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Liquid–liquid equilibrium data for ternary aqueous mixtures containing 1-pentanol and 2-methyl-1-propanol at (298.15, 323.15, and 348.15) K

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ABSTRACT

Liquid–liquid equilibrium (LLE) tie-line data of ternary aqueous mixtures containing 1-pentanol and 2-methyl-1-propanol were reported separately at $T = (298.15, 323.15$ and $348.15)$ K under normal pressure in this article. Meanwhile, a type II LLE phase diagram for the investigated system at each constant temperature was given and the effect of temperature on LLE phase behavior was discussed. The well-known Othmer–Tobias, Bachman and Hand correlations were used to test the reliability of the experimental data. In addition, both the NRTL ($\alpha = 0.2$) and UNIQUAC models were applied to correlate the measured data to obtain the binary interaction parameters between each pair of components valid for the range of temperature studied. All of the root-mean-square deviation (*RMSD*) between the measured and calculated data was less than 0.0056. The results of this study can be used to design and optimize the liquid–liquid separation process of aqueous solution containing 2-methyl-1-propanol and 1-pentanol.

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1. Introduction

In order to solve the energy crisis and environmental contamination, organic alcohols have gradually become a substitute for fossil fuel, which can be thought as an environment-friendly fuel. The organic alcohol can be obtained from diluted solution produced in biomass fermentation process, which is the only renewable carbon source. The recovery of mixed alcohol from aqueous–organic mixtures can be completed by extraction, which is considered as a kind of high efficiency and energy saving method. The successful implementation of the above processes is dependent on the accurate liquid–liquid equilibrium (LLE) data, which are also fundamental and important to simulate and design the extraction process.

At present, LLE phase behavior has been researched thoroughly by many famous experts to collect a large number of useful data that are of significant importance in most chemical processes. The retrieval, correlation and prediction methods for LLE data have been summarized and reported by Sørensen et al. in the previous literatures [1–3]. The LLE data for the binary systems containing alkanol and water have been accumulated and reviewed by Góral et al. [4], which would provide an important theoretical and methodological basis for the design of the separation of the related binary system. The investigations of LLE for the aqueous solution containing organic alcohols have been carried out in recent years and some valuable scientific achievements have been made to enlarge the application of biomass fermentation fuel and reduce fossil fuel consumption [5–23]. Among the work, the influence of the temperature on the LLE of the ternary system 1-pentanol + 1-propanol + water has been detected by Fernández et al. [11]. For the same system, LLE data for the system have been determined experimentally at 298.15 and 323.15 K by Ghizellaoui et al. [20]. Ternary equilibrium data of mixtures consisting of 2-butanol, water, and heavy alcohols at $T = 298.2$ K are measured by Ghanadzadeh Gilani and his co-workers [23], and experimental and correlated tie-line data for aqueous mixtures of 2-butanol with 2-ethyl-1-hexanol at various temperatures also have been reported by Ghanadzadeh Gilani et al. [21]. All of the above LLE data can be used to the extraction of alcohols from aqueous mixtures containing alcohols, especially biomass fermentation solution. However, LLE data for some ternary mixtures composed of water and alcohols could not be found in the present literature. LLE data for the ternary system of 1-butanol + 3-methyl-1-butanol + water at different temperatures and the system containing 2-methyl-1-propanol, 3-methyl-1-butanol and water at $T = (298.15, 323.15$ and $348.15)$ K had been reported [24,25]. In addition, LLE data for ternary aqueous mixtures containing 2-methyl-1-propanol and 2-propanol over the temperature range of (298.15–348.15) K had been given in our previous work [26]. In this work, LLE for the ternary system 2-methyl-1-propanol + 1-pentanol + water will be studied in detail.

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Table 1
Sample table.

Components	Supplier	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
Ethanol	Sinopharm Chemical Reagent Co., Ltd.	0.997	None	–	GC[a]
2-Methyl-1-propanol	Tianjin Bodi Chemical Holding Co., Ltd.	0.995	None	–	GC[a]
1-Pentanol	Tianjin Bodi Chemical Holding Co., Ltd.	0.990	None	–	GC[a]

[a] Gas chromatography.

Table 2
CAS number (CAS), mole weights (M), boiling temperatures (T_b), densities (ρ) and refractive indices (n) at $T = 293.15$ K under atmospheric pressure.[a]

Component	CAS	M (g mol^{-1})	T_b (K)	ρ (g cm^{-3})		n	
				Exp.	Lit. [30]	Exp.	Lit. [30]
Water	7732-18-5	18.00	373.20	0.9984	0.9982	1.3328	1.3330
Ethanol	64-17-5	46.07	351.55	0.7900	0.7893	1.3616	1.3614
2-Methyl-1-propanol	78-83-1	74.12	380.15	0.8017	0.8020	1.3955	1.3960
1-Pentanol	71-41-0	88.15	410.95	0.8137	0.8144	1.4087	1.4090

[a] Standard uncertainties u are $u(\rho) = 0.0005$ g cm^{-3}, $u(n) = \pm 0.0002$, and $u(T) = 0.05$ K.

Liquid–liquid phase equilibrium was studied in detail for the ternary system consisted of 2-methyl-1-propanol, 1-pentanol and water at $T = (298.15, 323.15$ and $348.15)$ K to observe the effect of temperature on the ternary system and get useful tie-line data, respectively. The ternary systems can be classified as Treybal's type II [27] because they have two partially miscible binaries, that is, 2-methyl-1-propanol and water, and 1-pentanol and water. It is expected that the corresponding miscibility region will be affected by temperature as well.

The accuracy of simulation calculation is closely related to the value of model parameters. Both the simulation calculation and the prediction of LLE data can be affected by the selection of parameter values. The model parameter was obtained by the regression of experimental data. The NRTL (non-random two liquid) [28] and UNIQUAC (universal quasi-chemical) [29] models describing the Gibbs energy of mixing are functions of the composition and temperature. Satisfactory data association results will be obtained by using the two models to regress the LLE data of aqueous systems containing alcohols. Therefore, in order to ensure the accuracy of the simulation, the UNIQUAC and NRTL models were chosen and the model parameters of corresponding system were determined by Aspen Plus physical parameter regression system using the LLE experimental data in this paper.

2. Experimental

2.1. Materials and instruments

The analytical grade chemicals without further purification were chosen in this research, and their purity was checked by gas chromatograph. The suppliers and mass fraction for all of the materials are given in Table 1. The homemade double deionized water with specific conductance of 1.0×10^{-4} S m^{-1} was used in the experiment. The specific conductance of the deionized water was measured by the DDSJ-308A conductivity meter produced by Shanghai Precision and Scientific Instrument Co., Ltd., with the estimated measurement uncertainty less than ±0.5% FS. The refractive index of all the materials at 293.15 K was measured using a WAY Abbe refractometer whose measurement range was 1.3000–1.7000. Water was used to calibrate the refractometer and the uncertainty of the measurements for all the chemicals was not more than ±0.0002. The SDT301 densimeter with measurement accuracy of 0.0005 g cm^{-3} produced by SANI Measuring Instruments (Zhong Shan) Co., Ltd. was chosen to measure the density for the chemicals at 293.15 K. The measured and literature data [30] of the CAS number, molar mass, boiling temperature, density and refractive index for the materials used in this research at 293.15 K under 1 atm are shown in Table 2.

2.2. Equilibrium measurements

The detailed methods and procedures of LLE experiments have been referred to in the previous literatures [8,9]. Therefore, only a brief description of the experimental apparatus and approach was provided. The LLE experiment was conducted at three different constant temperatures under atmospheric pressure, respectively, and the maximum temperature fluctuation range was within 0.1 K. The volume for one pure substance was usually fixed and those for the other two were varied with one increased and the other decreased correspondingly during the mixing of three kinds of pure components to make the LLE data cover the entire two-phase region as far as possible. The change interval for volume of the pure components was 5–10 mL each time. First, the mixtures with known component were prepared in a 100 mL glass container and stirred violently at least 1 h to make the sample mix completely. Then, the sample was sealed with a glass stopper and kept standing at a constant temperature about 20 h until it reached equilibrium state. The CS501-3C super constant temperature water bath produced by Chongqing Huida Experimental Equipment Co., Ltd. was used to keep the experimental temperature constant with fluctuation range of ±0.05 K. The conical flask should be filled up by liquid mixtures as much as possible during the course of the whole experiment, which aimed at avoiding the appearance of additional vapor phase that could be easily generated at high temperatures. After

Table 3
The operating conditions for the gas chromatography.

Name	Characteristic	Description
Column	Type	The length is 20 m and the diameter is 6 mm.
	Packing	Porapak Q–S 80/100
	Temperature	453.15 K
Carrier gas	Type	Hydrogen
	Flow rate	70 mL min^{-1}
	Pressure	0.3 MPa
Injector	Injection volume	1 μL
	Split ratio	5:1
	Temperature	473.15 K
Detector	Type	Thermal conductivity detector (TCD)
	Current	100 mA
	Temperature	473.15 K (TCD)

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