

Measurement and correlation of isobaric vapour–liquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa



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ABSTRACT

Isobaric vapour–liquid equilibrium (VLE) data for binary systems containing o-cresol (OC) + m-cresol (MC), OC + 2, 6-dimethylphenol (DMP), and MC + DMP at 20.0 kPa were measured by using a modified Othmer still. Its reliability was confirmed by measuring the saturated vapour pressure data for the components of MC and DMP. Herington area test was used to confirm the thermodynamic consistency for these binary systems, and the results showed good thermodynamic consistency. The binary VLE experimental data were correlated and predicted by Wilson, NRTL, and UNIFAC models. The results correlated by Wilson and NRTL models agree well with the experimental values. The results predicted by UNIFAC are in accordance with experimental data with rational deviations for systems OC + MC and OC + DMP but show relatively large deviations between the predicted values and experimental data for MC + DMP system. By defining the group =COH in DMP and MC as two different groups, the experimental data were correlated, and new groups with binary interaction parameters were obtained. The results calculated by UNIFAC with new defining groups are in accordance with the experimental data.

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1. Introduction

O-cresol (OC), m-cresol (MC), and 2,6-dimethylphenol (DMP) are important organic synthesis materials. OC is mainly used as synthetic resin and as a raw material for the synthesis of pesticides, plastic antioxidants, and polymerization inhibitors et al. [1] MC can be used to manufacture antioxidants, pesticides, and vitamin E et al. [2] DMP is used as a monomer to synthesize engineering plastic PPO, the raw material for the synthesis of pesticide intermediates 2, 6-diphenylamine and antiarrhythmic drugs [3,4].

OC, MC, and DMP are mainly derived from chemical synthesis and byproduct of coal tar fractionation. Separation or purification of these phenols is important due to their wide application. In general, vacuum distillation can be used to separate OC and MC/DMP due to their relatively high boiling point difference (about 10.0 K), namely, 464.15 K for OC, 475.35 K for MC, and 474.15 K for DMP [5]. Separating MC and DMP using ordinary distillation is difficult because the normal boiling point of DMP is close to that of MC. However, according to the comparison of their saturated vapour pressure data, we found that the difference of boiling point between MC and

DMP gradually increases with pressure reduction (see details in the next section). In this case, vacuum distillation could be used to separate MC and DMP. Vapour–liquid equilibrium (VLE) data are important on the design and optimization of distillation process. According to literature and Dortmund databank, Fox et al. [6] measured the $T-x$ experimental data (bubble point) for the system of OC + MC at 101.0 kPa in 1917. Ye et al. [7] measured the $T-x-y$ experimental data of OC + DMP at 10.0 and 25.0 kPa in 1998. To our knowledge, the VLE data for DMP + MC are limited and may not meet the requirements of designing the separation process.

In this work, the reliability of the modified Othmer still was confirmed by measuring the saturated pressure data for the components of MC and DMP. Isobaric VLE data for the binary systems OC + MC, OC + DMP, and DMP + MC at 20.0 kPa were measured by using the equilibrium apparatus. Herington area test was used to confirm the thermodynamic consistency of these binary systems. Wilson [8] and NRTL [9] models were used to correlate the VLE data, and the interaction parameters involved in models were obtained. UNIFAC [10] model was used to predict the VLE of these three binary systems. The groups of =COH were distinguished as two different groups in the system of DMP + MC, and the group binary interaction parameters were obtained by correlating the binary VLE data.

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Table 1
Mass fraction purity of the chemical reagent used.

Material	Source	CAS RN	Mass fraction purity	Purification method	Analysis method
O-Cresol	Sinopharm Chemical Regent Co., Ltd.	95-48-7	≥0.990	none	GC
M-Cresol	Sinopharm Chemical Regent Co., Ltd.	108-39-4	≥0.990	none	GC
2, 6-Dimethylphenol	Aladdin Reagent Co., Ltd	576-26-1	≥0.990	none	GC

2. Experimental

2.1. Materials

The chemicals used in this work were OC, MC, and DMP. The OC (≥99.0% purity of mass fraction) and MC (≥99.0% purity of mass fraction) were supplied by Sinopharm Chemical Regent Co., Ltd., and DMP (≥99.0% purity of mass fraction) was provided by Aladdin Reagent Co., Ltd. These chemicals were stated pure from factory. Detailed information on these chemicals is listed in Table 1. All reagents were used without further purification in this work.

2.2. VLE measurements

A modified Othmer still (c.f., Fig. 1.) was used to measure the VLE of systems consisting of OC + MC, OC + DMP, and MC + DMP. In this still, both liquid and condensed vapour phases were recirculated successively to sufficiently mix the phases, thus ensuring that equilibrium state could be achieved as early as possible. System pressure and temperature were measured by using a U-shaped differential manometer (filled with mercury) with uncertainty of ±0.0665 kPa and a high precision mercury thermometer with uncertainty of ±0.05 K. In each VLE measurement, the mixed solution

was placed into the boiling chamber at first, and the system pressure was fixed and held constant by using a vacuum pump (2XZ-4, Shanghai Instrument, China). Heat was provided, and a suitable power of heater was defined to achieve reasonable condensation reflux rate (i.e., about 2–3 drops per second). When constant temperature and pressure were maintained for more than 50 min, the equilibrium state was assumed, and the samples can be taken from the sampling ports at this time.

Vapour pressure data for the components of DMP and MC was measured to determine the reliability of equilibrium apparatus (Table 2). For the convenience of evaluation, the experimental data of this work were compared with previously published experimental results, and the compared results are shown in Fig. 2. In this figure, the experimental data of vapour pressure are in good agreement with those in literature [11–15]. Therefore, verification showed that the equilibrium was reliable.

2.3. Sample analysis

The gas chromatograph (Agilent 7890B) equipped with a Flame Ionization Detector and a HP-ULTRA 2 (25 m × 0.320 mm × 0.52 μm) chromatographic column was used to analyze the vapour and liquid samples. The temperatures of

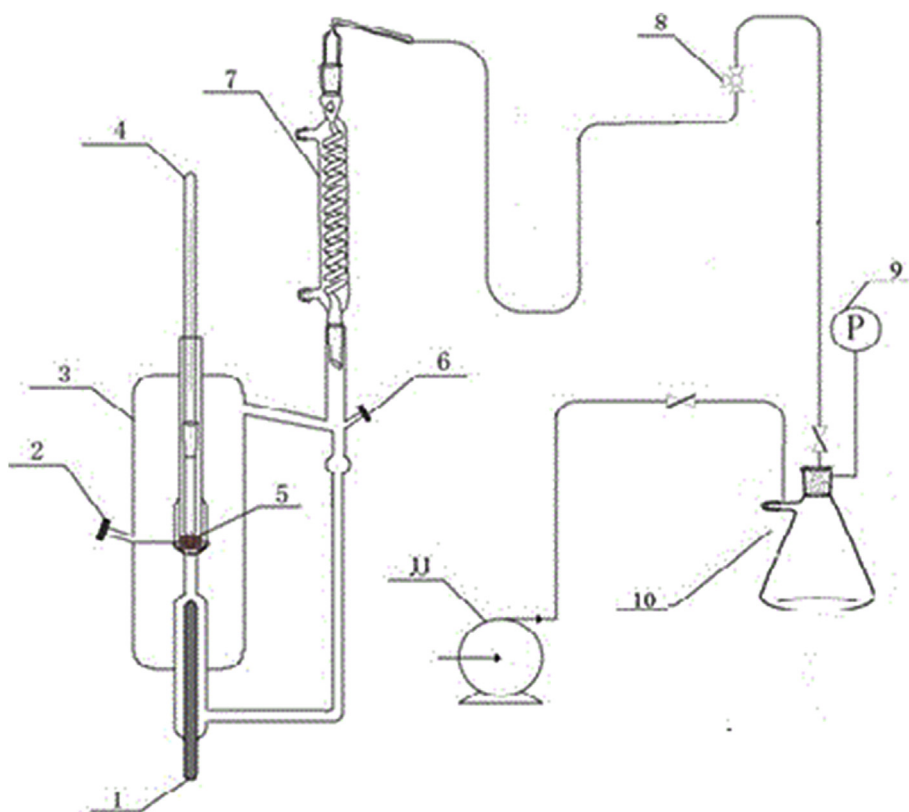


Fig. 1. Experimental device for VLE measurement. 1. heating rod; 2. liquid phase sampling port; 3. equilibrium chamber; 4. mercury thermometer; 5. glycerol; 6. vapour phase sampling port; 7. condensing coil; 8. valve; 9. buffer bottle (erlenmeyer flask); 10. U-shaped differential manometer; 11. vacuum pump.

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