Fluid Phase Equilibria 425 (2016) 188–195

Contents lists available at ScienceDirect

Fluid Phase Equilibria

journal homepage: www.elsevier.com/locate/fluid

Vapour-liquid equilibrium for tripropylene glycol + aromatic hydrocarbons binary systems: Measurements and modelling

Elena M. Fendu*, Marilena Nicolae, Florin Oprea

Petroleum Processing and Environmental Engineering Department, Petroleum – Gas University, Bd. București, 39 No., 100680, Ploiești, Romania

ARTICLE INFO

Article history:
Received 12 April 2016
Received in revised form
31 May 2016
Accepted 31 May 2016
Available online 3 June 2016

Keywords:
VLE
Tripropylene glycol
Aromatic hydrocarbons
Regression

ABSTRACT

Vapour-liquid equilibrium (VLE) data are reported for five binary systems involving aromatic hydrocarbons (toluene, ethylbenzene, *o*-xylene, *m*-xylene, and *p*-xylene) and tripropylene glycol (2-[2-(2-hydroxypropoxy)propoxy]propan-1-ol). VLE data was determined by using a static method for the binary mixtures at temperatures within 305.15 K–496.15 K. The *p-T-x* experimental data obtained were correlated using the NRTL model, in order to obtain the binary interaction parameters for each mixture. We compared the *T-x-y* diagrams determined based on the NRTL resulted parameters with the diagrams calculated using the UNIFAC predictive model and IDEAL model. We observed differences between the *T-x* curves calculated with the NRTL model that includes the binary interaction parameters resulting from the experimental VLE data and the *T-x* curves calculated with UNIFAC predictive model and IDEAL model.

1. Introduction

Liquid-liquid extraction and the extractive distillation are widely used in refineries and petrochemical plants in order to produce aromatic hydrocarbons. An optimized planning and realization of the extraction and extractive distillation plants will require comprehensive qualitative and quantitative phase equilibrium data between aliphatic and aromatics hydrocarbons and the used solvents [1]. The solvents used in aromatics extraction process should provide some qualities like: affinity for aromatics, density and boiling point higher than the aromatics who want to be extracted, considerable polarity, water solubility [2,3]. Many solvents for the liquid-liquid extraction were studied over time, such as sulfolane [4–7], *n*-methyl-2-pyrrolidone [8–10], *N*-formylmorpholine [11–13] or dimethyl-sulfoxide [14]. Recently published studies shows a special interest for using glycols (ethylene and propylene) as solvents in the processes mentioned above.

For ethylene glycols (mono-, di-, tri-, tetra), there are few data about the liquid-liquid and vapour–liquid equilibrium for the mixtures ethylene glycols–hydrocarbons in the literature [10,15–17].

Regarding the use of propylene glycols as solvents, our research group developed a large program to study the possibility of their use in extractive distillation and liquid-liquid extraction. The first step of our study was the separation of propylene glycols from their mixtures. In order to perform a proper separation of the propylene glycols mixtures we have experimentally determined the vapour-liquid equilibrium data for the involved binary systems: water + propylene glycols [18] and between propylene glycols [19]. Another step was the use of the propylene glycols as solvents in new processes for the extraction of aromatics hydrocarbons from mixtures. We investigated the liquid-liquid equilibrium (LLE) of hydrocarbon + 1,2-propylene glycol (MPG) binary systems [20,21]. For dipropylene glycol we determined: (1) the liquid-liquid equilibrium data for eleven binary systems formed by 4-oxa-2,6-heptandiol (dipropylene glycol, DPG) with paraffinic, naphthenic and aromatic hydrocarbons [22], (2) the vapour-liquid equilibrium data for the binary mixtures of DPG with benzene, toluene, ethylbenzene, *o*-xylene, *m*-xylene, and *p*-xylene [23] and (3) the solvency properties of dipropylene glycol [24].

Equilibrium data for the systems formed by tripropylene glycol (2-[2-(2-hydroxypropoxy)propoxy]propan-1-ol) and aromatic was not previously documented.

In this study, we report *p-T-x* experimental VLE data for binary mixtures formed by tripropylene glycol (TPG) and aromatic hydrocarbons having up to eight carbon atoms: toluene, ethylbenzene, *o*-xylene, *m*-xylene and *p*-xylene. Vapour–liquid equilibrium for the binaries mentioned above was determined by measuring the vapour pressure of the mixtures with a static equilibrium apparatus build in our laboratory described in detail in our

---

* Corresponding author.
E-mail address: fendu.elena@gmail.com (E.M. Fendu).

http://dx.doi.org/10.1016/j.fluid.2016.05.032
0378-3812/

Table 1
Specifications of the used chemicals.

Chemical name	Source	Mass fraction purity
Toluene	Chemical Company, Romania	0.993
Ethylbenzene	Merck KGaA, Germany	>0.99
o-xylene	Merck KGaA, Germany	0.98
m-xylene	Merck KGaA, Germany	>0.99
p-xylene	Merck KGaA, Germany	>0.99
Tripropylene glycol	Dow Chemical, Germany	0.9993

previous work [18,19,23,25]. The VLE experimental data was regressed with the NRTL (Non Random Two-Liquid) model [26,27]. The NRTL binary interaction parameters obtained could be used in the liquid-liquid extraction or extractive distillation processes designs, using a simulation software for the chemical processes [28]. The VLE data obtained with NRTL for each binary are compared with data calculated with IDEAL [29] and UNIFAC (UNIquac Functional-group Activity Coefficients) [30] models.

2. Experimental

The specifications and the suppliers of all chemical substances used in this work are presented in Table 1. The pressure was measured using a DPI 705 sensor with the measuring range between 0 and $0.35 \cdot 10^5$ Pa and the temperature was measured with VWR International, LLC, NIST traceable digital thermometer (±0.05% accuracy and 0.001 K resolution).

We used a static apparatus in our laboratory, built to determine *p-T-x* equilibrium data, by measuring the vapour pressure. The operation of this apparatus have been described in our previous articles [18,19,25]. The experimental procedure used to determine the VLE data involving aromatic hydrocarbons and propylene glycols has been described in detail in our previous article in which we used dipropylene glycol [23].

The ELV experimental data for toluene + TPG, ethylbenzene + TPG, *o*-xylene + TPG, *m*-xylene + TPG and *p*-xylene + TPG were obtained for five mixture compositions (around the values of 0.1, 0.3, 0.5, 0.7 and 0.9 mol fraction of hydrocarbon).

Table 2
Experimental VLE data for temperature T, pressure p with standard uncertainty $u(p)$ and mole fraction x_1 for the binary system toluene (1) + TPG (2).[a]

T/K	p/kPa	$u(p)$/kPa	T/K	p/kPa	$u(p)$/kPa	T/K	p/kPa	$u(p)$/kPa
$x_1 = 0.0000$								
350.15	0.039	0.003	385.15	0.330	0.004	420.15	1.803	0.011
357.15	0.063	0.008	392.15	0.477	0.005	427.15	2.435	0.011
364.15	0.098	0.004	399.15	0.680	0.008	434.15	3.251	0.016
371.15	0.150	0.009	406.15	0.953	0.009	441.15	4.297	0.022
378.15	0.224	0.004	413.15	1.320	0.014	448.15	5.624	0.033
$x_1 = 0.1018$								
383.15	15.369	0.011	403.15	25.209	0.026	423.15	38.084	0.030
388.15	17.727	0.011	408.15	27.838	0.022	428.15	42.095	0.025
393.15	20.221	0.013	413.15	30.753	0.020	433.15	46.752	0.029
398.15	22.790	0.018	418.15	34.313	0.021	440.15	54.159	0.041
$x_1 = 0.3008$								
305.15	2.871	0.010	345.15	12.636	0.022	385.15	39.685	0.031
313.15	3.976	0.009	353.15	16.013	0.023	393.15	48.913	0.040
321.15	5.548	0.008	361.15	20.527	0.021	401.15	59.646	0.037
329.15	7.520	0.013	369.15	26.110	0.025	409.15	71.014	0.042
337.15	9.827	0.017	377.15	32.329	0.027	417.15	82.717	0.051
$x_1 = 0.4998$								
315.15	6.110	0.013	345.15	19.467	0.023	375.15	47.230	0.032
321.15	7.880	0.012	351.15	23.368	0.027	381.15	56.080	0.033
327.15	9.929	0.018	357.15	27.940	0.031	389.15	69.863	0.029
333.15	12.486	0.015	363.15	33.087	0.024	397.15	84.810	0.040
339.15	15.550	0.014	369.15	39.511	0.021	405.15	99.724	0.039
$x_1 = 0.7005$								
315.15	7.110	0.011	340.15	18.976	0.018	365.15	44.231	0.034
320.15	8.733	0.013	345.15	22.647	0.026	370.15	51.639	0.024
325.15	10.683	0.017	350.15	27.105	0.015	375.15	59.915	0.036
330.15	12.994	0.021	355.15	32.070	0.019	380.15	68.995	0.045
335.15	15.714	0.026	360.15	37.643	0.029	385.15	79.418	0.039
$x_1 = 0.9010$								
321.15	10.111	0.010	345.15	26.231	0.019	370.15	60.799	0.019
325.15	12.109	0.012	350.15	31.338	0.024	375.15	70.444	0.023
330.15	14.903	0.014	355.15	37.273	0.018	379.15	79.308	0.019
335.15	18.013	0.017	360.15	44.183	0.025	383.15	88.892	0.030
340.15	21.799	0.014	365.15	51.980	0.026	387.15	98.642	0.034
$x_1 = 1.0000$								
315.15	8.622	0.006	340.15	24.269	0.014	365.15	57.883	0.016
320.15	10.769	0.012	345.15	29.224	0.018	370.15	67.745	0.028
325.15	13.343	0.005	350.15	34.971	0.022	375.15	78.898	0.016
330.15	16.404	0.016	355.15	41.599	0.024	380.15	91.457	0.030
335.15	20.022	0.012	360.15	49.203	0.024	385.15	105.543	0.022

[a] Standard uncertainties u are $u(T) = 0.01$ K and $u(x) = 0.0002$.