46	0.17	0.59	1.79	0.09	0.00	11.4	2.9	20.9	203.3
24.63	1.92	2.37	1.27	0.53	66.34	0.00	0.41	0.39	0.11	0.55	1.71	0.07	0.00	12.3	2.9	26.1	195.9
43.79	2.65	3.77	2.00	0.49	41.01	0.00	1.34	0.56	0.26	0.63	1.89	0.06	0.00	7.0	2.3	10.3	125.9
7.53	0.44	0.70	0.29	0.02	20.72	70.12	0.72	0.63	0.19	0.80	1.99	0.01	0.07	14.8	2.8	29.2	992.1
5.74	0.32	0.50	0.19	0.01	16.02	77.14	0.69	0.70	0.17	0.94	2.04	0.00	0.09	18.1	2.9	41.7	1595.4
11.26	0.62	1.00	0.37	0.03	19.67	66.81	0.92	0.70	0.23	0.86	2.07	0.01	0.10	13.8	2.8	28.4	796.5
7.96	0.40	0.66	0.24	0.02	14.52	76.08	1.18	0.80	0.26	1.04	2.08	0.00	0.12	13.4	2.7	28.8	918.8
20.42	1.09	1.65	0.75	0.08	20.09	55.00	1.39	0.71	0.27	0.80	1.88	0.01	0.11	9.6	2.4	15.5	332.9
19.17	1.10	1.62	0.67	0.08	18.66	57.95	1.19	0.69	0.28	0.83	2.01	0.04	0.10	10.2	2.8	19.7	424.3
15.16	0.79	1.23	0.47	0.05	13.77	68.20	1.50	0.73	0.35	0.97	1.94	0.07	0.14	9.4	2.9	21.0	428.2
11.91	0.65	1.04	0.37	0.03	22.43	63.02	0.67	0.57	0.20	0.73	1.52	0.15	0.00	15.3	3.4	35.4	826.7
15.76	0.91	1.49	0.48	0.05	20.84	59.68	0.88	0.68	0.26	0.75	1.49	0.05	0.00	13.3	3.1	28.0	569.4
31.37	2.17	3.15	1.61	0.38	15.67	42.48	2.34	0.79	0.43	0.98	3.49	0.14	0.00	4.8	1.8	8.1	122.9

Table 2. Extract Phase Molar Percentages, x^I_i, Raffinate Phase Molar Percentages, x^{II}_i, and Selectivities, β_{12}, β_{13}, β_{14}, β_{15} and β_{16}, for *m*-Cresol (1) + *o*-Tolunitrile (2) + *o*-Toluidine (3) + Indene (4) + Pseudocumene (5) + Undecane (6) + Triethylene Glycol (7) + Water (8) + Hexane (9) at 313.15 K and 101.3 kPa

x^I_1	x^I_2	x^I_3	x^I_4	x^I_5	x^I_6	x^I_7	x^I_8	x^{II}_1	x^{II}_2	x^{II}_3	x^{II}_4	x^{II}_5	x^{II}_6	x^{II}_7	x^{II}_8	β_{12}	β_{13}	β_{14}	β_{15}	$10^{-2}\beta_{16}$
14.77	0.65	0.53	1.19	0.08	0.00	12.09	69.30	2.27	1.10	0.77	4.50	1.46	1.13	0.32	0.25	11.0	4.2	55.2	125.5	464.3
8.47	0.28	0.24	0.69	0.05	0.00	13.28	76.38	1.65	0.91	0.74	4.28	1.42	1.19	0.30	0.14	16.6	5.5	93.0	146.4	418.4
6.32	0.24	0.16	0.52	0.01	0.00	13.41	78.97	1.53	1.07	0.74	4.25	1.41	1.15	0.97	0.13	18.4	5.9	110.8	443.9	523.3
4.98	0.20	0.12	0.44	0.03	0.00	14.78	79.14	0.85	1.06	0.58	4.40	1.46	1.14	0.25	0.10	31.1	7.8	211.5	276.9	545.1
3.51	0.15	0.11	0.44	0.02	0.00	14.91	80.55	0.53	1.11	0.68	4.38	1.54	1.17	0.65	0.09	48.2	10.3	260.1	641.2	607.4
23.35	1.26	1.03	1.94	0.16	0.02	18.46	51.44	1.66	1.00	0.71	3.97	1.34	1.09	0.10	0.15	11.2	5.2	54.3	119.1	9.7
15.86	0.96	0.54	1.35	0.13	0.00	21.22	58.25	1.05	1.15	0.68	3.79	1.95	1.41	0.17	0.12	18.1	7.6	105.4	225.4	46.6
10.49	0.54	0.55	0.99	0.05	0.00	22.92	63.89	0.68	0.88	0.51	3.96	1.43	1.14	0.11	0.15	25.2	7.9	111.7	429.7	327.6
8.19	0.44	0.34	0.82	0.04	0.00	24.73	64.74	0.49	0.91	0.45	3.96	1.41	1.16	0.21	0.06	34.8	9.2	196.2	614.6	53.9
14.28	0.72	0.60	1.31	0.07	0.00	20.63	61.19	0.98	0.95	0.57	4.07	1.40	1.15	0.24	0.09	19.2	6.3	99.2	300.6	42.8
7.18	0.32	0.22	0.66	0.03	0.00	16.16	74.97	0.95	0.95	0.59	4.22	1.42	1.17	0.19	0.13	22.6	6.8	145.5	372.2	34.8
9.33	0.64	0.93	1.04	0.14	0.01	13.89	73.21	3.04	3.28	1.73	15.51	6.02	5.36	0.31	0.54	15.7	5.1	50.9	127.8	15.1
6.44	0.43	0.60	0.70	0.08	0.00	13.71	77.65	2.65	3.29	1.51	15.79	6.23	5.55	0.52	0.57	18.4	5.2	63.7	184.7	39.2
4.55	0.32	0.36	0.49	0.04	0.00	12.74	81.13	2.61	3.44	1.59	18.85	6.85	5.44	0.19	0.55	19.1	5.6	92.2	277.2	28.3
8.94	0.32	0.23	0.71	0.03	0.00	13.46	75.77	1.16	0.86	0.58	3.30	1.09	0.85	0.14	0.14	20.5	6.3	113.1	250.6	39.1
14.78	0.58	0.46	1.12	0.07	0.00	11.94	69.63	1.83	0.86	0.66	3.29	1.10	0.86	0.14	0.22	12.0	4.8	57.4	129.3	19.1
6.45	0.22	0.15	0.50	0.01	0.00	14.35	77.91	0.73	0.85	0.54	3.31	1.10	0.87	0.21	0.12	33.3	9.4	200.3	726.6	49.7
4.82	0.17	0.11	0.41	0.01	0.00	14.82	79.33	0.72	0.85	0.51	3.37	1.15	0.86	0.10	0.10	33.0	8.3	213.2	895.2	46.8
3.31	0.12	0.07	0.31	0.01	0.00	15.04	80.76	0.59	0.85	0.47	3.50	1.15	0.86	0.07	0.10	39.3	8.4	265.8	1260.6	71.2
22.26	1.05	0.93	1.83	0.11	0.01	17.52	53.29	1.33	0.78	0.60	3.14	1.10	0.87	0.19	0.13	12.4	5.5	56.4	163.7	15.0
14.50	0.65	0.48	1.26	0.06	0.00	21.79	59.95	0.81	0.75	0.49	3.07	1.07	0.85	0.11	0.09	20.6	6.9	115.1	304.5	51.6
10.50	0.46	0.34	0.90	0.04	0.00	24.21	62.78	0.67	0.76	0.47	3.15	1.12	0.87	0.01	0.07	25.8	8.1	143.5	476.3	75.8
8.31	0.37	0.28	0.79	0.02	0.00	23.76	66.03	0.49	0.77	0.41	3.31	1.17	0.92	0.11	0.08	35.4	8.8	197.5	984.5	316.8
5.90	0.30	0.21	0.60	0.02	0.00	24.29	68.52	0.28	0.69	0.32	3.33	1.16	0.91	0.05	0.06	47.1	11.1	332.8	1087.7	694.1
9.14	0.57	0.69	0.99	0.08	0.00	13.66	73.95	1.95	2.05	1.15	10.96	3.74	3.09	0.07	0.11	16.8	5.4	74.7	211.6	32.6
24.03	1.37	1.62	2.29	0.21	0.02	35.25	31.91	0.66	0.85	0.47	4.90	1.44	1.13	0.05	0.07	22.6	7.5	110.1	251.7	23.8
22.77	0.95	0.71	1.56	0.08	0.01	17.35	52.57	1.26	0.62	0.54	2.62	0.88	0.70	0.05	0.14	11.9	6.2	66.9	198.4	18.6
15.03	0.57	0.42	1.18	0.04	0.00	22.07	58.97	0.71	0.65	0.42	2.64	0.87	0.70	0.01	0.08	24.3	7.6	132.9	427.6	89.3
10.72	0.42	0.34	0.96	0.04	0.00	23.62	62.90	0.58	0.65	0.41	3.02	0.91	0.70	0.01	0.06	28.9	8.0	165.4	467.7	43.6
8.27	0.35	0.23	0.75	0.03	0.00	23.88	65.74	0.46	0.64	0.36	2.63	0.91	0.72	0.04	0.06	33.3	8.6	207.6	607.8	102.0
5.70	0.24	0.18	0.52	0.02	0.00	23.89	69.08	0.38	0.64	0.31	2.62	0.89	0.70	0.02	0.05	40.2	9.0	220.2	549.2	105.8
15.38	0.51	0.36	1.03	0.04	0.00	12.13	68.28	1.45	0.73	0.60	2.67	0.90	0.69	0.06	0.09	15.2	6.2	78.3	221.9	25.1
8.85	0.28	0.16	0.61	0.01	0.00	13.32	75.92	1.00	0.70	0.54	3.03	0.87	0.68	0.07	0.13	22.3	7.8	171.5	708.2	49.0
6.31	0.20	0.11	0.46	0.01	0.00	13.95	78.53	0.86	0.73	0.49	2.67	0.90	0.69	0.01	0.49	27.3	7.9	173.7	661.9	98.7
4.85	0.15	0.09	0.40	0.01	0.00	14.43	79.86	0.68	0.72	0.45	2.68	0.90	0.70	0.01	0.53	33.1	8.0	217.0	845.9	162.6
3.33	0.11	0.07	0.28	0.01	0.00	14.68	81.36	0.58	0.71	0.40	2.74	0.88	0.70	0.04	0.49	38.4	8.3	219.6	724.0	110.0
32.08	3.10	6.00	3.76	1.28	0.29	23.48	22.42	2.41	1.74	1.12	11.93	5.09	5.51	0.05	0.31	7.5	4.0	26.5	53.0	2.5
23.31	2.24	4.03	2.80	0.83	0.10	33.50	29.97	1.09	1.67	0.81	12.00	5.27	5.45	0.03	0.14	15.9	6.2	63.7	135.4	11.3
17.86	1.77	3.25	2.17	0.61	0.06	36.60	34.78	0.84	1.62	0.66	12.31	5.94	6.47	0.01	0.11	19.6	6.5	80.8	208.6	22.5
14.34	1.44	2.74	1.84	0.48	0.05	39.66	37.64	0.63	1.40	0.54	11.59	5.82	5.96	0.23	0.09	22.2	6.7	96.0	277.7	27.6
10.65	1.10	2.19	1.31	0.38	0.04	42.94	40.00	0.39	1.21	0.36	10.51	5.73	6.22	0.02	0.07	30.1	7.7	131.9	416.6	42.7
33.85	1.62	1.25	2.71	0.20	0.01	26.27	24.84	1.17	0.62	0.50	2.64	0.88	0.69	0.01	0.08	11.0	5.3	61.0	129.5	13.8
24.41	1.16	0.96	2.10	0.13	0.01	35.37	33.01	0.64	0.59	0.39	2.61	0.88	0.72	0.01	0.04	19.5	7.0	104.2	262.9	21.7
18.23	0.89	0.78	1.73	0.10	0.01	39.52	36.74	0.36	0.55	0.33	2.51	0.90	0.70	0.01	0.04	31.4	9.7	165.3	463.6	35.9
14.99	0.79	0.73	1.47	0.07	0.00	41.35	38.91	0.25	0.53	0.26	2.47	0.90	0.70	0.01	0.03	41.0	10.9	206.9	786.6	86.3
10.81	0.65	0.65	1.12	0.08	0.01	44.68	40.97	0.18	0.51	0.22	2.40	0.87	0.70	0.02	0.03	47.7	12.2	222.6	638.4	56.7
44.17	2.61	3.15	4.02	0.50	0.09	32.88	0.00	1.24	0.83	0.59	3.63	1.32	1.13	0.03	0.00	11.3	5.2	40.9	93.7	4.6
27.70	1.87	2.61	2.93	0.32	0.04	58.54	0.00	0.35	0.68	0.37	3.52	1.35	1.31	0.01	0.00	28.7	9.9	106.9	335.6	24.5
34.16	2.37	2.89	3.53	0.39	0.05	49.03	0.00	0.33	0.72	0.36	3.73	1.41	1.20	0.02	0.00	31.4	10.7	133.9	372.1	25.9
23.80	1.72	2.41	2.54	0.33	0.06	64.12	0.00	0.26	0.67	0.30	3.68	1.38	1.19	0.02	0.00	35.7	10.8	140.4	377.8	17.5
17.86	1.46	2.15	2.13	0.32	0.05	72.47	0.00	0.13	0.51	0.20	3.33	1.33	1.18	0.05	0.00	45.9	12.4	205.6	557.5	31.9
45.00	2.29	2.46	3.93	0.40	0.06	34.57	0.00	1.18	0.73	0.55	3.01	1.05	0.86	0.04	0.00	12.1	5.3	46.5	100.0	5.5
34.44	1.93	2.01	3.24	0.29	0.03	50.34	0.00	0.49	0.65	0.39	2.97	1.07	0.90	0.00	0.00	23.8	8.5	104.5	262.8	23.8
27.85	1.65	1.90	2.75	0.24	0.02	58.90	0.00	0.31	0.57	0.29	2.85	1.08	0.94	0.00	0.00	31.2	9.4	135.3	408.4	44.9
23.71	1.49	1.80	2.46	0.22	0.02	65.26	0.00	0.25	0.57	0.27	2.78	1.06	0.86	0.00	0.00	36.8	10.5	148.9	461.6	40.6
17.40	1.23	1.88	1.98	0.20	0.02	71.66	0.00	0.15	0.48	0.20	2.65	1.07	0.89	0.00	0.00	46.1	12.3	168.4	641.1	53.6
45.07	2.20	2.07	3.62	0.32	0.05	35.43	0.00	1.17	0.62	0.48	2.60	0.89	0.71	0.00	0.00	10.8	5.1	48.4	106.4	5.1
35.55	1.99	1.71	3.32	0.34	0.04	52.48	0.00	0.50	0.51	0.32	2.47	0.96	0.69	0.00	0.00	18.4	6.9	103.3	199.9	11.5
28.41	1.61	1.74	2.80	0.27	0.05	58.82	0.00	0.29	0.51	0.27	2.41	0.86	0.73	0.00	0.00	31.1	9.4	135.4	313.2	13.9
23.40	1.48	1.77	2.47	0.21	0.04	63.95	0.00	0.20	0.47	0.22	2.36	0.86	0.68	0.02	0.00	36.8	10.4	155.2	475.2	20.5
18.05	1.16	2.21	1.91	0.50	0.20	72.63	0.00	0.15	0.44	0.19	1.91	0.73	0.66	0.01	0.00	45.9	11.9	104.7	175.4	4.0
7.26	0.60	0.94	0.85	0.10	0.00	23.86	66.19	0.88	2.49	0.82	16.54	7.32	6.29	0.57	0.56	34.3	7.9	145.6	632.8	233.4
6.96	0.53	0.60	0.79	0.06	0.00	23.80	66.99	0.49	1.49	0.56	9.22	3.63	3.00	0.12	0.30	40.3	10.1	218.3	847.0	263.9
6.94	0.43	0.39	0.75	0.05	0.00	23.83	67.38	0.37	1.08	0.45	5.67	2.08	1.70	0.01	0.13	46.9	11.1	269.4	706.4	330.8
6.82	0.36	0.31	0.71	0.03	0.00	23.68	66.66	0.32	0.86	0.43	4.28	1.51	1.21	0.47	0.05	50.7	13.1	291.3	937.9	213.9
6.80	0.36	0.30	0.68	0.03	0.00	24.67	65.63	0.30	0.68	0.32	3.08	1.09	1.01	0.01	0.04	43.5	10.9	233.2	748.8	104.2
19.69	1.30	1.74	2.14	0.33	0.08	68.95	0.00	0.16	0.45	0.19	2.28	0.87	0.70	0.01	0.04	43.4	11.2	163.2	331.2	10.4
12.31	0.64	0.79	1.18	0.13	0.01	41.91	38.29	0.21	0.50	0.24	2.30	0.83	0.68	0.01	0.03	45.9	12.1	169.7	369.1	27.0
6.71	0.30	0.25	0.62	0.04	0.00	23.81	66.10	0.38	0.60	0.32	2.53	0.87	0.68	0.01	0.06	35.3	8.9	176.4	370.3	62.8
4.06	0.13	0.07	0.32	0.01	0.00	14.46	80.03	0.66	0.74	0.43	2.76	0.93	0.72	0.01	0.05	34.3	8.2	234.1	709.9	54.4
2.82	0.07	0.03	0.21	0.00	0.00	10.76	85.88	0.73	0.77	0.50	2.86	0.93	0.73	0.01	0.07	42.3	9.1	381.0	1607.1	140.2
24.30	1.15	1.02	2.17	0.13	0.01	34.82	33.68	0.63	0.71	0.42	3.14	1.08	0.87	0.01	0.05	24.0	7.5	119.0	317.3	33.6
18.20	0.96	0.99	1.76	0.10	0.01	37.71	35.63	0.34	0.66	0.35	3.04	1.09	0.88	0.01	0.04	37.0	10.7	164.3	577.2	65.6
35.37	1.73	1.63	2.92	0.23	0.03	27.60	25.05	1.22	0.75	0.57	3.13	1.10	0.87	0.01	0.10	12.5	5.6	55.4	139.8	10.1

Table 2 (Continued)

x^{I}_{1}	x^{I}_{2}	x^{I}_{3}	x^{I}_{4}	x^{I}_{5}	x^{I}_{6}	x^{I}_{7}	x^{I}_{8}	x^{II}_{1}	x^{II}_{2}	x^{II}_{3}	x^{II}_{4}	x^{II}_{5}	x^{II}_{6}	x^{II}_{7}	x^{II}_{8}	β_{12}	β_{13}	β_{14}	β_{15}	$10^{-2}\beta_{16}$
14.51	0.85	0.90	1.56	0.09	0.01	41.43	38.15	0.25	0.63	0.30	2.93	1.11	0.89	0.01	0.05	42.3	11.1	187.0	721.1	98.0
10.34	0.67	0.70	1.08	0.08	0.01	43.20	40.14	0.16	0.59	0.23	2.91	1.17	0.91	0.01	0.03	56.6	13.6	263.6	903.5	73.6
31.84	1.86	2.14	3.19	0.30	0.02	24.12	33.30	1.15	0.83	0.45	3.79	1.35	1.15	0.05	0.08	12.2	3.9	48.8	123.0	13.5
18.13	1.13	1.20	1.83	0.17	0.03	37.98	35.73	0.43	0.77	0.42	3.90	1.43	1.15	0.01	0.04	28.6	9.6	136.5	353.9	17.7
14.83	0.96	1.17	1.50	0.18	0.03	40.18	37.95	0.31	0.70	0.35	3.62	1.36	1.14	0.04	0.04	35.1	11.0	147.6	365.2	16.2
12.37	0.83	1.06	1.34	0.15	0.02	41.82	40.37	0.22	0.70	0.29	3.71	1.43	1.21	0.01	0.03	47.2	12.0	195.4	533.0	28.9
10.83	0.74	0.92	1.15	0.17	0.02	43.43	40.52	0.18	0.68	0.26	3.72	1.38	1.17	0.01	0.02	54.7	13.4	238.4	490.9	28.0
20.93	1.44	1.91	2.20	0.30	0.07	70.24	0.00	0.19	0.49	0.23	2.67	0.97	0.87	0.00	0.01	37.6	11.4	152.9	351.5	12.8
12.52	0.78	0.88	1.33	0.14	0.03	42.88	39.92	0.20	0.56	0.25	2.79	1.02	0.86	0.02	0.03	46.0	12.2	203.1	464.5	20.4
20.17	1.57	2.36	2.24	0.38	0.12	69.12	0.00	0.18	0.55	0.23	3.17	1.25	1.19	0.01	0.01	39.9	11.9	152.7	368.2	10.8
4.10	0.14	0.09	0.35	0.01	0.00	14.63	80.21	0.66	0.86	0.48	3.48	1.15	0.91	0.01	0.07	38.0	8.4	252.0	822.1	48.6
4.21	0.17	0.12	0.40	0.01	0.00	14.52	80.01	0.60	1.08	0.55	4.39	1.46	1.18	0.02	0.09	45.0	9.5	260.3	942.2	70.7
15.33	1.24	1.97	1.70	0.44	0.05	20.78	56.15	1.82	2.64	1.23	17.00	6.41	6.49	0.04	0.24	18.0	6.1	72.8	122.1	10.7
10.79	0.91	1.43	1.22	0.22	0.02	22.34	62.38	1.15	2.33	0.99	15.19	6.32	5.76	0.02	0.16	24.0	7.6	99.4	267.0	29.0
8.50	0.72	1.11	0.98	0.16	0.01	23.84	64.20	0.91	2.30	0.80	14.89	6.17	5.63	0.02	0.13	30.1	7.7	125.4	370.0	42.4
12.01	1.24	2.56	1.51	0.37	0.04	42.23	38.60	0.47	1.43	0.42	12.17	6.62	6.61	0.03	0.24	29.3	7.1	121.5	457.8	40.9
5.71	0.55	1.08	0.71	0.15	0.01	22.81	67.33	0.58	2.49	0.59	16.58	9.39	8.34	0.03	0.15	44.9	8.3	151.2	626.1	56.0
4.34	0.29	0.38	0.47	0.08	0.00	14.72	79.58	1.76	3.31	1.24	16.17	6.05	5.63	0.03	0.28	28.3	6.6	103.8	188.2	42.8
3.42	0.23	0.27	0.38	0.02	0.00	14.34	81.21	1.56	3.08	1.16	16.10	6.25	5.20	0.05	0.23	29.1	6.7	132.3	554.1	52.1
5.85	0.45	0.58	0.66	0.07	0.00	23.66	68.46	0.40	1.42	0.53	8.76	3.51	2.95	0.05	0.07	46.8	11.9	220.3	748.6	87.0
8.65	0.64	0.82	0.95	0.09	0.01	23.01	64.93	0.77	1.70	0.69	9.76	4.01	3.25	0.01	0.10	29.9	8.2	133.3	490.6	43.9
10.92	0.79	1.00	1.16	0.12	0.01	22.66	61.69	0.99	1.73	0.83	9.98	3.77	3.09	0.00	0.13	24.1	7.9	110.6	336.4	26.1

Table 3. Extract Phase Molar Percentages, x^{I}_{i}, Raffinate Phase Molar Percentages, x^{II}_{i}, and Selectivities, $\beta_{(123)4}$, $\beta_{(123)5}$, and $\beta_{(123)6}$, for 2,4-Xylenol (1) + 3,5-Xylenol (2) + 3,4-Xylenol (3) + Indane (4) + Naphthalene (5) + Dodecane (6) + Triethylene Glycol (7) + Water (8) + Hexane (9) at 313.15 K and 101.3 kPa

x^{I}_{1}	x^{I}_{2}	x^{I}_{3}	x^{I}_{4}	x^{I}_{5}	x^{I}_{6}	x^{I}_{7}	x^{I}_{8}	x^{II}_{1}	x^{II}_{2}	x^{II}_{3}	x^{II}_{4}	x^{II}_{5}	x^{II}_{6}	x^{II}_{7}	x^{II}_{8}	$\beta_{(123)4}$	$\beta_{(123)5}$	$\beta_{(123)6}$
3.52	1.93	1.96	0.11	1.18	0.03	14.33	76.39	1.63	0.66	0.59	3.28	16.61	9.21	0.15	0.53	77.4	36.3	9.0
1.92	1.03	1.04	0.05	0.51	0.03	14.45	80.69	1.21	0.47	0.39	3.14	16.69	8.84	0.22	0.48	133.3	62.8	6.2
1.38	0.74	0.74	0.03	0.34	0.02	14.42	82.07	0.99	0.32	0.33	3.49	17.10	9.38	0.06	0.49	221.6	89.0	10.2
1.09	0.57	0.56	0.02	0.26	0.00	14.91	82.52	0.90	0.30	0.24	3.25	16.30	8.81	0.23	0.17	273.1	97.8	103.0
0.75	0.39	0.38	0.01	0.20	0.00	15.62	82.60	0.74	0.24	0.20	3.33	17.06	9.10	0.25	0.13	684.8	113.2	80.8
2.54	1.57	1.58	0.02	0.27	0.01	14.01	79.77	0.81	0.31	0.29	0.87	4.78	2.45	0.09	0.15	180.8	70.3	19.7
1.57	0.90	0.93	0.02	0.16	0.03	14.65	81.61	0.62	0.23	0.21	0.89	4.88	2.42	0.11	0.11	164.1	96.6	2.3
1.17	0.67	0.66	0.00	0.10	0.00	14.69	82.61	0.54	0.19	0.15	0.91	4.82	2.38	0.02	0.10	1036.6	143.2	19.5
0.91	0.53	0.53	0.01	0.08	0.00	14.94	82.86	0.46	0.15	0.12	0.89	4.77	2.47	0.04	0.10	386.0	169.4	38.4
0.67	0.36	0.36	0.00	0.07	0.00	15.18	83.24	0.37	0.12	0.11	0.91	4.85	2.60	0.11	0.06	496.3	154.2	22.7
3.04	1.70	1.76	0.04	0.52	0.01	13.96	78.62	1.00	0.40	0.36	1.39	7.40	3.90	0.22	0.19	125.2	52.4	21.6
1.79	0.91	1.05	0.01	0.24	0.00	14.78	81.03	0.75	0.35	0.26	1.44	7.57	3.97	0.19	0.12	265.8	87.3	126.6
1.28	0.70	0.72	0.01	0.17	0.00	15.05	82.00	0.60	0.20	0.17	1.43	7.48	3.84	0.03	0.12	512.1	120.9	22.4
1.05	0.53	0.55	0.01	0.14	0.01	14.70	82.89	0.58	0.18	0.15	1.41	7.55	3.99	0.12	0.07	349.0	127.6	17.8
0.72	0.38	0.38	0.01	0.12	0.00	15.28	83.05	0.43	0.13	0.14	1.41	7.18	3.87	0.46	0.06	575.9	124.8	30.3
1.67	0.99	1.11	0.01	0.18	0.00	10.13	85.67	1.13	0.46	0.43	1.09	6.17	3.12	0.17	0.25	168.3	65.6	24.3
1.73	0.97	1.04	0.00	0.19	0.00	14.24	81.54	0.62	0.22	0.20	1.06	5.66	2.97	0.12	0.12	2950.2	110.4	27.8
1.26	0.69	0.71	0.00	0.14	0.01	14.95	82.09	0.55	0.18	0.16	1.11	5.96	3.15	0.07	0.08	1968.6	124.7	17.8
0.98	0.54	0.54	0.01	0.11	0.00	15.05	82.54	0.50	0.16	0.14	1.15	6.27	3.22	0.07	0.07	473.6	142.2	95.4
0.71	0.39	0.39	0.01	0.09	0.00	16.10	82.11	0.41	0.15	0.13	1.12	5.92	3.19	0.05	0.05	386.6	143.9	37.0
3.09	1.81	1.88	0.03	0.42	0.01	14.05	78.30	0.82	0.32	0.27	1.13	5.83	3.01	0.05	0.16	184.7	67.8	28.3
3.31	1.81	1.75	0.04	0.64	0.00	24.76	67.31	0.39	0.13	0.16	1.13	5.66	2.94	0.17	0.06	309.2	90.4	104.3
2.34	1.24	1.26	0.03	0.50	0.00	24.91	69.44	0.31	0.09	0.19	1.08	5.71	3.01	0.20	0.04	351.4	93.7	126.7
1.89	1.00	1.02	0.01	0.46	0.00	25.30	70.01	0.27	0.09	0.08	1.14	5.97	3.18	0.04	0.05	754.2	113.6	125.2
1.27	0.65	0.68	0.02	0.32	0.00	25.37	71.50	0.20	0.07	0.06	1.10	5.85	3.12	0.06	0.04	407.9	144.4	166.7
3.14	1.67	1.76	0.04	0.65	0.01	23.33	68.64	0.48	0.13	0.14	1.37	7.15	3.93	0.20	0.15	274.3	95.3	24.9
5.90	3.22	3.39	0.11	1.41	0.01	22.59	62.51	0.63	0.20	0.20	1.45	7.49	4.04	0.12	0.15	160.5	64.4	63.6
2.46	1.30	1.36	0.04	0.63	0.01	25.31	68.54	0.35	0.12	0.10	1.45	7.21	4.05	0.11	0.07	343.5	101.3	32.7
1.73	1.04	0.98	0.03	0.56	0.00	24.90	70.51	0.27	0.10	0.10	1.43	7.24	3.97	0.15	0.07	391.9	103.2	235.6
1.30	0.69	0.69	0.03	0.41	0.00	25.16	71.52	0.28	0.09	0.09	1.46	7.28	4.11	0.20	0.10	284.8	103.5	121.7
5.12	2.87	3.04	0.08	0.81	0.03	22.14	65.12	0.57	0.21	0.18	0.88	4.73	2.47	0.06	0.08	134.4	67.4	8.3
3.00	1.65	1.64	0.05	0.78	0.00	34.04	58.32	0.25	0.09	0.08	0.90	4.63	2.51	0.10	0.04	273.9	88.8	84.6
2.25	1.21	1.22	0.03	0.39	0.00	24.87	69.71	0.33	0.11	0.09	0.89	4.80	2.52	0.17	0.07	300.7	107.4	46.4
0.69	0.37	0.38	0.01	0.09	0.00	15.14	83.19	0.40	0.12	0.11	1.11	5.90	3.20	0.14	0.07	377.8	158.1	16.7
1.26	0.64	0.65	0.02	0.30	0.00	25.37	71.55	0.19	0.06	0.07	0.91	4.72	2.52	0.31	0.08	400.0	128.2	59.1
5.58	3.07	3.19	0.07	1.09	0.01	22.30	63.98	0.60	0.21	0.19	1.08	5.72	3.05	0.26	0.10	174.7	62.5	44.9
3.10	1.75	1.71	0.03	0.51	0.01	23.55	68.60	0.43	0.15	0.14	0.88	4.73	2.51	0.19	0.06	265.4	84.3	18.1
2.55	1.33	1.36	0.07	1.25	0.01	24.91	68.08	0.50	0.17	0.15	3.22	16.21	9.56	0.25	0.09	281.5	82.6	56.0
1.81	0.96	0.98	0.03	0.36	0.03	25.35	70.09	0.25	0.08	0.08	0.91	4.74	2.46	0.07	0.05	266.3	124.9	7.9
1.40	0.70	0.71	0.05	0.83	0.00	25.26	70.84	0.33	0.10	0.09	3.29	15.20	9.82	0.22	0.06	348.7	99.7	632.8
8.23	4.56	4.78	0.13	1.96	0.05	35.79	42.54	0.51	0.18	0.16	0.89	4.72	2.49	0.05	0.08	137.2	49.7	10.9
5.74	3.09	3.18	0.13	1.67	0.03	42.17	42.44	0.30	0.12	0.10	0.88	4.51	2.52	0.24	0.05	153.0	62.4	22.6
4.49	2.31	2.32	0.17	1.55	0.02	45.17	42.81	0.20	0.07	0.08	0.85	4.40	2.42	0.05	0.04	135.5	74.6	30.9
3.39	1.77	1.81	0.13	1.39	0.02	47.05	43.38	0.19	0.06	0.06	0.86	4.32	2.52	0.21	0.03	146.9	70.6	26.6
2.50	1.29	1.24	0.12	1.24	0.02	47.47	45.22	0.09	0.02	0.05	0.85	4.19	2.50	0.10	0.03	225.1	103.4	42.1
8.03	4.28	4.20	0.13	1.84	0.01	29.47	50.47	0.44	0.19	0.17	1.09	5.59	3.25	0.11	0.08	166.5	62.5	64.5
5.94	3.15	3.22	0.12	1.89	0.04	43.06	40.79	0.38	0.12	0.11	1.09	5.45	2.97	0.07	0.07	182.5	57.9	15.7

Table 3 (Continued)

x^{I}_{1}	x^{I}_{2}	x^{I}_{3}	x^{I}_{4}	x^{I}_{5}	x^{I}_{6}	x^{I}_{7}	x^{I}_{8}	x^{II}_{1}	x^{II}_{2}	x^{II}_{3}	x^{II}_{4}	x^{II}_{5}	x^{II}_{6}	x^{II}_{7}	x^{II}_{8}	$\beta_{(123)4}$	$\beta_{(123)5}$	$\beta_{(123)6}$
4.36	2.28	2.34	0.12	1.84	0.01	45.14	42.67	0.22	0.08	0.06	1.07	5.30	3.22	0.05	0.09	218.4	73.4	59.2
3.56	1.88	1.89	0.11	1.72	0.02	47.10	42.42	0.19	0.07	0.06	1.06	5.17	3.08	0.20	0.05	229.0	69.2	44.0
2.43	1.29	1.29	0.10	1.53	0.04	47.72	44.56	0.13	0.04	0.04	1.15	5.04	3.20	0.10	0.03	290.6	80.1	20.4
9.73	5.26	5.24	0.26	3.77	0.07	37.33	34.93	0.62	0.20	0.20	1.37	7.10	3.98	0.18	0.07	102.6	37.2	10.6
4.59	2.34	2.35	0.15	2.45	0.05	45.22	41.14	0.21	0.06	0.07	1.35	6.79	3.82	0.40	0.05	258.4	76.9	20.7
3.60	1.88	1.87	0.14	2.05	0.02	46.91	42.37	0.23	0.08	0.07	1.38	6.93	4.10	0.09	0.03	185.2	65.1	45.9
2.58	1.31	1.29	0.11	1.77	0.01	47.44	44.49	0.12	0.04	0.04	1.38	6.57	4.25	0.12	0.04	339.0	101.0	191.1
9.61	5.17	5.22	0.20	2.64	0.03	36.40	37.78	0.46	0.17	0.14	1.10	5.63	3.12	0.11	0.11	147.2	55.7	29.9
1.01	0.59	0.62	0.01	0.09	0.00	10.70	86.80	0.96	0.37	0.32	1.07	5.90	2.97	0.06	0.19	231.8	92.0	8.4
0.74	0.40	0.42	0.00	0.05	0.00	10.44	87.80	0.88	0.34	0.29	1.06	5.75	2.95	0.06	0.18	287.1	110.7	7.4
0.59	0.34	0.35	0.01	0.05	0.02	10.85	87.71	0.71	0.25	0.21	1.18	5.85	2.99	0.08	0.15	105.6	136.9	2.0
0.44	0.25	0.25	0.00	0.04	0.00	10.98	87.82	0.55	0.18	0.16	1.06	5.68	2.98	0.06	0.15	429.8	170.3	32.9
6.20	3.23	3.23	0.15	1.96	0.02	23.00	60.76	0.74	0.26	0.24	2.00	9.90	5.65	0.05	0.16	134.8	51.3	28.1
3.73	1.85	1.89	0.07	1.13	0.01	24.26	66.43	0.48	0.15	0.14	1.94	9.68	5.45	0.12	0.10	251.8	83.0	77.6
2.43	1.25	1.30	0.05	0.83	0.01	24.85	68.83	0.37	0.13	0.12	1.94	9.90	5.45	0.50	0.09	310.0	94.9	43.8
1.94	0.99	1.03	0.04	0.77	0.01	26.01	68.79	0.37	0.11	0.09	2.09	10.29	6.05	0.12	0.14	380.8	91.9	69.4
1.31	0.68	0.70	0.03	0.59	0.02	26.24	69.94	0.22	0.07	0.07	1.93	9.55	5.42	0.14	0.12	433.6	119.7	18.0
10.29	5.39	5.52	0.41	5.36	0.08	35.31	33.82	0.59	0.21	0.20	1.91	9.56	5.55	0.15	0.12	100.1	38.0	15.7
6.38	3.27	3.24	0.21	3.24	0.01	45.04	37.37	0.24	0.07	0.06	1.29	6.26	3.93	0.06	0.04	215.9	66.7	103.9
6.40	3.21	3.22	0.20	3.91	0.03	43.24	38.12	0.28	0.09	0.08	1.98	8.83	5.75	0.09	0.05	278.3	64.8	51.5
4.64	2.34	2.22	0.18	3.45	0.02	44.38	41.64	0.21	0.07	0.08	2.06	8.33	5.91	0.10	0.07	284.3	61.7	76.6
3.99	1.84	1.81	0.17	3.11	0.02	44.37	43.19	0.16	0.04	0.05	1.78	7.85	5.59	0.17	0.08	311.7	73.6	74.9
2.40	1.25	1.21	0.14	2.23	0.01	47.22	44.64	0.11	0.03	0.03	1.88	7.40	5.76	0.11	0.09	372.3	91.3	227.9
3.01	1.76	1.80	0.05	0.60	0.01	13.43	78.95	1.16	0.44	0.38	2.09	10.43	5.46	0.57	0.26	126.4	57.5	20.9
1.85	1.05	1.05	0.02	0.31	0.00	14.69	80.83	0.99	0.30	0.26	1.95	10.18	5.34	0.08	0.17	233.0	83.9	87.7
1.38	0.73	0.75	0.01	0.22	0.00	14.87	81.88	0.73	0.23	0.20	2.11	10.32	5.33	0.10	0.14	355.5	114.7	90.6
1.15	0.55	0.56	0.06	0.18	0.00	14.68	82.58	0.81	0.33	0.23	1.87	10.24	5.73	0.13	0.12	54.2	94.1	103.5
0.67	0.37	0.37	0.05	0.14	0.00	14.75	83.27	0.70	0.26	0.14	1.84	14.50	5.59	0.19	0.11	49.7	135.5	79.5

Experimental Section

Materials. Triethylene glycol, mesitylene, pseudocumene, and *o*-tolunitrile with a stated purity of 97%, benzonitrile and *o*-toluidine with a stated purity of 98%, aniline with a stated purity of 99%, and indane, indene, and dodecane with a stated purity of better than 95% were obtained from Fluka Co. 5-Ethyl-2-methylpyridine and naphthalene with a stated purity of 98% were supplied by Aldrich Chemical Co. Phenol with a stated purity of 99.5% and *m*-cresol with a stated purity of better than 99% were obtained from Riedel-de-Haen. 2,4-Xylenol, 3,4-xylenol, and 3,5-xylenol with a stated purity of 98% were purchased from Merck. Analytical reagent grade hexane was obtained from NT Laboratories. All the chemicals were used without further purification. The water was glass distilled.

Apparatus. The batch extraction tests were carried out in standard 250 mL glass separating funnels which were placed in a water bath. The water in the bath was circulated and kept at 313.15 K (±0.5 K) by means of a Haake D1 thermostat.

Procedure. Known masses, measured with a precision of ±0.001 g, of the pure feed components, triethylene glycol, water, and hexane were separately added to the separating funnels. The separating funnels were sealed and shaken for 30 s. The funnels were then positioned in the water bath so that the level of the funnel contents was below the level of the water. The portion of the funnel protruding above the water level was covered with insulation material. The funnels remained in the bath for a minimum of 24 h. They were shaken at regular intervals.

Upon removal from the water bath, the high-boiling solvent (extract) and countersolvent (raffinate) phases were quickly drained and stored in glass bottles with screw caps. The mass of each phase was measured with a precision of ±0.001 g and diluted to prevent secondary-phase separation at ambient temperature. Care was taken throughout to minimize evaporation losses. Samples of each phase were analyzed.

Analysis. The composition of each of the resulting batch extraction phases was determined with a Hewlett-Packard 5890A gas chromatograph (GC) with a flame ionization detector (FID). Integration was performed with a Delta computerized integration system. A 60 m Zebron D68H5 capillary column (inner diameter 0.25 mm) was used. Response factors were determined using solutions of known concentrations. From material balances over each of the solutes, the accuracy of solute mass measurements in each phase was estimated to be within ±1.7% for phenol, ±1.0% for *m*-cresol, ±1.4% for 2,4-xylenol, ±1.3% for 3,5-xylenol, ±1.3% for 3,4-xylenol, ±1.3% for aniline, ±1.4% for benzonitrile, ±1.5% for 5-ethyl-2-methylpyridine, ±1.3% for mesitylene, ±0.7% for *o*-toluidine, ±0.8% for *o*-tolunitrile, ±0.8% for indene, ±0.8% for pseudocumene, ±1.0% for undecane, ±1.2% for indane, ±1.2% for dodecane, ±1.2% for naphthalene, ±1.3% for triethylene glycol, and ±1.6% for hexane. Each analysis was repeated at least twice to ensure repeatability.

Table 4. NRTL Binary Interaction Parameters, b_{ij} and b_{ji}, for the System Hexane (1) + Water (2) + Mesitylene (3) + 5-Ethyl-2-methylpyridine (4) + Aniline (5) + Benzonitrile (6) + Phenol (7) + Triethylene Glycol (8)[a]

i	j	b_{ij}	b_{ji}	i	j	b_{ij}	b_{ji}
1	2	1883.5	3579.9	3	5	−139.9	6691.5
1	3	−1500.6	6366.4	3	6	1758.8	2330.3
1	4	2012.6	5960	3	7	−261.3	6656.4
1	5	481.5	503.2	3	8	1326.6	−1419
1	6	2233.4	−131.2	4	5	−955.2	1674.8
1	7	1019.9	84.91	4	6	2469.8	2340
1	8	2164.5	1559	4	7	1510.5	1105.1
2	3	351	750.5	4	8	2546.4	1440.1
2	4	2996.2	5230.9	5	6	1044	−129.9
2	5	950.4	62.63	5	7	1630	−709
2	6	2602.8	6205.8	5	8	278.6	−450.3
2	7	1403.2	−211.3	6	7	1057.7	996.5
2	8	−248	6668.6	6	8	3561	1335.6
3	4	1445.5	−199.3	7	8	−216.7	−267.6

[a] $\alpha_{ij} = \alpha_{ii} = 0.2$.

The water concentrations in each of the resulting batch extraction phases were determined by means of Karl Fischer volumetric titrations using a Metrohm 701 Titrino. From mass balances, the accuracy of the measured water masses was estimated to be within 1.2%.

Table 5. NRTL Binary Interaction Parameters, b_{ij} and b_{ji}, for the System Hexane (1) + Water (2) + Pseudocumene (3) + Undecane (4) + Indene (5) + *o*-Tolunitrile (6) + *o*-Toluidine (7) + *m*-Cresol (8) + Triethylene Glycol (9)[a]

i	j	b_{ij}	b_{ji}	i	j	b_{ij}	b_{ji}	i	j	b_{ij}	b_{ji}
1	2	1883.50	3579.90	2	7	884.57	4488.94	4	8	340.62	4720.85
1	3	−437.90	1147.24	2	8	819.63	270.04	4	9	4254.79	−1580.61
1	4	−2141.75	5842.71	2	9	−248.00	6668.60	5	6	572.44	−402.76
1	5	253.27	−375.26	3	4	4392.00	−1842.83	5	7	283.68	−297.57
1	6	−83.02	2566.88	3	5	876.64	−1976.36	5	8	3276.01	−598.45
1	7	51.95	622.62	3	6	−71.69	3764.98	5	9	487.42	−409.63
1	8	2163.74	−568.34	3	7	15.29	−1003.18	6	7	−1950.24	−372.27
1	9	2164.50	1559.00	3	8	1871.94	152.37	6	8	572.15	−897.22
2	3	4457.22	4746.21	3	9	5835.40	472.06	6	9	2886.06	−366.29
2	4	1842.81	3365.84	4	5	−1057.01	4502.56	7	8	38.47	−788.81
2	5	4043.78	636.41	4	6	−780.20	6189.99	7	9	1265.30	−969.67
2	6	1070.77	538.48	4	7	−324.53	−440.49	8	9	4578.41	−597.35

[a] $\alpha_{ij} = \alpha_{ii} = 0.2$.

Table 6. NRTL Binary Interaction Parameters, b_{ij} and b_{ji}, for the System Hexane (1) + Water (2) + Indane (3) + Dodecane (4) + Naphthalene (5) + 2,4-Xylenol (6) + 3,5-Xylenol (7) + 3,4-Xylenol (8) + Triethylene Glycol (9)[a]

i	j	b_{ij}	b_{ji}	i	j	b_{ij}	b_{ji}	i	j	b_{ij}	b_{ji}
1	2	1883.50	3579.90	2	7	3283.26	2930.22	4	8	5256.00	3294.94
1	3	662.80	7109.68	2	8	3178.45	3969.44	4	9	1382.00	−67.09
1	4	4451.29	−1369.38	2	9	−248.00	6668.60	5	6	9086.92	7457.86
1	5	231.44	−326.19	3	4	348.86	−601.99	5	7	2556.49	990.98
1	6	2276.17	4526.16	3	5	475.00	2684.98	5	8	1952.95	1169.98
1	7	3852.82	4099.85	3	6	846.48	−856.57	5	9	536.95	−359.80
1	8	2798.49	4831.69	3	7	4356.92	933.42	6	7	2602.12	2082.25
1	9	2164.50	1559.00	3	8	828.30	598.99	6	8	2100.01	1775.39
2	3	2351.00	4756.21	3	9	−68.27	356.75	6	9	3932.52	334.66
2	4	6977.00	434.00	4	5	119.00	4015.97	7	8	2574.91	2488.55
2	5	3817.02	699.93	4	6	9100.17	540.55	7	9	2850.13	785.22
2	6	2544.85	5852.87	4	7	4963.00	−157.25	8	9	2176.37	876.55

[a] $\alpha_{ij} = \alpha_{ii} = 0.2$.

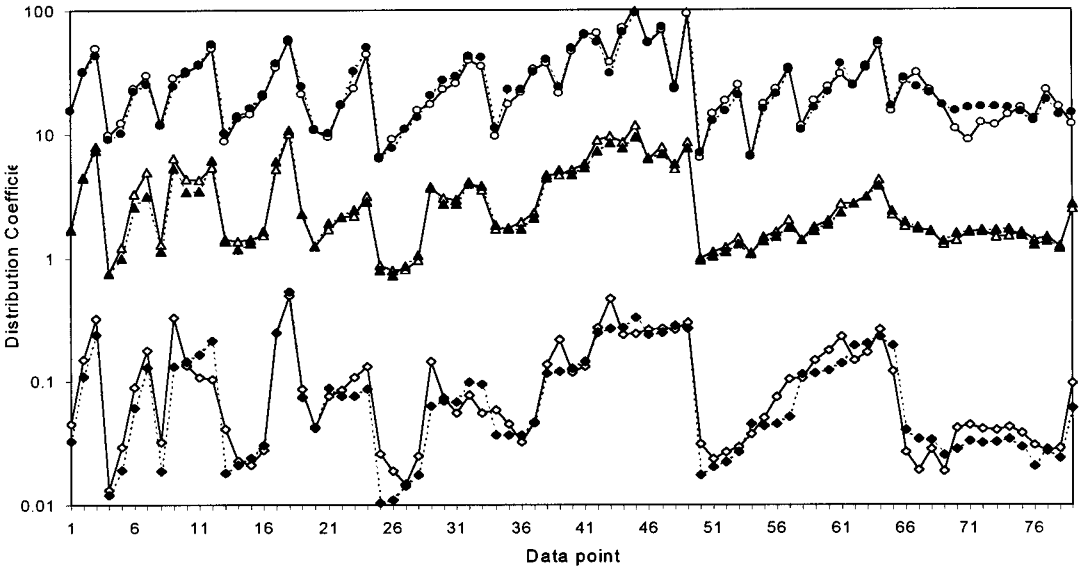

Figure 1. Experimental and simulated cistribution coefficients obtained for phenol, benzonitrile, and mesitylene for the system hexane + water + mesitylene + 5-ethyl-2-methylpyridine + aniline + benzonitrile + phenol + triethylene glycol at 313.15 K and 101.3 kPa: ●, phenol experimental; ○, phenol simulated; ▲, benzonitrile experimental; △, benzonitrile simulated; ◆, mesitylene experimental; ◇, mesitylene simulated.

The measured and analytically determined masses of the extract and raffinate phases on average differed by ±1.2% and ±1.7%, respectively. Overall mass balances for each batch extraction yielded an average error of 1.7%.

Models and Predictions. For a multicomponent two-phase liquid−liquid extraction system, the equilibrium activities of each component in both phases must be equal. Thus

$$\gamma_i^{\mathrm{E}} x_i^{\mathrm{E}} = \gamma_i^{\mathrm{R}} x_i^{\mathrm{R}} \tag{1}$$

where γ_i^{E} and γ_i^{R} are the activity coefficients and x_i^{E} and x_i^{R} are the molar concentrations of component i in the extract and raffinate phases, respectively.

The distribution coefficient K_i may thus be expressed in terms of either the activity coefficients or the equilibrium molar concentrations of component i in both phases:

$$K_i = x_i^{\mathrm{E}}/x_i^{\mathrm{R}} = \gamma_i^{\mathrm{R}}/\gamma_i^{\mathrm{E}} \tag{2}$$

The activity coefficients for a two-phase liquid−liquid extraction system may be modeled with the three-param-

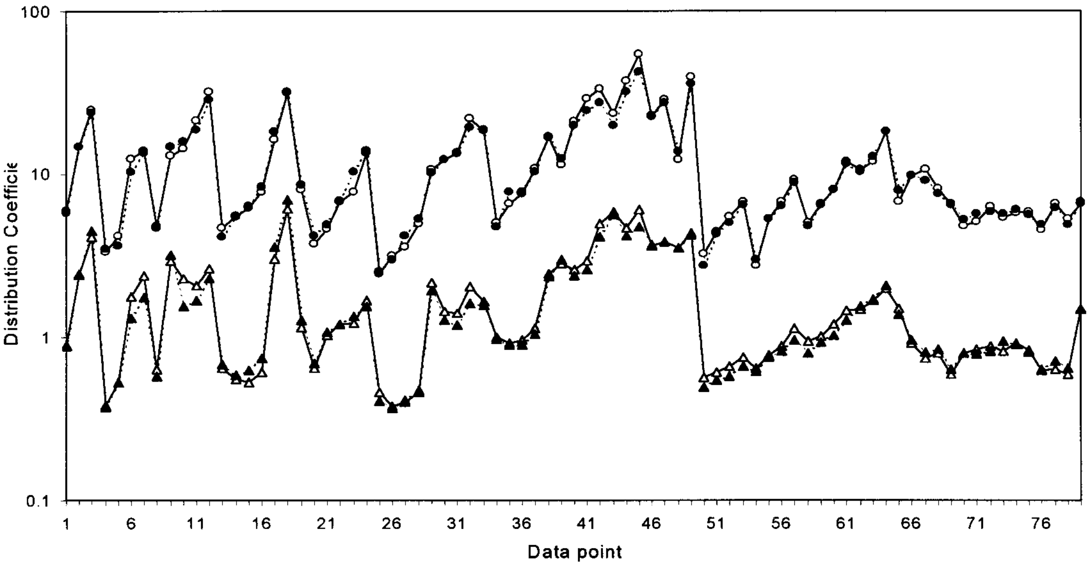

Figure 2. Experimental and simulated distribution coefficients obtained for aniline and 5-ethyl-2-methylpyridine for the system hexane + water + mesitylene + 5-ethyl-2-methylpyridine + aniline + benzonitrile + phenol + triethylene glycol at 313.15 K and 101.3 kPa: ●, aniline experimental; ○, aniline simulated; ▲, 5-ethyl-2-methylpyridine experimental; △, 5-et-2-me-pyridine, simulated.

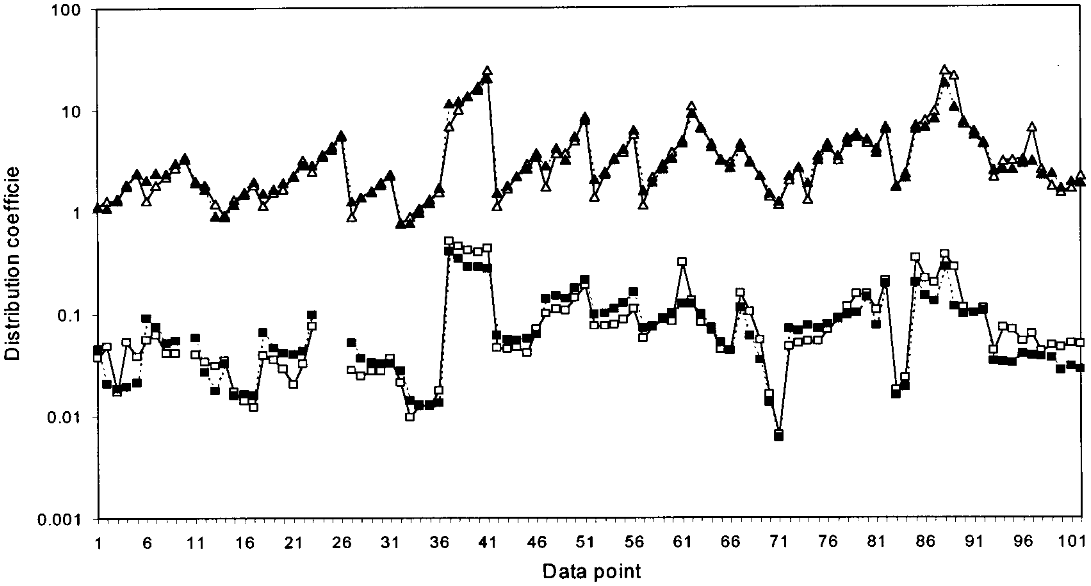

Figure 3. Experimental and simulated distribution coefficients obtained for *o*-toluidine and pseudocumene for the system hexane + water + pseudocumene + undecane + indene + *o*-tolunitrile + *o*-toluidine + *m*-cresol + triethylene glycol at 313.15 K and 101.3 kPa: ▲, *o*-toluidine experimental; △, *o*-toluidine simulated; ■, pseudocumene experimental; □, pseudocumene simulated.

eter nonrandom two-liquid (NRTL)[7] model using an appropriate set of binary interaction parameters, b_{ij} and α_{ij}.

Results and Discussion

The suitability of a solvent for a desired separation depends on its ability to preferentially extract a desired solute from a mixture of solutes. The selectivity of a solvent for solute *i* relative to *j*, β_{ij}, is analogous to the relative volatility in the distillation:

$$\beta_{ij} = K_i/K_j \tag{3}$$

where K_i and K_j are the distribution coefficients of components *i* and *j*, respectively.

The distribution coefficient can have any value—even less than one—and the extraction will still be feasible. The higher the separation factor, the easier the liquid extraction will be.[3]

The evaluation of triethylene glycol as an effective solvent is based on the selectivities obtained for each phenolic compound with respect to the neutral oils and nitrogen bases present in the respective multicomponent liquid−liquid system.

The measured equilibrium molar compositions for the three systems studied are listed in Tables 1−3. The selectivities obtained for phenol with respect to benzonitrile, aniline, mesitylene, and 5-ethyl-2-methylpyridine are listed in Table 1. The selectivites obtained for *m*-cresol with respect to *o*-tolunitrile, *o*-toluidine, pseudocumene, indene, and undecane are listed in Table 2, while those obtained for 2,4-, 3,4-, and 3,5-xylenol with respect to naphthalene, indane, and dodecane are listed in Table 3.

It can be seen from Tables 1−3 that very high selectivities are obtained for the component pairs *m*-cresol−indene, xylenol−naphthalene, xylenol−indane, and especially phenol−mesitylene, *m*-cresol−pseudocumene, and xylenol−

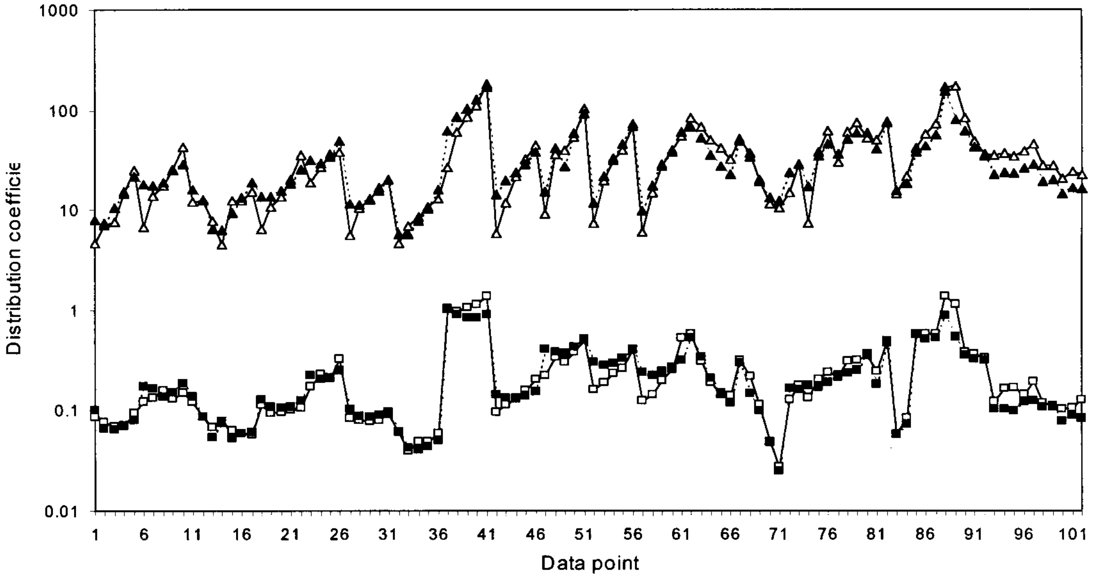

Figure 4. Experimental and simulated distribution coefficients obtained for *m*-cresol and indene for the system hexane + water + pseudocumene + undecane + indene + *o*-tolunitrile + *o*-toluidine + *m*-cresol + triethylene glycol at 313.15 K and 101.3 kPa: ▲, *m*-cresol experimental; △, *m*-cresol simulated; ■, indene experimental; □, indene simulated.

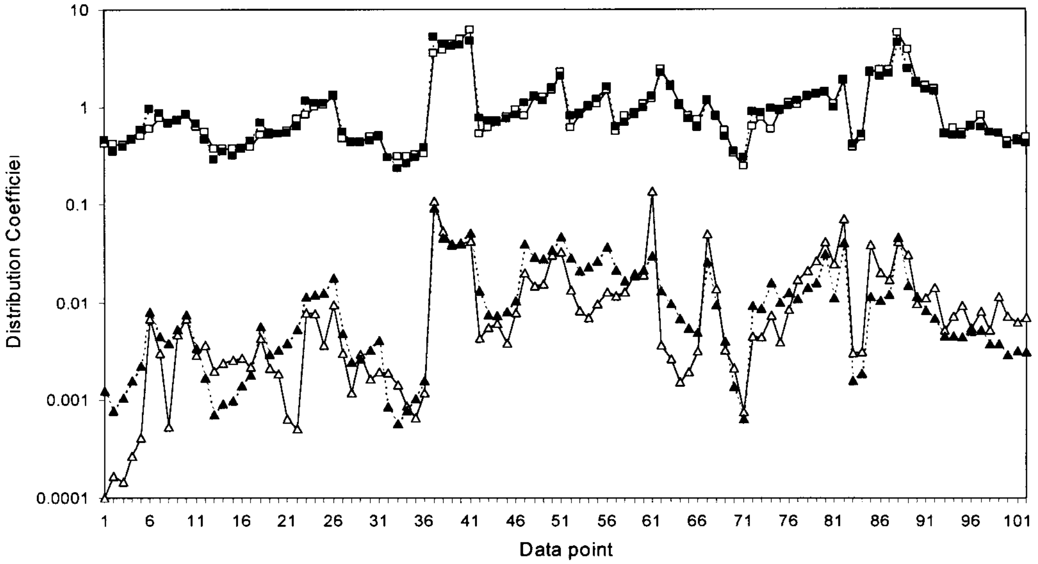

Figure 5. Experimental and simulated distribution coefficients obtained for *o*-tolunitrile and undecane for the system hexane + water + pseudocumene + undecane + indene + *o*-tolunitrile + *o*-toluidine + *m*-cresol + triethylene glycol at 313.15 K and 101.3 kPa: ■, *o*-tolunitrile experimental; □, *o*-tolunitrile simulated; ▲, undecane experimental; △, undecane simulated.

dodecane. It can be concluded that the corresponding separations are trivial using the proposed liquid–liquid extraction system.

The selectivities obtained for phenol–benzonitrile, phenol–aniline, phenol–5-ethyl-2-methylpyridine, *m*-cresol–*o*-tolunitrile, and *m*-cresol–*o*-toluidine are highly satisfactory.

It can therefore be concluded that the proposed solvent system is effective in separating phenolic compounds from neutral oils and nitrogen bases.

The NRTL equation was fitted to the experimental data listed in Tables 1–3 using a computer program which incorporated a particle swarm method followed by the Levenberg–Marquardt algorithm to minimize the value of the following objective function:

$$F = \sum_i w_i \epsilon_i^2 \qquad (4)$$

where F is the goal function to be minimized, w_i is a constant, and ϵ_i is defined as

$$\epsilon_i = \frac{\gamma_i^{E} x_i^{E} - \gamma_i^{R} x_i^{R}}{\frac{1}{2}(\gamma_i^{E} x_i^{E} + \gamma_i^{R} x_i^{R})} \times 100 \qquad (5)$$

The parameter α_{ij} was assumed to equal α_{ji} and was assigned a value of 0.2 for all component pairs.

The optimum binary interaction parameters, b_{ij}, determined according to eq 4 for the three systems studied are listed in Tables 4–6.

Each LLE data point was simulated with the process simulator, PRO/II version 5.11 (Simulation Sciences Inc. 2000), using the sets of binary parameters obtained through regression. The root-mean-square-deviation (RMSD) for each multicomponent system was calculated from the experimental and simulated equilibrium molar fractions

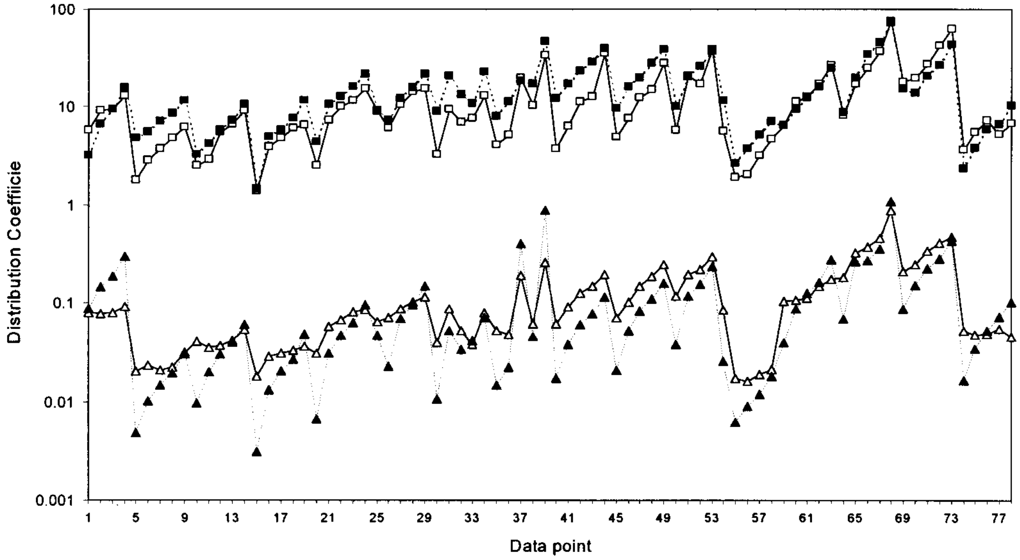

Figure 6. Experimental and simulated distribution coefficients obtained for 3,5-xylenol and naphthalene for the system hexane + water + indane + dodecane + naphthalene + 2,4-xylenol + 3,5-xylenol + 3,4-xylenol + triethylene glycol at 313.15 K and 101.3 kPa: ■, 3,5-xylenol experimental; □, 3,5-xylenol simulated; ▲, naphthalene experimental; △, naphthalene simulated.

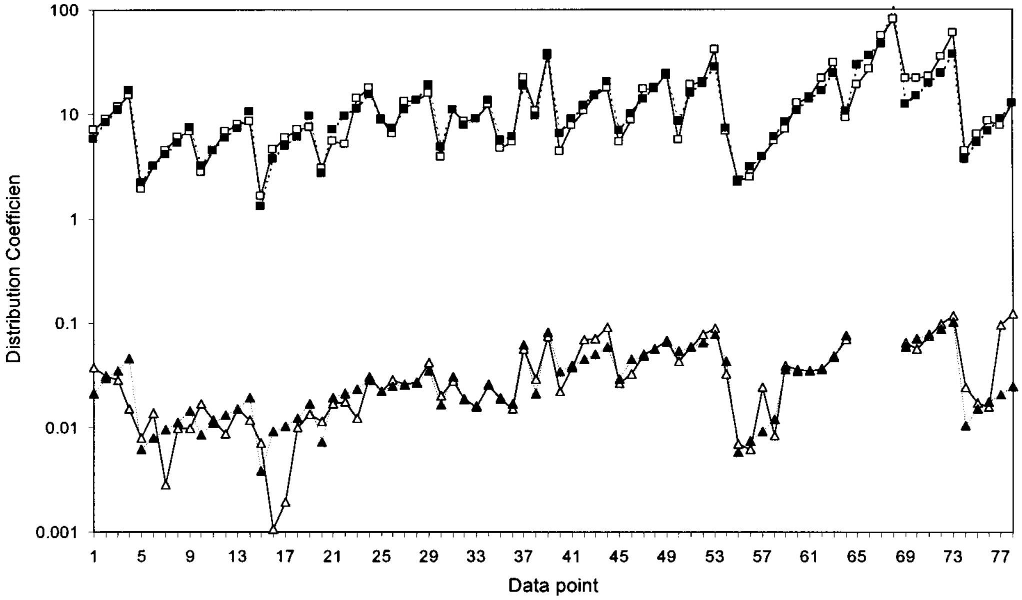

Figure 7. Experimental and simulated distribution coefficients obtained for hexane + water + indane + dodecane + naphthalene + 2,4-xylenol + 3,5-xylenol + 3,4-xylenol + triethylene glycol at 313.15 K and 101.3 kPa: ■, 3,4-xylenol experimental; □, 3,4-xylenol simulated; ▲, indane experimental; △, indane simulated.

of each component in the two resulting liquid phases according to the following equation:

$$\mathrm{RMSD} = \left[\sum_{n}\frac{\sum_{i}(x_{i,\mathrm{exp}}{}^{\mathrm{E}} - x_{i,\mathrm{sim}}{}^{\mathrm{E}})^2 + \sum_{i}(x_{i,\mathrm{exp}}{}^{\mathrm{R}} - x_{i,\mathrm{sim}}{}^{\mathrm{R}})^2}{2kn}\right]^{1/2} \tag{6}$$

where n is the number of data points, k is the number of components, $x_{i,\mathrm{exp}}{}^{\mathrm{E}}$ and $x_{i,\mathrm{sim}}{}^{\mathrm{E}}$ are the experimental and simulated molar fractions of component i in the extract phase, and $x_{i,\mathrm{exp}}{}^{\mathrm{R}}$ and $x_{i,\mathrm{sim}}{}^{\mathrm{R}}$ are the experimental and simulated molar fractions of component i in the raffinate phase.

The experimental and simulated distribution coefficients for the system hexane + water + mesitylene + 5-ethyl-2-methyl-pyridine + aniline + benzonitrile + phenol + triethylene glycol are shown in Figures 1 and 2. The RMSD value calculated for the system is 0.0037. The experimental and simulated distribution coefficients for the system hexane + water + pseudocumene + undecane + indene + *o*-tolunitrile + *o*-toluidine + *m*-cresol + triethylene glycol are shown in Figures 3−5, while those for the system hexane + water + indane + dodecane + 2,4-xylenol + 3,4-xylenol + 3,5-xylenol + triethylene glycol are shown in Figures 6−8. The RMSD values calculated for the two systems are 0.010 and 0.0058, respectively.

From Figures 1−8 and Tables 4−6, it can be concluded that the equilibrium data can accurately be correlated with the NRTL model.

Conclusions

Liquid−liquid equilibria and selectivities for the systems triethylene glycol + hexane + water + (phenol + aniline

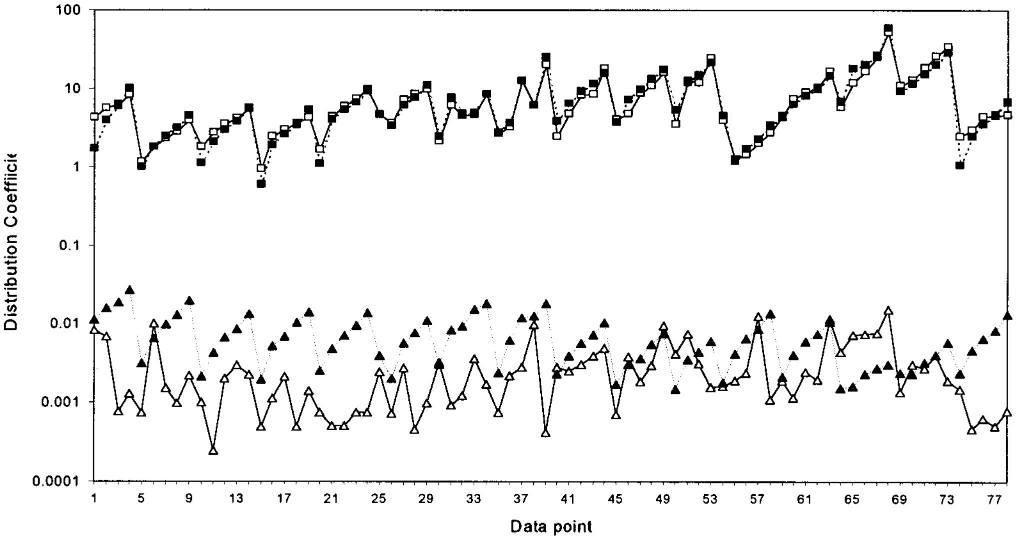

Figure 8. Experimental and simulated distribution coefficients obtained for 2,4-xylenol and dodecane for the system hexane + water + indane + dodecane + naphthalene + 2,4-xylenol + 3,5-xylenol + 3,4-xylenol + triethylene glycol at 313.15 K and 101.3 kPa: ■, 2,4-xylenol experimental; □, 2,4-xylenol simulated; ▲, dodecane experimental; △, dodecane simulated.

+ benzonitrile + 5-ethyl-2-methylpyridine + mesitylene) or (*m*-cresol + *o*-tolunitrile + *o*-toluidine + indene + pseudocumene + undecane) or (2,4-xylenol + 3,4-xylenol + 3,5-xylenol + indane + naphthalene + dodecane) have been determined at 313.15 K in order to evaluate their suitability in separating phenolic compounds from neutral oils and nitrogen bases.

The separation of phenolic compounds from paraffins, indane, indene, naphthalene, and trimethylbenzene isomers is trivial using the proposed solvent system. The selectivities obtained for phenol with regard to benzonitrile, aniline, and 5-ethyl-2-methylpyridine as well as those obtained for *m*-cresol with regard to *o*-tolunitrile and *o*-toluidine are highly satisfactory.

It can therefore be concluded that the triethylene glycol, hexane, and water are effective solvents for the separation of phenolic compounds from neutral oils and nitrogen bases.

Optimum binary parameters for the NRTL equation were determined by regression of the equilibrium data obtained for each of the three systems investigated. RMSD values of 0.0037, 0.0100, and 0.0058 were respectively calculated for the multicomponent systems containing phenol, *m*-cresol, and the xylenol isomers. A good correlation between the distribution coefficients predicted using the NRTL equation and those determined experimentally was obtained.

Nomenclature

b = binary parameter for NRTL equation
F = regression goal function
k = number of components
K = distribution coefficient
n = number of data points
w = regression constant
x = equilibrium molar fraction
α = binary parameter for NRTL equation
β = selectivity
ϵ = regression error function
γ = liquid-phase activity coefficient

Subscripts

i = component i
j = component j

Subscripts

E = extract (water-rich) phase
R = raffinate (hexane-rich) phase

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Received for review October 12, 2000. Accepted March 6, 2001.

JE0003389