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Vapor-liquid equilibrium in the binary and ternary systems containing ethyl propionate, ethanol and alkane at 101.3 kPa

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ABSTRACT

The vapor-liquid equilibria at 101.3 kPa of seven binary systems: ethanol (1) + cyclohexane (2), ethanol (1) + n-hexane (2), ethanol (1) + n-octane (2), cyclohexane (1) + ethyl propionate (2), n-hexane (1) + ethyl propionate (2), n-octane (1) + ethyl propionate (2) and ethanol (1) + ethyl propionate (2), three ternary systems: ethanol (1) + cyclohexane (2) + ethyl propionate (3), ethanol (1) + n-hexane (2) + ethyl propionate (3) and ethanol (1) + n-octane (2) + ethyl propionate (3) at temperatures from 332.15 to 396.85 K were studied, all the binary VLE data passed the Herington test. Wilson, NRTL and UNIQUAC models were used to correlate experimental VLE data of the all systems to obtain interaction parameters through the MATLAB software and the experimental values were compared with the regression results. The Wilson and NRTL models reproduced the experimental values very well. Ternary VLE behavior were successfully predicted by the correlated binary parameters. The VLE data for the binary and ternary systems predicted by the correlated interaction parameters were in good agreement with all the experimental data.

1. Introduction

The ethyl propionate is a kind of raw material and solvent [1] that can be widely used in organic synthetic and used to dissolve cellulose esters, ethers, all kinds of natural or synthetic resin. It has aromatic odor and can be used as a spice and a variety of flavors [2]. It can also be used as the organic intermediates in producing antimalarial ethyl amine pyridine. Therefore, the research on ethyl propionate will be of great significance. Ethyl propionate is produced from alcohol and propionic acid as raw material, alkane as water-carrying agent, catalyst synthesis [3]. In the previous research of producing ethyl propionate, cyclohexane, n-hexane, and n-octane were used as water-carrying agent because that different water-carrying agent leaded to different temperature of esterification reaction. Ethyl propionate in the product would be mixed with ethanol and water-carrying agent, so we needed to purify ethyl propionate by rectification process [4].

Vapor-liquid equilibrium data for the system can provide the basis for the design and optimization of chemical processes in heterogeneous (vapor-liquid) systems; it plays a very important role in chemical process design. It's necessary to carry out the rectification by steam to separate ethyl propionate, ethanol and water-carrying agent. Studying on vapor liquid equilibrium of ethyl propionate, ethanol and water-carrying agent is of great importance for the separation of the mixture. Unfortunately despite a practical importance of ethyl propionate the data sets on equilibrium properties of system ethyl propionate + ethanol + alkane (water-carrying agent) are very limited. Ortega et al. set out vapor-liquid equilibria of the similar systems composed of a propyl ester (ethanoate, propanoate, butanoate) + an n-alkane (C_7, C_9) [5].

In this paper, vapor liquid equilibrium of ethyl propionate, ethanol and water-carrying were studied, the binary and ternary VLE data of the three systems were correlated by the Wilson [6,7], NRTL [8,9] and UNIQUAC models [10].

2. Experimental

2.1. Chemicals

The chemical reagents used in this work were ethyl propionate,

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Table 1
Specification of chemical samples.

Chemical	Source	CAS#	Mass fraction purity	Analysis method	Purification method	Boiling point (K) at 101.3 kPa[b]	Molar volume (cm^3/mol)
Ethyl propionate	Macklin	105-37-3	0.989	GC[a]	None	372.15	114.52
Ethanol	Tianjin Fengchuan Chemical Co.,Ltd	64-17-5	0.997	GC	None	351.45	59.08
Cyclohexane	Tianjin Fengchuan Chemical Co.,Ltd	110-82-7	0.995	GC	None	353.85	108.75
N-hexane	Tianjin Fuyu Fine Chemical Co.,Ltd	110-54-3	0.970	GC	None	342.15	131.61
N-octane	Aladdin	111-65-9	0.960	GC	None	398.95	160.53

[a] GC = gas chromatograph.
[b] Ref [11,12].

Table 2
The main experimental instruments.

Instrument	Model	Manufacturer
Gas chromatograph	GC-7980	Agilent Technologies Inc
Mercury thermometer	50–150 °C	Beijing Heng Aode Instrument Co., Ltd.
Electronic balance	FA2004	Shanghai Hengping Instrume nt and Meter Factory
Circulation pump	DLSB-5/25	Gongyi Jinghua Instruments Co., Ltd.

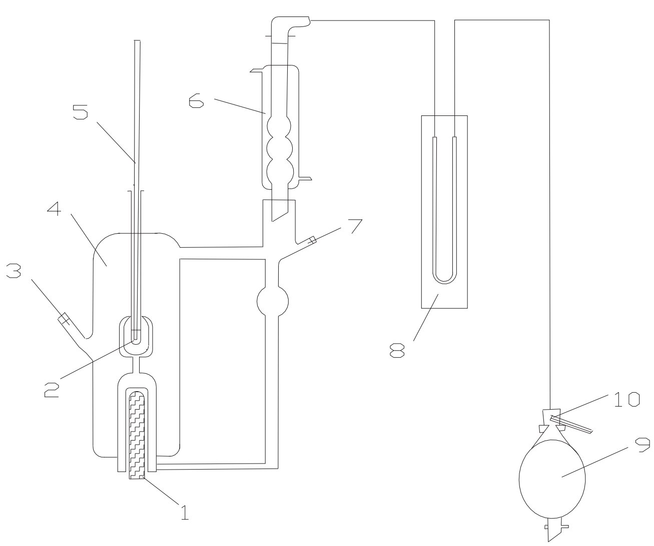

Fig. 1. Modified Othmer still. 1, heating bar; 2, silicone oil; 3, liquid-phase sampling port; 4, equilibrium chamber; 5, mercury thermometer; 6, condenser; 7, vapor-phase sampling port; 8, differential pressure gauge; 9, pneumatic ball; 10, triple valves.

ethanol, cyclohexane, n-hexane and n-octane. The purities of ethyl propionate, ethanol, cyclohexane, n-hexane and n-octane were checked by gas chromatograph (GC-7890 B). The specifications of chemicals used were listed in Table 1 and the main experimental instruments used were shown in Table 2.

2.2. Apparatus and procedure

A double circulation vapor-liquid equilibrium still (a modified Othmer still) was used in the measurement of the isobaric VLE data, as shown in Fig. 1. It includes a liquid-phase sampling port, a vapor-phase sampling port, an equilibrium chamber, a condenser, a pressure control system and a heating bar. This equipment maintained pressure at 101.3 kPa via a pressure control system, with the system's pressure measured using a differential pressure gauge with a standard uncertainty of 0.1 kPa. The details of the vapor-liquid equilibrium still were described by Yuan et al. [13].

For each binary and ternary point tested, a fresh mixture of 40 mL prepared via weighing with an electronic balance was added in the still before the external heater was turned on. When the liquid of the equilibrium still was boiling stably (boiling temperature and the condensate return flow were stable, respectively), remain for 30 min [14], it was considered to have been reached the vapor-liquid equilibrium. The boiling temperature was the vapor-liquid equilibrium temperature measured using a mercury thermometer (thermometer with a precision of 0.1 K), with a standard uncertainty of 0.1 K. Take out the vapor and liquid samples at the same time and place them in the sample bottles prepared before, lid tightly in order to prevent the volatilization.

Gas chromatography was used to determine the composition of the samples, the injection volume of each sample into the GC was

Table 3
Antoine equation[a] parameters[b] for the reagents.

Chemical	A	B	C	D	E
Ethyl propionate	43.754	−3477.4	−12.477	1.6521×10^{-11}	3.9087×10^{-6}
Ethanol	23.844	−2864.2	−5.0474	3.7448×10^{-11}	2.7361×10^{-7}
Cyclohexane	48.553	−3087.4	−15.521	7.383×10^{-3}	6.3563×10^{-12}
N-hexane	69.738	−3627.8	−23.927	1.281×10^{-2}	-16844×10^{-13}
N-octane	29.095	−3011.4	−7.2653	-2.2696×10^{-11}	1.468×10^{-6}

[a] Antoine equation: $logP_i^s = A + \frac{B}{T} + C \times lgT + D \times T + E \times T^2$, with: P ($\frac{101.3}{760}$kPa) and T (K).
[b] Ref. [19].

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