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Removal of aromatic hydrocarbons from hydrocarbon mixture using glycols at 303.15 K and 333.15 K and atmospheric pressure: Experimental and calculated data by NRTL and UNIQUAC models

Francisca Maria Rodrigues Mesquita, Regiane Silva Pinheiro, Hosiberto B. de Sant'Ana, Rílvia S. Santiago-Aguiar *

Grupo de Pesquisa em Termofluidodinâmica Aplicada, Chemical Engineering Department, Federal University of Ceará, Campus do Pici, Bloco 709, 60455-760 Fortaleza, CE, Brazil

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ABSTRACT

Aromatic hydrocarbons are usually extracted from reformed naphtha, which are multicomponent mixtures with aliphatic hydrocarbons. These components have very close boiling point, which makes distillation process not so efficient and economically infeasible. For this reason, aromatics compounds are usually separated from aliphatic compounds by intermediate of solvent extraction unit operation. In this work, liquid–liquid equilibrium (LLE) data for systems containing decane + toluene + diethylene glycol (DEG) and decane + toluene + triethylene glycol (TEG) at T = (303.15 and 333.15) K and atmospheric pressure were studied. It was observed that temperature hardly influence the size of the two-phase region. Distribution coefficient and selectivity have been calculated from those experimental data. For all systems studied, selectivity parameter showed values greater than 1 indicating that the extraction is possible by using DEG and TEG as extractor solvents. Additionally, selectivity values increase with increasing glycol carbon chain. LLE have been correlated by intermediate of NRTL and UNIQUAC activity coefficients.

1. Introduction

Benzene, toluene and xylene, known as BTX's, are very important components to petrochemical and petroleum industries. These aromatics are been used in the fabrication of solvents, polyesters, plastics, resins and among other products [1]. The aromatics are commonly derived from reformed naphtha, which are a multicomponent mixture with aliphatic hydrocarbons [2,3].

Aromatic and aliphatic hydrocarbons have boiling points very close. Numerous combinations of mixing these components form azeotropes, which complicates the separation of BTX's by using a simple distillation process [4]. Due to its limitations, distillation those mixtures are not separate by distillation unit operation. For this reason, aromatic aliphatic hydrocarbons is separate by intermediate of conventional liquid–liquid extraction process, also known as solvent extraction.

The solvents used in aromatics extraction process must present some important features such as considerable polarity, water solubility, affinity for aromatics, density and boiling point higher than the aromatics desired to extract [5]. For this process organic solvents such as sulfolane [6–32], dimethylsulfoxide [33], *N*-methylpyrrolidone [34], *N*-formylmorpholine [31,35–41] and glycols [42–48] are used.

A vast number of papers presenting liquid–liquid equilibrium data of systems including aliphatics + aromatics + sulfolane [6,28–32] have been published in the literature. Nevertheless, only few data of systems containing aliphatics + aromatics + glycols [43–48] is available. For this reason, experimental LLE data for systems containing decane + toluene + glycols at different temperatures were studied in this paper.

The main aim of this paper is to generate new LLE data for decane + toluene + (diethylene glycol (DEG) or triethylene glycol (TEG)) systems at T = (303.15 and 333.15) K and atmospheric pressure and to correlate experimental results with the NRTL [49] and UNIQUAC [50] models. Furthermore, this study also investigates the influence glycol carbon chain in the efficiency

* Corresponding author. Tel.: +55 85 3366 9611; fax: +55 85 33669610.
E-mail address: rilvia@ufc.br (R.S. Santiago-Aguiar).

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Table 1
Source, CAS no., purities and density of the chemicals used in the study.[a]

Chemical name	Source	CAS no.	Purity mass fraction	Density (g cm^{-3})
Decane	Sigma–Aldrich	124-18-5	≥99%	0.722439
Toluene	Sigma–Aldrich	108-88-3	99.8%	0.857606
Diethylene glycol	Sigma–Aldrich	111-46-6	99%	1.109165
Triethylene glycol	Sigma–Aldrich	112-27-6	99%	1.116052

[a] Standard uncertainty are $\sigma(T) = 0.001$ K; $\sigma(\rho) = 0.00008$.

of toluene extraction process. For that, distribution coefficient and selectivity parameters have been calculated.

2. Experimental

2.1. Chemicals

Chemical analysis of chemical compounds used in this study (decane, toluene, diethylene glycol – DEG and triethylene glycol – TEG) has been reported in Table 1.

2.2. LLE determination

All ternary mixtures were prepared using Shimadzu analytical balance with an uncertainty of ±0.0001 g. The density of the pure components and mixtures were obtained by using an Anton Paar DSA-5000 digital vibrating tube densimeter with uncertainty of ±0.00008 g cm^{-3}. The standard uncertainty of the measured temperature of the densimeter is ±0.001 K. It should be reminded that all density measurements were performed in triplicate.

Glass cells of approximately 60 mL, Stragevitch and dÁvila model [51], were used for experimental LLE data determination. In order to maintain a constant temperature, the cells were jacketed and connected a thermostatic bath (Tecnal TE-184) with uncertainty of ±0.1 K.

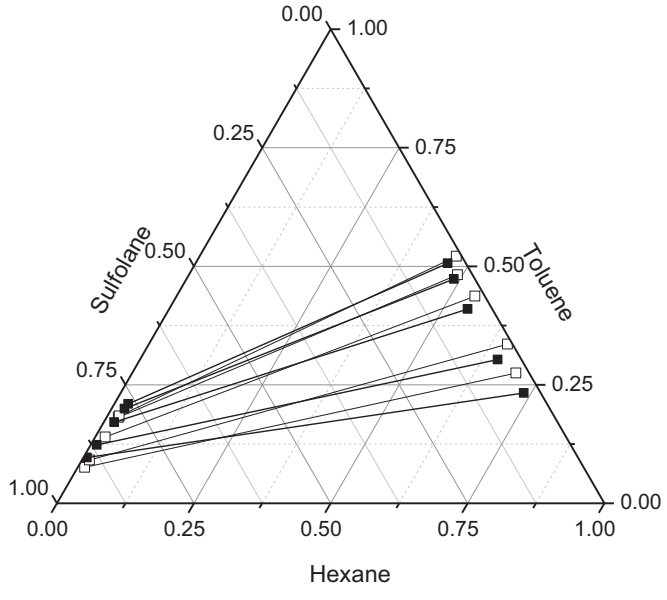

Fig. 1. Validation of the methodology test at 303.15 K. Experimental data (■) and Kamankesh et al. data [54] (□).

Table 2
Binodal curves for systems including decane (1) + toluene (2) + diethylene glycol-DEG (3) at 303.15 K and 333.15 K.[a]

w_1	w_2	Density (g cm^{-3})
Decane (1) + toluene (2) + diethylene glycol (3) at 303.15 K		
0.0070	0.0206	1.100440
0.0305	0.1267	1.074578
0.0893	0.2279	1.072891
0.1408	0.3043	1.011921
0.0751	0.1948	1.065057
0.1846	0.3931	0.867165
0.2675	0.4693	0.800938
0.4418	0.4477	0.783812
0.5800	0.3566	0.766984
0.7298	0.2463	0.750984
0.8501	0.1309	0.737565
0.9455	0.0279	0.725737
Decane (1) + toluene (2) + diethylene glycol (3) at 333.15 K		
0.0112	0.1386	0.714270
0.7833	0.1963	0.720990
0.6694	0.2872	0.732598
0.5647	0.3765	0.744407
0.1953	0.4028	0.757690
0.2850	0.4234	0.769354
0.1917	0.4087	0.779227
0.1323	0.3515	0.794267
0.1882	0.4300	0.864175
0.1066	0.3374	1.019718
0.0454	0.2018	1.046286
0.0856	0.2753	1.048992
0.0092	0.0000	1.084783

[a] Standard uncertainties are $\sigma(T) = 0.1$ K; $\sigma(w) = 0.001$; $\sigma(\rho) = 0.00008$.

Table 3
Binodal curves for systems including decane (1) + toluene (2) + triethylene glycol-TEG (3) at 303.15 K and 333.15 K.[a]

w_1	w_2	Density (g cm^{-3})
Decane (1) + toluene (2) + triethylene glycol (3) at 303.15 K		
0.9950	0.0000	0.722552
0.8624	0.1238	0.736542
0.7295	0.2442	0.751658
0.5978	0.3828	0.768236
0.4907	0.4895	0.783347
0.3494	0.5837	0.800741
0.2162	0.6008	0.817495
0.1517	0.5294	0.939834
0.0982	0.4511	0.948860
0.0788	0.3454	1.059489
0.0322	0.2384	1.063080
0.0250	0.1264	1.074016
0.0088	0.0000	1.113572
Decane (1) + toluene (2) + triethylene glycol (3) at 333.15 K		
0.9968	0.0000	0.699772
0.8611	0.1339	0.713634
0.7380	0.2502	0.726818
0.6123	0.3726	0.742440
0.4902	0.4927	0.757545
0.3614	0.6008	0.776492
0.2269	0.6239	0.790666
0.1349	0.5399	0.800413
0.0915	0.4548	0.860413
0.0645	0.3534	1.005218
0.0894	0.3423	1.029363
0.0275	0.2099	1.036933
0.0748	0.2369	1.038833
0.0233	0.1388	1.049873
0.0126	0.0663	1.071123
0.0078	0.0000	1.088977

[a] Standard uncertainties are $\sigma(T) = 0.1$ K; $\sigma(w) = 0.001$; $\sigma(\rho) = 0.00008$.