



# Isobaric vapor–liquid equilibrium for binary and ternary systems with toluene, 2-methoxyethanol and dimethyl sulfoxide at 101.3 kPa



Shuo Zhao, Peng Bai\*, Chang Sun

School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, PR China

## ARTICLE INFO

### Article history:

Received 10 January 2014

Received in revised form 23 April 2014

Accepted 25 April 2014

Available online 4 May 2014

### Keywords:

Vapor–liquid equilibrium

Toluene

2-Methoxyethanol

Dimethyl sulfoxide

## ABSTRACT

Isobaric vapor–liquid equilibrium (VLE) data for binary systems of toluene + 2-methoxyethanol, 2-methoxyethanol + dimethyl sulfoxide (DMSO) and toluene + DMSO were obtained by using a Fischer VLE 602 equipment at 101.3 kPa, as well as for the ternary system of toluene + 2-methoxyethanol + DMSO. The binary VLE data were considered to be thermodynamically consistent according to the Wisniak's modification of the Herington test and the Wisniak's *L–W* test. It was determined that toluene and 2-methoxyethanol form binary azeotrope at 379.08 K, 70.2 mol% toluene at 101.3 kPa. The binary VLE data were correlated by using Wilson, NRTL and UNIQUAC models with minor deviations. The ternary system was well predicted from binary interaction parameters and passed both the Wisniak–Tamir's modification of McDermott–Ellis test and the Wisniak's *L–W* test. Besides, the ternary VLE data were also satisfactorily correlated by using Wilson, NRTL and UNIQUAC models. Moreover, the change of phase equilibria behavior of toluene and 2-methoxyethanol due to the addition of DMSO is significant. Therefore, DMSO is recommended as a promising entrainer for the separation of toluene and 2-methoxyethanol azeotropic mixture by extractive distillation.

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## 1. Introduction

Toluene and 2-methoxyethanol are important solvents and fine chemicals in various industrial applications. Toluene is a widely used raw material in the chemical and pharmaceutical production process. Besides, it can be used as a solvent in dyes, varnishes and inks, and also can be used as a cleaner in electrochemical industries [1]. 2-Methoxyethanol, known as glycol ether, is notable for its ability to dissolve a variety of chemical compounds. It is a good diluent and solvent in paints, varnishes and printing inks. It has also attracted much attention as a solvent in electrochemical industries [2]. Then, the related processes, such as dyestuffs, varnishes, printing inks and electrochemical industries, may produce a large volume of toluene and 2-methoxyethanol solution. Therefore, a suitable and efficient method to separate toluene and 2-methoxyethanol is indispensable in the above-mentioned processes. Separation of them with a conventional distillation process is very difficult due to the homogeneous azeotrope [3]. Extractive distillation is a practical way of separating azeotropic systems and approximate boiling point systems [4,5]. The entrainer is added

to the liquid mixture to alter the relative volatility and make the separation more efficient.

Based on our previous work, dimethyl sulfoxide (DMSO) was proposed as a promising entrainer in extractive distillation for the separation of an ethylbenzene and 2-ethoxyethanol mixture [6]. In this work, DMSO was also expected to break the azeotropic point formed by toluene and 2-methoxyethanol as an entrainer. For simulating and designing the separation process, it is essential to determine the vapor–liquid equilibrium (VLE) data for the binary and ternary systems and study their correlating models. Radhama et al. [7] reported isobaric VLE data for the binary system of toluene and DMSO at 95.3 kPa. Nissema and Karvo [8] reported isothermal VLE data for the binary system of toluene and DMSO at 323.14 K. However, these data are obviously not sufficient for designing the separation process.

This work was carried out to provide fundamental data for the separation of toluene and 2-methoxyethanol by extractive distillation using DMSO as the entrainer. The isobaric VLE data for binary systems of toluene + 2-methoxyethanol, 2-methoxyethanol + DMSO, toluene + DMSO, and the ternary system of toluene + 2-methoxyethanol + DMSO were measured at 101.3 kPa with a Fischer VLE 602 equipment. The thermodynamic consistency of the experimental VLE data was checked out by means of the Wisniak's modification [9] of the Herington test [10] and the Wisniak's *L–W* test [11] for the binary systems, and the

\* Corresponding author. Tel.: +86 022 27406186.

E-mail address: [chemeng114.tju@163.com](mailto:chemeng114.tju@163.com) (P. Bai).

$a, b$	binary interaction parameters
$A_1 - G_7$	coefficients of the extended Antoine equation
$F$	objective function
$N$	number of data points
$n_D$	refractive index
$p$	pressure (kPa)
$q$	UNIQUAC area parameter
$r$	UNIQUAC volume parameter
$R$	universal gas constant ( $\text{J mol}^{-1} \text{K}^{-1}$ )
$T$	absolute temperature (K)
$u$	uncertainty
$V$	molar volume ( $\text{cm}^3 \text{mol}^{-1}$ )
$x$	mole fraction in the liquid phase
$y$	mole fraction in the vapor phase
<b>Greek letters</b>	
$\alpha$	non-randomness parameter of NRTL model
$\alpha_{12}$	relative volatility of toluene to 2-methoxyethanol
$\rho$	density
$\gamma$	activity coefficient
$\sigma$	standard deviation
<b>Subscripts</b>	
$b$	normal boiling
$i, j$	component $i, j$
$k$	data number
<b>Superscripts</b>	
$az$	azeotrope
$cal$	calculated property
$exp$	experimental property
$L$	liquid phase property
$s$	saturation property
$V$	vapor phase property

Wisniak–Tamir’s modification [12] of the McDermott–Ellis test [13] and the Wisniak’s  $L$ – $W$  test [11] for the ternary system, respectively. Wilson [14], NRTL [15] and UNIQUAC [16] models were used to correlate the VLE data of the binary and ternary systems. With the parameters obtained from the correlations of the binary systems, the prediction for the ternary system was also studied and discussed.

## 2. Experimental

### 2.1. Chemicals

Analytical reagents, toluene, 2-methoxyethanol and DMSO, purchased from Tianjin Guangfu Technology Development Co., Ltd., China. All of the reagents were further purified with batch distillation and dehydrated with 3 Å molecular sieve. The purities of all the chemicals were checked by a gas chromatograph (GC) equipped with a flame ionization detector (FID). The water content in chemicals was determined using a Karl Fischer moisture titrator. The purity and water content are listed in Table 1. The purity of the chemicals was further confirmed by comparing their physical properties with the corresponding literature values as shown in Table 2. The normal boiling points were measured by a Fischer VLE 602 equipment with an uncertainty of 0.01 K. The densities of the pure components were measured at 293.15 K using a KEM DA-510 density meter, and the refractive indexes were measured at 293.15 K using an ATAGO RX-5000 Abbe refractometer. The uncertainties in

density and refractive index measurements were  $2.0 \times 10^{-5} \text{ g cm}^{-3}$  and 0.00001, respectively.

### 2.2. Apparatus and procedure

The equilibrium device used in the measurements (Labodest VLE 602) was an all-glass dynamic-recirculating still equipped with a Cottrell-pump, manufactured by Fischer Labor und Verfahrenstechnik (Germany). The Cottrell-pump ensured that both liquid and vapor phases were in intimate contact during the boiling process and also in contact with the temperature sensing element. The equilibrium temperature was measured with a precise glass temperature sensor PT-100 with a standard uncertainty of 0.01 K. A Fisher M101 pressure control system was used to control and measure the pressure and the heating power. The pressure in the still was maintained at  $101.3 \pm 0.1 \text{ kPa}$  during the measurement process. The temperature and pressure sensors were calibrated to guarantee the correct operation.

For each binary and ternary point tested, the pressure was fixed, and the immersion heater and the stirring system of the liquid mixture were turned on. All experiments were carried out under an inert atmosphere of dry nitrogen to avoid exposure to moisture and oxygen. The still was operated at constant pressure until equilibrium was reached. Equilibrium conditions were assumed when the fluctuation in vapor temperature was within 0.1 K in a time period of 30 min or longer. Then the liquid and vapor condensate samples were taken simultaneously for analysis. The sampling was carried out using special syringes that allowed withdrawal of small volume samples ( $0.5 \mu\text{L}$ ). At least three consecutive samples were taken for analysis at each experimental point. And, three analyses were made for each sample.

### 2.3. Sample analysis

All the samples of the equilibrium phases were analyzed using an Agilent 7890A Gas Chromatography (GC) equipped with a HP-5 capillary column ( $30 \text{ m} \times 0.32 \text{ mm} \times 0.25 \mu\text{m}$ ) and a flame ionization detector (FID). Nitrogen with a purity of 99.999% was used as the carrier gas at a constant flow rate of  $1 \text{ mL min}^{-1}$ . The temperature of injector was  $200^\circ\text{C}$ , the same as that of detector. The oven temperature program was as follows:  $45^\circ\text{C}$  (1 min), increased to  $120^\circ\text{C}$  ( $3.75 \text{ min}$ ) at  $20^\circ\text{C min}^{-1}$ , and at last  $120^\circ\text{C}$  (1 min).

The gas chromatograph was calibrated with a set of mixtures of known compositions that were prepared gravimetrically by an electronic balance (uncertainty of  $\pm 0.0001 \text{ g}$ ). For each sample, the final composition was determined from the average of three replications. With repeated measurements, the standard uncertainty of compositions determination was estimated to be 0.001 in mole fraction.

## 3. Results and discussion

### 3.1. Experimental data

The VLE data for the three binary systems such as toluene + 2-methoxyethanol, 2-methoxyethanol + DMSO and toluene + DMSO were obtained at 101.3 kPa, as listed in Table 3. Also, the VLE data for the ternary system toluene + 2-methoxyethanol + DMSO were measured at 101.3 kPa, as shown in Table 4 and Fig. 4. The location of the azeotropic points of the toluene (1) + 2-methoxyethanol (2) system could be obtained by using  $y_1 - x_1$  versus  $x_1$  diagrams in order to determine azeotropic composition in mole fraction of toluene at  $y_1 - x_1 = 0$  together with  $T$  versus  $x_1$  diagrams where the azeotropic temperature should be the extremum at azeotropic composition in mole fraction of toluene [24]. The experimental data confirm that

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