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Effects of salt on the LLE and tie-line data for furfuryl alcohol — n-butanol–water at T = 298.15 K

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ABSTRACT

Solubility and tie-line data for the systems containing water + furfuryl alcohol + n-butanol + NaCl were measured at T = 298.15 K and atmospheric pressure. The NRTL and UNIQUAC models were employed to compare the experimental liquid–liquid equilibrium (LLE) data. The binary interaction parameters were determined. The Othmer–Tobias, Hand and Bachman correlation equations were applied to validate the LLE data for these systems. Distribution coefficients and separation factors were calculated. It was noted that enlargement of the two-phase region occurred when the concentration of salt increased in the initial aqueous phase. Adding salt to the system proved beneficial in separating furfuryl alcohol from water.

1. Introduction

In recent years, great interest has been shown in the liquid–liquid equilibrium (LLE) and salting-out effect on the liquid–liquid equilibrium for various ternary systems. LLE [1–10] and salt effect [11–15] have been much used in chemical engineering processes and waste water treatment due to their application in industry and economical usage. In the process of evaluating solvent extraction, it is important that research into mixtures of furfuryl alcohol (FAL) with organic solvents be carried out. Thus, for the separation of FAL from aqueous solutions to be most effective, accurate data is vital [16,17].

FAL is an important chemical well known in the polymer industry. It is mainly used for the production of thermostatic resins, liquid resins (for strengthening ceramics), as well as in the production of various synthetic fibers, rubber-resins and farm chemicals. In addition, it is used as a chemical intermediate, employed for the manufacture of lysine, vitamin C, lubricants, dispersing agents and plasticizers [18].

Potentially, FAL can be used as a precursor for components in "P series" alternative fuels [19,20]. FAL is prepared from furfural by catalytic hydrogenation in gas or liquid phase [21]. If the hydrogenation of furfural is performed in water as a solvent, one possibility for separation of FAL from water is extraction [22]. However, furfuryl alcohol is a toxic component and may contaminate industrial wastewater. The National Institute for Occupational Safety and Health (NIOSH) listed furfuryl alcohol as a carcinogen [23,24]. Due to the toxicity of furfuryl alcohol together with its adverse environmental impact, separation of furfuryl alcohol from water and wastewater, before its discharge, is highly important.

Among the first to do research on liquid liquid equilibrium of furfuryl alcohol were Negadi et al. [17]. Wongsawa et al. also carried out an important research into liquid liquid equilibrium data of furfuryl alcohol with various organic solvents (MIBK, ethyl acetate, furfural or n-butanol) [15]. Many investigations into varying organic solvents have been undertaken for the separation of furfuryl alcohol from water. Nevertheless, more research needs to be assembled. As yet, research on LLE data for the systems containing FAL + water + n-butanol + NaCl has not been collated in the literature.

In this paper, the solubility and tie-line data for the systems consisting water, FAL, n-butanol and various concentration of NaCl at T = 298.15 K and atmospheric pressure are presented. Using the tie-line data, separation factors and distribution coefficients were evaluated. The reliability of the experimental tie-line data was validated by the Othmer–Tobias [25], Hand [26] and Bachman correlation equations [27]. Both the UNIQUAC [28–31] and the NRTL [32–36] models were used to correlate the experimental LLE data.

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Table 1
Source and mass fraction of the chemical reagent.

Component	Supplier	Mass fraction purity	Analysis method
Furfuryl alcohol	Sigma-Aldich	0.99	GC
n-Butanol	Erba Lachema	0.995	GC
Water	–	–	–
NaCl	Merck	–	–

2. Experimental

2.1. Materials

The chemicals furfuryl alcohol and n-butanol were purchased from Sigma-Aldich and Erba Lachema Co. Ltd. Throughout all the experiments, distilled and deionized water was used. All materials received were used without any further purification. The chemicals used in this study along with literature values are listed in Table 1.

Table 2
Experimental solubilitydata in mass fraction for water (w_1) + FAL (w_2) + n-butanol (w_3) at different temperatures and $P = 101.325$ kPa[a].

$T = 298.15$ K			$T = 308.15$ K			$T = 318.15$ K			$T = 328.15$ K		
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
0.8363	0.0000	0.1637	0.0791	0.0000	0.9209	0.0843	0.0000	0.9157	0.0860	0.0000	0.9140
0.7464	0.0846	0.1690	0.0653	0.1557	0.7790	0.0701	0.1688	0.7611	0.0672	0.1618	0.7710
0.6697	0.1484	0.1819	0.0767	0.2415	0.6818	0.0848	0.2482	0.6670	0.0823	0.2565	0.6612
0.5995	0.2045	0.1960	0.0982	0.3159	0.5859	0.10554	0.32406	0.5704	0.0951	0.3326	0.5723
0.5263	0.2624	0.2113	0.1206	0.3770	0.5024	0.1289	0.3803	0.4908	0.1281	0.3660	0.5059
0.4340	0.3327	0.2333	0.1520	0.4272	0.4208	0.1596	0.4100	0.4304	0.1641	0.3980	0.4379
0.3812	0.3701	0.2487	0.1917	0.4464	0.3619	0.2100	0.4302	0.3598	0.2185	0.4140	0.3675
0.3274	0.4068	0.2658	0.2554	0.4365	0.3081	0.2638	0.4231	0.3131	0.2768	0.4060	0.3172
0.2463	0.4463	0.3074	0.3251	0.4001	0.2748	0.3226	0.3936	0.2838	0.3286	0.3834	0.2808
0.1851	0.4529	0.3620	0.3856	0.3621	0.2523	0.3925	0.3539	0.2536	0.3849	0.3540	0.2611
0.1444	0.4271	0.4285	0.4397	0.3225	0.2378	0.4396	0.3142	0.2462	0.4471	0.3059	0.2470
0.1130	0.3841	0.5029	0.5251	0.2547	0.2202	0.5264	0.2465	0.2271	0.5144	0.2592	0.2264
0.0882	0.3212	0.5906	0.6049	0.1953	0.1998	0.6048	0.1870	0.2082	0.5905	0.2018	0.2077
0.0715	0.2515	0.6770	0.6751	0.1408	0.1841	0.6702	0.1391	0.1907	0.6788	0.1338	0.1874
0.0591	0.1688	0.7721	0.7511	0.0746	0.1743	0.7464	0.0697	0.1839	0.7281	0.0884	0.1835
0.0628	0.0000	0.9372	0.8275	0.0000	0.1725	0.8197	0.0000	0.1803	0.8114	0.0000	0.1886

[a] Standard uncertainties u are $u(w) = 0.01$, $u(P) = 0.01$ kPa and $u(T) = 0.1$ K.

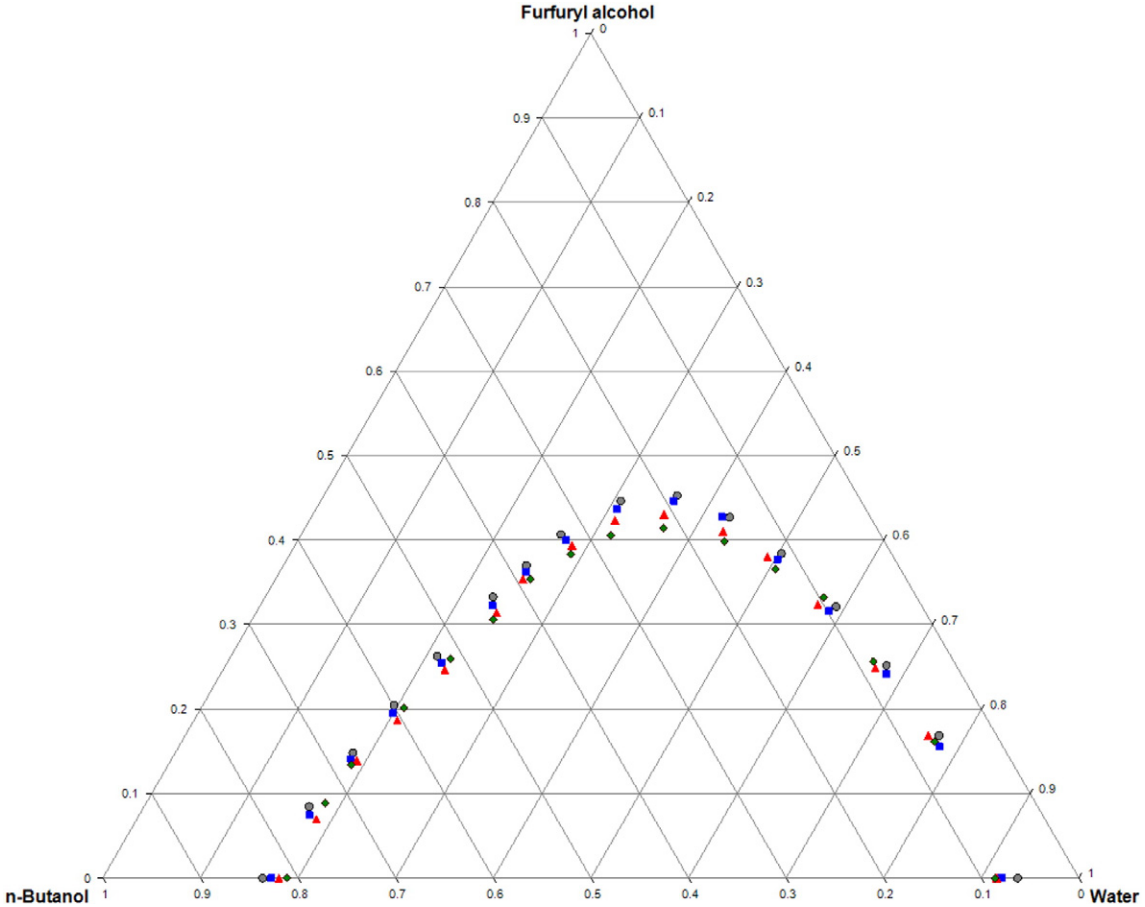

Fig. 1. Binodal curves diagram for water + FAL + n-butanol at temperature; (●) 298.15 K, (■) 308.15 K, (▲) 318.15 K and (◆) 328.15 K at atmosphereric pressure.