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Measurement, correlation and COSMO-SAC prediction of liquid-liquid equilibrium for the ternary systems, mesityl oxide + *o*-, *m*-, *p*-cresol + water, at 333.2K and 353.2 K

Shaoming Zhou, Libo Li, Youchang Wang, Yun Chen*

Department of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou, 510640, PR China

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ABSTRACT

In this work, liquid-liquid equilibrium (LLE) data for the ternary systems, mesityl oxide + *o*-, *m*-, *p*-cresol + water, were determined at 333.2 K and 353.2 K under 101 kPa. The high distribution coefficient and selectivity calculated by the experimental tie-line data indicate excellent efficiency for mesityl oxide extracting cresols from aqueous solutions. The NRTL and UNIQUAC models were used to correlate the experimental LLE data, with root mean square deviations (RMSDs) below 2.1% and 1.5%, respectively. The COSMO-SAC model was also employed to calculate the LLE data, which agreed with the experimental results quite well.

1. Introduction

Coal gasification, a clean and high efficient coal utilization technology, is playing an significant role in the energy-hungry world due to the increasing demand of natural gas [1,2]. However, the widely used coal gasification processes [3], e.g. lurgi coal gasification process, usually generates a great amount of wastewater, which contains highly concentrated phenolic compounds and other toxic compounds [1,4]. With high toxicity even at low concentration, phenolic compounds cause serious damage to human beings, animals and plants if discharging without treatment [5]. Cresols are the primary phenolic compounds in the coal gasification wastewater [6], and are listed as priority pollutants by the EU and the USA-EPA [7]. Removing cresols from water with conventional recovery process, e.g. distillation or evaporation, is not energy efficient in the industry because of the high boiling point of cresols and the high heat of evaporation of water [8]. Other newly developed methods to remove cresols, e.g. adsorption [9,10], biodegradation [1,11] and chemical oxidation [12], also suffer from various flaws. For instance, adsorption is only applied in treating low concentrated phenolic effluents (less than 200 ppm) due to the high price of activated carbon, the most widely used adsorbents [13]. Biodegradation alone can not be used to treat phenolic wastewater because: (1) microorganisms would be poisoned by the highly concentrated phenolic compounds, (2) degrading cresols is quite time-consuming, which usually takes a few days. Chemical oxidation, a destructive treatment, cannot recycle cresols, which are important industrial materials widely used as antioxidants, herbicides, surfactants, dyes and pigments [14].

Liquid-liquid extraction has been used to recovered polar compounds from aqueous solutions [15,16], showing a series of advantages over other phenolic wastewater treatment methods, such as high throughput, versatility, low energy cost and high commercial efficiency. Such method has been used to treat industrial phenolic wastewater in USA [17], South Africa [17] and China [17–19]. The key problem to design a liquid-liquid extraction process is to develop an appropriate extractant with low water solubility, low price and high efficiency to separate cresols from water. However, such study or data is quite scarce at present, with just a few solvents (or extractants) having been reported [20–24]: at 298.2 K, the distribution coefficient (D) and selectivity (S) of methyl tert-butyl ether for cresols are 800–1200 and 3500–13700, those of methyl isopropyl ketone are 390–1450 and 1300–7800 and

* Corresponding author.
E-mail address: yunchen@scut.edu.cn (Y. Chen).

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Table 1
Supplier, purity and UNIQUAC parameters of the reagents used in this work.

component	Supplier	Mass fraction	UNIQUAC parameter	
			r	q
Mesityl oxide	Xiya Reagent	>0.99	4.43632	3.8600
o-Cresol	Xiya Reagent	>0.995	4.2867	3.2480
m-Cresol	Xiya Reagent	>0.995	4.2867	3.2480
p-Cresol	Xiya Reagent	>0.99	4.2867	3.2480
water	deionized water		0.9200	1.4000
n-propyl acetate	Xiya Reagent	>0.99	–	–
Methanol	Xiya Reagent	>0.99	–	–

those of methyl propyl ketone are 530–1450 and 1900–8900. As a polar organic solvent, Mesityl oxide have shown high efficiency in extracting phenol from the aqueous solution [26]. In addition, it is usually easier to extract cresols from aqueous solutions than to extract phenol [24,25,27–29]. Therefore, it is of practical significance to study the performance of mesityl oxide to extract cresols from wastewater. In industrial practice, especially in coal gasification plants, the operation temperature of the extraction column is often above 333 K, so that the extraction installation would not be clogged by the paraffin (melting point ranges from 328.5 K to 335.15 K) in the wastewater. However, the LLE equilibrium data for phenolic compounds above 333 K are very scarce at present, not to mention data for cresols [25]. Hence, in this work, the extraction performance of mesityl oxide for cresols was investigated above 333 K.

In the present work, the liquid-liquid equilibrium (LLE) data of the mesityl oxide + *o*-, *m*-, *p*-cresol + water ternary systems and corresponding distribution coefficients and selectivities were determined at 333.2 K and 353.2 K, under 101 kPa. LLE data were correlated by the non-random two liquid (NRTL) [30] and universal quasi-chemical (UNIQUAC) [31] models. The conductor-like screening model for segment activity coefficient (COSMO-SAC) [32], a quantum chemical based prediction model, was also employed to predict the liquid-liquid equilibrium data.

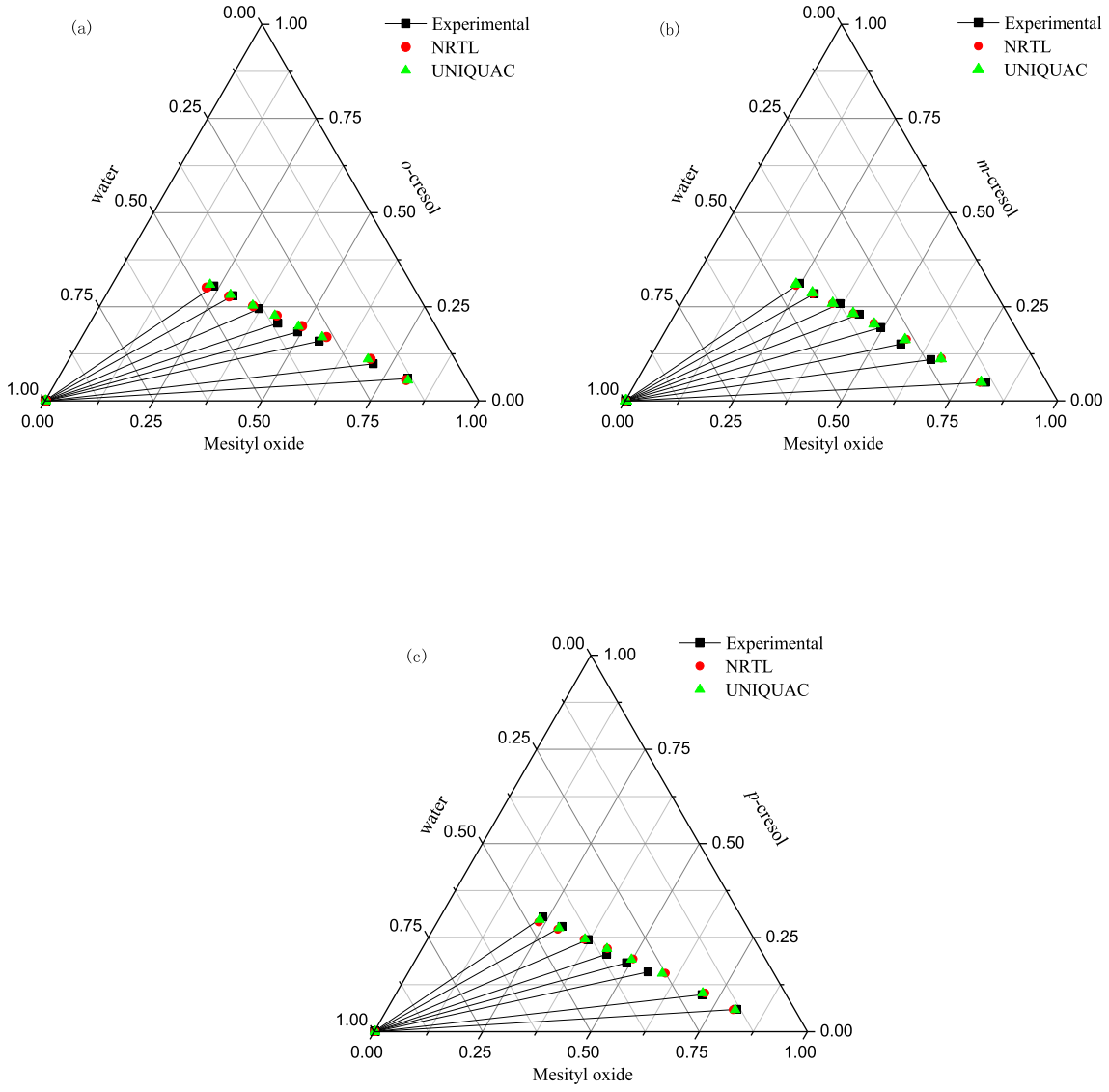

Fig. 1. Ternary diagram for experimental LLE data and the corresponding NRTL and UNIQUAC calculated data of the ternary system, Mesityl oxide(1) + Cresol(2) + Water(3), at 333.2 K; (a) *o*-cresol, (b) *m*-cresol, (c) *p*-cresol.