1 **Measurement and thermodynamic modeling of**
2 **ternary (liquid + liquid) equilibrium for**
3 **extraction of *o*-cresol, *m*-cresol or *p*-cresol from**
4 **aqueous solution with 2-pentanone**

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ABSTRACT

The (liquid + liquid) equilibrium (LLE) data are vital for the liquid extraction of cresols from aqueous solution with 2-pentanone as an extraction agent. Therefore, the ternary LLE data for {2-pentanone + *o*-cresol, *m*-cresol or *p*-cresol + water} were determined at $T = (298.15 \text{ and } 323.15) \text{ K}$ and $p = 101.3 \text{ kPa}$. And the reliability of the LLE data was ascertained by using the Othmer-Tobias and Hand equations. The distribution coefficients and separation factors were calculated to evaluate the effectiveness of extracting cresols from water. The thermodynamic NRTL and UNIQUAC models were used to correlate the experimental LLE data of the studied systems, and the binary interaction parameter values were obtained from the data correlation.

Keywords: Ternary (liquid + liquid) equilibrium; Cresols; 2-Pentanone; NRTL; UNIQUAC

1. Introduction

Coal gasification has been an important alternative for the production of base chemicals including gaseous fuels, especially in developing country, e.g. in China, and various commercial coal gasification technologies have been applied in the coal chemical plants around the world in the last few decades [1-2]. However, a number of phenols would also be produced as by-products during the coal gasification process and washed out with water in the washing step, appearing as pollutants in the effluents discharged by coal gasification plants. Cresols are among the principal components in the phenols-containing coal gasification wastewaters [3]. Cresols in the wastewaters are highly toxic even at low concentration [4], and have been listed as the priority pollutants by the U.S. EPA and the EU [5]. However, as primary organic pollutants in the coal gasification wastewaters, there are only a few studies concerning cresols removal from coal gasification wastewaters, thus further investigation of cresols removal from wastewaters was needed for the consideration of the sustainable development of the coal chemical industry and the ecological environment.

(Liquid + liquid) extraction technology are a desirable method in the abatement of phenolic compounds from wastewaters, which has a range of advantages over other kinds of organic wastewater treatment methods, such as high through put, ease of automatic operation and scale up [6], handling high concentration of phenolic wastewater effectively [5], and

providing economic benefits by recovering cresols, for the reason that the isomers of cresols are very useful materials in the production of various kinds of chemicals, such as epoxy resins (by *o*-cresol), disinfectants (by *m*-cresol), light-resistant antioxidants (by *p*-cresol), etc. [7]. (Liquid + liquid) extraction has been used to treat phenolic wastewater in industry [2]. And it should be noted that, after the extraction process, a solvent stripping process is usually used to recover the solvent from the aqueous phase to avoid significant solvent loss, and the extraction solvent's concentration in the aqueous phase could be reduced to below 0.001 % (mass percent) [8] after the stripping process.

Thermodynamic (liquid + liquid) equilibrium (LLE) data reflect the distribution of cresols between the aqueous phase and the solvent phase in extraction process, provide a good understanding of phase behavior and the thermodynamic properties for ternary systems of {organic solvent + cresols + water} [9], and thus are important thermodynamic properties for the design, operation and optimization of cresols extraction from wastewaters [10-11]. However, only a few studies have been reported for the LLE data in cresols extraction from aqueous solution till now [12-16], searching for a new and more suitable solvent for the removal of cresols is still the primary consideration. 2-Pentanone, as a polar solvent, has already been investigated as an extraction solvent of aliphatic acids including acetic acid and propanoic acid, and showed excellent extraction efficiency in extracting above organic acids [17-19]. Therefore, in this work, 2-pentanone were chose as a new solvent for cresols extraction from coal gasification wastewater, and investigated the (liquid + liquid) equilibrium and phase behavior involved in extracting cresols from aqueous solution with 2-pentanone adequately.

In this work, to explore the multicomponent phase behaviors of *o*-cresol, *m*-cresol or *p*-cresol in (2-pentanone + water) mixture and the distribution ratios between the water-rich phase and solvent-rich phase, the LLE data of the ternary systems {2-pentanone + *o*-cresol, *m*-cresol or *p*-cresol + water} were determined at $T = (298.15 \text{ and } 323.15) \text{ K}$ and $p = 101.3 \text{ kPa}$. To the best knowledge of the authors, these data have never been reported in any previous references. And, furthermore, the experimental LLE data were correlated by the thermodynamic activity coefficient models: NRTL (nonrandom two-liquid) [20] and UNIQUAC (universal quasi-chemical) [21] models, and the binary interaction parameters

were obtained through the model correlation.

2. Experimental

2.1. Materials

o-Cresol, *m*-cresol, *p*-cresol, 2-pentanone and 1, 3, 5-trimethylbenzene were all supplied by Xiya Reagent (Chengdu, China), except that the *n*-Butyl acetate was obtained from Kemiou Chemical Reagent (Tianjin, China). All these chemical were used without further purification, for their purity were confirmed by gas chromatography (GC) and no peaks of impurity was detected out. Distilled water was used throughout all the experiments. The details of chemicals used in this work are shown in table 1.

2.2. Apparatus and procedure

2.2.1. Mixture preparation

The LLE measurements for ternary systems {2-pentanone + *o*-cresol + water}, {2-pentanone + *m*-cresol + water}, and {2-pentanone + *p*-cresol + water} were carried out at $T = (298.15 \text{ and } 323.15) \text{ K}$ and $p = 101.3 \text{ kPa}$. To establish liquid phase equilibrium, a 100 mL glass cell was employed in this work, which was equipped with a magnetic stirrer and a jacket for water circulation to keep the temperature of the liquid mixture in the glass cell at a constant. A certain amount of 2-pentanone, cresol and water were loaded into the glass cell, and then the mixture was stirred vigorously for 2 hours and left for standing for at least 20 hours. The stirring and settling time in the above procedure were sufficient for the ternary mixture to separate into two liquid phases and reach (liquid + liquid) equilibrium.

2.2.2. Sample analyses

After the phase equilibrium was established, the samples of aqueous and organic phases were collected from the lower and upper phases by a syringe, respectively, and were then analyzed by a gas chromatograph (GC, Agilent 6820) equipped with a flame ionization detector (FID) and a DB-5MS capillary column ($30 \text{ m} \times 0.32 \text{ mm} \times 0.25 \text{ }\mu\text{m}$). The temperatures of the injection port and FID detector were set at 523.15 K and 543.15 K, respectively, and the GC oven's temperature was at first kept at 313.15 K for 2 minutes, then was increased from (313.15 to 433.15) K at a rate of $0.5 \text{ K} \cdot \text{s}^{-1}$, and finally kept at 433.15 K for another 2 minutes. The nitrogen flow rate for the separation column was set at $30 \text{ cm}^3 \cdot \text{min}^{-1}$. The mass fractions of 2-pentanone and cresols in samples of both the aqueous

1 phase and organic phase were measured by an internal standard method, with 1, 3,
2 5-trimethylbenzene as internal standard for cresols and *n*-butyl acetate for 2-pentanone, and
3 samples as well as the internal standards were all weighed by an analytical balance (Shimadzu
4 AUV220D) accurate to within ± 0.0001 g. The mass fraction of the third component (i.e.
5 water) in each phase was evaluated through mass balance, for the reason that the mass
6 fractions of 2-pentanone and cresol had been obtained by GC analysis. Three analyses at least
7 for each sample were made to obtain a mean value, which was reported in this work. The
8 uncertainty for each component, either in the aqueous phase or in the organic phase, was also
9 estimated according to the GUM and NIST guidelines [22, 23], and Appendix A provides the
10 corresponding equations.

11 **3 Results and discussion**

12 *3.1 Experimental LLE data*

13 The LLE data for ternary systems {2-pentanone + *o*-cresol + water}, {2-pentanone +
14 *m*-cresol + water}, and {2-pentanone + *p*-cresol + water} were determined at $T = (298.15$ and
15 $323.15)$ K and $p = 101.3$ kPa. The experimental LLE data for the studied systems at different
16 temperatures are presented in tables 2-4, and are also plotted in triangle diagrams as shown in
17 figures 1-6. All the studied {2-pentanone + *o*-cresol, *m*-cresol, or *p*-cresol + water} ternary
18 systems are supposed to be classified as Treybal's type II [24], where the two liquid pairs
19 (2-pentanone + water) and (cresol + water) are partially miscible. And as can be seen from the
20 phase diagrams in figures 1-6, temperature presents a minor effect on the size of the
21 two-phase region, by comparison of phase diagrams at different temperatures of the same
22 system. And isomer type of cresol (i.e. *o*-cresol, *m*-cresol, *p*-cresol) has a negligible influence
23 on the size of the two-phase region, this may be due to the very similar structures of three
24 kinds of cresols. The binary endpoints (water + 2-pentanone) and (water + isomeric cresols)
25 obtained in this work were tabulated in tables S1 and S2, and also plotted in figures S1 and S2
26 in the Supplementary data, along with the data taken from references [25-33]. Seen from
27 these tables and figures, the binary solubilities for (water + 2-pentanone) and (water +
28 isomeric cresols) agree with literature data quite well.

29 The distribution coefficients (D) and separation factors (S) were calculated to evaluate the
30 efficiency of 2-pentanone in extracting cresols from aqueous solution, defined as:

$$D = w_2^{\text{II}} / w_2^{\text{I}} \quad (1)$$

$$S = (w_2^{\text{II}} / w_2^{\text{I}}) / (w_3^{\text{II}} / w_3^{\text{I}}) \quad (2)$$

Here w_2^{I} and w_2^{II} denote cresol's mass fractions in the aqueous phase and the organic phase, respectively, while w_3^{I} and w_3^{II} denote the mass fractions of water in the above two phases, respectively. The distribution coefficients and separation factors are listed in table 5 and plotted in figures 7 and 8. Seen from the high distribution coefficients and separation factors in table 5, it could be concluded that 2-pentanone displays very excellent efficiency in extracting cresols from aqueous solution. And also, the extraction performance of 2-pentanone for the three isomers of cresol are similar. In addition, known from table 5, both the distribution coefficients and separation factors decrease a bit as the temperature increases among the studied temperature range, thus temperature could exert some influence on the distribution of cresols in (2-pentanone + water) mixture. The above conclusion reveals that, for the studied equilibrium systems, as the temperature rises, more cresols will transfer from the solvent phase to the aqueous phase before the new (liquid + liquid) phase equilibrium is formed, which is in agreement with the fact that the cresol's solubility in water increases with the rising of temperature. And there is also an evident decreasing tendency shown in distribution coefficients and separation factors with the increasing of cresol's concentration in the aqueous phase or in the organic phase at a certain temperature, indicating that concentration also put a vital effect on the distribution ratios of cresol among organic phase and aqueous phase and on the separation factors. Such temperature and concentration dependence could also be commonly observed in many other ternary systems, especially phenols containing systems [34-39]. It can also be seen from figures 7 and 8 that, the influence of the structure of cresol isomers on the extractive properties of 2-pentanone is insignificant, as the distribution coefficients and separation factors are very close for the three cresol isomers when using 2-pentanone as the extraction agent.

The extractive properties of cresols from water for the 2-pentanone were compared with other solvents, such as toluene [12, 40] and 2-methoxy-2-methylpropane [16], in terms of distribution coefficient. The comparisons were all made under similar temperature and cresol

concentration. Taking *o*-cresol as an example, the distribution coefficient of *o*-cresol in toluene ranges between 11.04 and 12.28 at $T = 293.15$ K, while that in 2-pentanone ranges 131.75~164.10 at $T = 298.15$ K for the similar *o*-cresol concentration range in the aqueous phase (0.002~0.004 in mass fraction) (see Supplementary data, figure S3). This indicates the efficiency of 2-pentanone in extracting cresol is much higher than that of toluene. In addition, the extractive properties of 2-pentanone for cresols from water were also compared with those of 2-methoxy-2-methylpropane. For example, when the concentration, expressed in mass fraction, of *m*-cresol in water ranges between 0.001~0.003 and the temperature is 298.15 K, the distribution coefficient of *m*-cresol in 2-pentanone ranges between 127.21~222.71, quite higher than those in 2-methoxy-2-methylpropane, ranging between 116.95~206.19 (see Supplementary data, figure S4). A minor exception is that, when the *m*-cresol concentration in the aqueous phase is far below 0.001 (mass fraction), 2-methoxy-2-methylpropane performed a bit better. On the whole, the extraction efficiency of 2-pentanone for cresols is better than 2-methoxy-2-methylpropane, since we seldom need to extraction cresols with concentrations far below 0.001. In addition, 2-pentanone, with higher boiling point, is more desirable than 2-methoxy-2-methylpropane when solvent extraction is carried out at higher temperatures [41].

The reliability of the experimental LLE data were verified by the Othmer-Tobias [42] and Hand [43] equations, which are defined as follows:

$$\ln[(1 - w_1^{\text{II}}) / w_1^{\text{II}}] = a_1 + b_1 \ln[(1 - w_3^{\text{I}}) / w_3^{\text{I}}] \quad (3)$$

$$\ln(w_2^{\text{II}} / w_1^{\text{II}}) = a_2 + b_2 \ln(w_2^{\text{I}} / w_3^{\text{I}}) \quad (4)$$

Where a_1 , b_1 , a_2 , and b_2 are fitting parameters of Othmer-Tobias and Hand equations, which are relevant to the type of system and the immiscibility, w_3^{I} and w_1^{II} denote the mass fractions of water in the aqueous phase and 2-pentanone in the organic phase, respectively, while w_2^{I} and w_2^{II} are mass fractions of cresol in the aqueous phase and in the organic phase, respectively. The fitting parameters together with the regression coefficients (R^2), for the three studied systems at different temperatures, are listed in table 6. And the Othmer-Tobias and Hand plots for the studied systems are shown in figures 9 and 10. The high linearity of the

plots in figures 9 and 10, together with the high regression coefficients (i.e. $R^2 > 0.97$) in table 6, indicates the good reliability of our experimental LLE data.

3.2. Correlation of LLE data

The thermodynamic NRTL [20] and UNIQUAC [21] models are local composition equations for the representation of the liquid mixtures' excess Gibbs energy, which are related to the activity coefficients of components in the liquid mixtures, and thus the two thermodynamic equations are commonly used to model the (liquid + liquid) phase equilibrium. The experimental LLE data for the studied systems in this work were correlated by the NRTL and UNIQUAC activity coefficient models. The thermodynamic criteria together with mass balance equation were applied for the LLE data correlation, shown as follows:

$$(x_i \gamma_i)^I = (x_i \gamma_i)^{II} \quad (5)$$

$$\sum_i x_i^I = 1, \text{ and } \sum_i x_i^{II} = 1 \quad (6)$$

Where the superscript I and II refer to the aqueous phase and the organic phase, and the subscript i refers to the number of components. The symbol x is the mole fraction of component in the ternary phase equilibrium systems, and γ is the activity coefficient for component, given by the thermodynamic models NRTL or UNIQUAC. The activity coefficient in the NRTL model for component i in multicomponent system is expressed as follows:

$$\ln \gamma_i = \frac{\sum_{j=1}^n \tau_{ji} G_{ji} x_j}{\sum_{k=1}^n G_{ki} x_k} + \sum_{j=1}^n \frac{x_j G_{ij}}{\sum_{k=1}^n G_{kj} x_k} \left(\tau_{ij} - \frac{\sum_{i=1}^n x_i \tau_{ij} G_{ij}}{\sum_{k=1}^n G_{kj} x_k} \right) \quad (7)$$

Here $G_{ji} = \exp(-\alpha_{ji} \tau_{ji})$, $G_{ij} = \exp(-\alpha_{ij} \tau_{ij})$, $\tau_{ji} = (g_{ji} - g_{ii})/RT = b_{ji}/T$, and $\tau_{ij} = (g_{ij} - g_{jj})/RT = b_{ij}/T$. α_{ij} is the non-randomness factor, and when correlating the experimental LLE data in this work using the NRTL model, α_{ij} was fixed to 0.2, except that value for (2-pentanone + cresol) binary pair, which was fixed to 0.3 instead, as listed in table 8. τ_{ji} and τ_{ij} are two adjustable parameters, related to the NRTL interaction

energies g_{ji} and g_{ij} between species i and j , and could be expressed by the binary interaction parameters b_{ji} and b_{ij} , which were yield by correlation of LLE data using the NRTL model.

The activity coefficient by the UNIQUAC model for component i in multicomponent system is expressed as:

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \quad (8)$$

Where γ_i^C are combinatorial activity coefficient, while γ_i^R are residual activity coefficient, defined as equation (9) and (10), respectively.

$$\ln \gamma_i^C = \ln \frac{\phi_i}{x_i} + \left(\frac{z}{2} \right) q_i \ln \frac{\theta_i}{\phi_i} + l_i - \frac{\phi_i}{x_i} \sum_{j=1}^n x_j l_j \quad (9)$$

$$\ln \gamma_i^R = q_i \left[1 - \ln \left(\sum_{j=1}^n \theta_j \tau_{ji} \right) - \sum_{j=1}^n \frac{\theta_j \tau_{ij}}{\sum_{k=1}^n \theta_k \tau_{kj}} \right] \quad (10)$$

Here $\phi_i = x_i r_i / (\sum_{i=1}^n x_i r_i)$, $\theta_i = x_i q_i / (\sum_{i=1}^n x_i q_i)$, $l_j = (z/2)(r_j - q_j) - (r_j - 1)$,

$\tau_{ji} = \exp[-(u_{ji} - u_{ii})/RT] = \exp(-a_{ji}/T)$, $\tau_{ij} = \exp[-(u_{ij} - u_{jj})/RT] = \exp(-a_{ij}/T)$. z

is the coordination number and is fixed to 10. ϕ_i and θ_i are the segment fraction and area fraction, and could be expressed in formula related to pure-component volume parameter, r_i , and area parameter, q_i , respectively, which were taken from reference [44] and are shown in table 7. Adjustable parameters τ_{ji} and τ_{ij} are related to the UNIQUAC interaction energies u_{ji} and u_{ij} between species i and j , and could be expressed by binary interaction parameters a_{ji} and a_{ij} obtained in UNIQUAC modeling of the experimental LLE data in this work.

The binary interaction parameters b_{ji} and b_{ij} in NRTL model, a_{ji} and a_{ij} for UNIQUAC model were obtained by minimizing the objective function (OF):

$$\text{OF} = \sum_{i=1}^3 \sum_{j=1}^2 \sum_{k=1}^n (w_{ijk}^{\text{exp}} - w_{ijk}^{\text{cal}})^2 \quad (11)$$

Where subscripts i, j , and k refer to the components, the phases and the tie lines, respectively, and n is the number of tie lines. w^{exp} is the experimental mass fraction, while w^{cal} is the calculated mass fraction. The optimized binary interaction parameters in NRTL and UNIQUAC models for the studied systems were shown in table 8. The correlated LLE data for ternary systems {2-pentanone + *o*-cresol + water}, {2-pentanone + *m*-cresol + water}, and {2-pentanone + *p*-cresol + water} are present in figures 1-6, with comparison to the experimental data. The root mean square deviation ($rmsd$) is used as a measure of the agreement between the experimental and calculated data, and are defined by the following equation:

$$rmsd\% = 100 \sqrt{\frac{\sum_{i=1}^3 \sum_{j=1}^2 \sum_{k=1}^n (w_{ijk}^{exp} - w_{ijk}^{cal})^2}{6n}} \quad (12)$$

The resulted $rmsd$ values for the studied systems are listed in table 8, in which the small $rmsd$ values (i.e. <0.4%) demonstrate the goodness of the correlation for the experimental data using both two thermodynamic models, though the $rmsd$ values for UNIQUAC model are slightly higher than the NRTL model. Also, seen from the calculated data represented in figures 1-6, there is a good coincidence between the calculated and experimental data.

4 conclusions

The experimental LLE data for the ternary systems {2-pentanone + *o*-cresol + water}, {2-pentanone + *m*-cresol + water}, and {2-pentanone + *p*-cresol + water}, were determined at $T = (298.15 \text{ and } 323.15) \text{ K}$ and $p = 101.3 \text{ kPa}$. The LLE data were fitted by the Othmer-Tobias and Hand equations with very high regression coefficients, which ascertained the experimental data to be highly reliable. The distribution coefficients and separation factors were calculated to evaluate the performance of 2-pentanone in cresols extraction. And 2-pentanone was shown to be a very promising extraction solvent to recover cresols from coal gasification wastewaters, for the distribution coefficients and separation factors for cresols extraction with 2-pentanone are high, which displays the excellent performance in cresols extraction of the selected extraction agent. The LLE data were then correlated by the thermodynamic models NRTL and UNIQUAC, which both described the phase behavior of the studied systems very accurately and yielded relevant binary interaction parameters. The

1 experimental LLE data and calculated binary interaction parameters in this work should be
2 useful for designing or optimizing the extraction process of cresols in the field of coal
3 gasification wastewater treatment.

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Appendix A

The mass fractions of 2-pentanone and cresols in samples from both the aqueous phase and organic phase were measured by an internal standard method. The proportionality factor for component i (2-pentanone or cresols) was calculated by:

$$F_i = \frac{A_{\text{std}} m_i}{A_i m_{\text{std}}} \quad (\text{A - 1})$$

The uncertainty for the proportionality factor was then estimated with:

$$\Delta F_i = \sqrt{\left(\frac{\partial F_i}{\partial A_{\text{std}}} \Delta A_{\text{std}}\right)^2 + \left(\frac{\partial F_i}{\partial A_i} \Delta A_i\right)^2 + \left(\frac{\partial F_i}{\partial m_i} \Delta m_i\right)^2 + \left(\frac{\partial F_i}{\partial m_{\text{std}}} \Delta m_{\text{std}}\right)^2} \quad (\text{A - 2})$$

Where A_i and A_{std} refer to the peak areas for component i and internal standard of component i in GC analysis, respectively, while m_i and m_{std} refer to the masses of component i and internal standard weighed by analytical balance. The uncertainty for the peak area was estimated by calculating relative standard deviation of the peak areas, which were obtained after injecting the samples for proportionality factor calculation consecutively for six times. The mass uncertainty was estimated to be equal to the reported uncertainty of the analytical balance.

The mass fraction for component i was calculated according to the equations as follows:

$$m_i = F_i \frac{A_i m_{\text{std}}}{A_{\text{std}}} \quad)$$

$$w_i = \frac{m_i}{m_{\text{sample}}} \quad)$$

Here the m_{sample} refers to the mass of the sample collected from the aqueous phase or the organic phase of the equilibrium systems and weighed by analytical balance. Correspondingly, the uncertainty for the mass fraction of component i was calculated as follows:

$$\Delta m_i = \sqrt{\left(\frac{\partial m_i}{\partial F_i} \Delta F_i\right)^2 + \left(\frac{\partial m_i}{\partial m_{\text{std}}} \Delta m_{\text{std}}\right)^2 + \left(\frac{\partial m_i}{\partial A_i} \Delta A_i\right)^2 + \left(\frac{\partial m_i}{\partial A_{\text{std}}} \Delta A_{\text{std}}\right)^2} \quad (\text{A - 5})$$

$$\Delta w_i = \sqrt{\left(\frac{\partial w_i}{\partial m_i} \Delta m_i\right)^2 + \left(\frac{\partial w_i}{\partial m_{\text{sample}}} \Delta m_{\text{sample}}\right)^2} \quad (\text{A - 6})$$

The above uncertainty calculation method was applied in this work for estimating the

uncertainties for components 2-pentanone $u(w_1)$ and cresols $u(w_2)$ in the studied ternary systems. Besides, the mass fraction for water (w_3) was obtained through mass balance [37, 39, 45, 46]:

$$w_3 = 1 - w_1 - w_2 \quad (\text{A - 7})$$

Thus the uncertainty for the mass fraction of water $u(w_3)$ was calculated with the following equation:

$$\Delta w_3 = \sqrt{\left(\frac{\partial w_3}{\partial w_1} \Delta w_1\right)^2 + \left(\frac{\partial w_3}{\partial w_2} \Delta w_2\right)^2} \quad (\text{A - 8})$$

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Caption of Tables and Figures

Tables

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Details of chemicals used in this work.

TABLE 2

(Liquid + liquid) equilibrium data in mass fraction for ternary system { 2-pentanone (1) + *o*-cresol (2) + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa.^a

TABLE 3

(Liquid + liquid) equilibrium data in mass fraction for ternary system { 2-pentanone (1) + *m*-cresol (2) + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa.^a

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(Liquid + liquid) equilibrium data in mass fraction for ternary system { 2-pentanone (1) + *p*-cresol (2) + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa.^a

TABLE 5

Distribution coefficients (D) and separation factors (S) for the ternary systems {2-pentanone (1) + *o*-cresol, *m*-cresol, or *p*-cresol (2) + water (3)} at $T = (298.15, 323.15)$ K.

TABLE 6

Othmer-Tobias and Hand equation parameters, a , b , and regression coefficients, R^2 for the studied systems {2-pentanone (1) + *o*-cresol, *m*-cresol, or *p*-cresol (2) + water (3)}.

TABLE 7

The UNIQUAC structural parameters (r and q) for pure components.

TABLE 8

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FIGURE 1. Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary system {2-pentanone (1) + *o*-cresol (2) + water (3)} at $T = 298.15$ K and $p = 101.3$ kPa: (■-■) experimental data, (Δ---Δ) NRTL model, and (×····×) UNIQUAC model.

FIGURE 2. Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary system {2-pentanone (1) + *o*-cresol (2) + water (3)} at $T = 323.15$ K and $p = 101.3$ kPa: (■-■)

1 experimental data, (Δ --- Δ) NRTL model, and ($\times$... $\times$) UNIQUAC model.

2 **FIGURE 3.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
3 system {2-pentanone (1) + *m*-cresol (2) + water (3)} at $T = 298.15$ K and $p = 101.3$ kPa: ($\blacksquare$ - $\blacksquare$)
4 experimental data, (Δ --- Δ) NRTL model, and ($\times$... $\times$) UNIQUAC model.

5 **FIGURE 4.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
6 system {2-pentanone (1) + *m*-cresol (2) + water (3)} at $T = 323.15$ K and $p = 101.3$ kPa: ($\blacksquare$ - $\blacksquare$)
7 experimental data, (Δ --- Δ) NRTL model, and ($\times$... $\times$) UNIQUAC model.

8 **FIGURE 5.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
9 system {2-pentanone (1) + *p*-cresol (2) + water (3)} at $T = 298.15$ K and $p = 101.3$ kPa: ($\blacksquare$ - $\blacksquare$)
10 experimental data, (Δ --- Δ) NRTL model, and ($\times$... $\times$) UNIQUAC model.

11 **FIGURE 6.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
12 system {2-pentanone (1) + *p*-cresol (2) + water (3)} at $T = 323.15$ K and $p = 101.3$ kPa: ($\blacksquare$ - $\blacksquare$)
13 experimental data, (Δ --- Δ) NRTL model, and ($\times$... $\times$) UNIQUAC model.

14 **FIGURE 7.** Distribution coefficient of cresol plotted versus mass fraction of cresol in the aqueous
15 phase at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa: ($\blacksquare$) *o*-cresol, at $T = 298.15$ K, ($\square$) *o*-cresol, at $T =$
16 323.15 K, ($\bullet$) *m*-cresol, at $T = 298.15$ K, ($\circ$) *m*-cresol, at $T = 323.15$ K, ($\blacktriangle$) *p*-cresol, at $T = 298.15$ K,
17 ($\triangle$) *p*-cresol, at $T = 323.15$ K.

18 **FIGURE 8.** Separation factor of cresol plotted versus mass fraction of cresol in the aqueous phase at T
19 $= (298.15, 323.15)$ K and $p = 101.3$ kPa: ($\blacksquare$) *o*-cresol, at $T = 298.15$ K, ($\square$) *o*-cresol, at $T = 323.15$ K,
20 ($\bullet$) *m*-cresol, at $T = 298.15$ K, ($\circ$) *m*-cresol, at $T = 323.15$ K, ($\blacktriangle$) *p*-cresol, at $T = 298.15$ K, ($\triangle$)
21 *p*-cresol, at $T = 323.15$ K.

22 **FIGURE 9.** Othmer-Tobias plots for the ternary systems {2-pentanone (1) + *o*-cresol, *m*-cresol, or
23 *p*-cresol (2) + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa: ($\blacksquare$) *o*-cresol, at $T = 298.15$ K, ($\square$)
24 *o*-cresol, at $T = 323.15$ K, ($\bullet$) *m*-cresol, at $T = 298.15$ K, ($\circ$) *m*-cresol, at $T = 323.15$ K, ($\blacktriangle$) *p*-cresol, at
25 $T = 298.15$ K, ($\triangle$) *p*-cresol, at $T = 323.15$ K.

26 **FIGURE 10.** Hand plots for the ternary systems {2-pentanone (1) + *o*-cresol, *m*-cresol, or *p*-cresol (2)
27 + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa: ($\blacksquare$) *o*-cresol, at $T = 298.15$ K, ($\square$) *o*-cresol, at
28 $T = 323.15$ K, ($\bullet$) *m*-cresol, at $T = 298.15$ K, ($\circ$) *m*-cresol, at $T = 323.15$ K, ($\blacktriangle$) *p*-cresol, at $T = 298.15$
29 K, ($\triangle$) *p*-cresol, at $T = 323.15$ K.

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1 **TABLE 1**
2 Details of chemicals used in this work.

Chemical name	Supplier	Mass fraction	Purification	Purity analysis	CAS
		purity	method	method	
<i>o</i> -Cresol	Xiya Reagent (Chengdu, China)	>0.995	None	GC ^a	95-48-7
<i>m</i> -Cresol	Xiya Reagent (Chengdu, China)	>0.995	None	GC	108-39-4
<i>p</i> -Cresol	Xiya Reagent (Chengdu, China)	>0.99	None	GC	106-44-5
2-Pentanone	Xiya Reagent (Chengdu, China)	>0.99	None	GC	107-87-9
<i>n</i> -Butyl acetate	Kemiou Chemical Reagent (Tianjin, China)	>0.99	None	GC	123-86-4
1, 3, 5-Trimethylbenzene	Xiya Reagent (Chengdu, China)	>0.99	None	GC	108-67-8

3 ^a Gas chromatography.

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1 **TABLE 2**

2 (Liquid + liquid) equilibrium data in mass fraction for ternary system { 2-pentanone (1) + *o*-cresol (2)
3 + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa.^a

Aqueous phase			Organic phase		
w_1^I	w_2^I	w_3^I	w_1^{II}	w_2^{II}	w_3^{II}
$T = 298.15$ K					
0.03985	0.00023	0.95992	0.8791	0.0817	0.0392
0.03268	0.00050	0.96682	0.7911	0.1634	0.0455
0.02771	0.00082	0.97147	0.7100	0.2387	0.0513
0.02412	0.00128	0.97460	0.6438	0.2997	0.0565
0.02151	0.00182	0.97667	0.5950	0.3449	0.0601
0.01893	0.00231	0.97876	0.5584	0.3791	0.0625
0.01667	0.00325	0.98008	0.5049	0.4282	0.0669
$T = 323.15$ K					
0.02879	0.00028	0.97093	0.8696	0.0830	0.0474
0.02354	0.00058	0.97588	0.7873	0.1595	0.0532
0.02027	0.00105	0.97868	0.7067	0.2348	0.0585
0.01815	0.00162	0.98023	0.6412	0.2939	0.0649
0.01676	0.00235	0.98089	0.5853	0.3458	0.0689
0.01403	0.00291	0.98306	0.5496	0.3786	0.0718
0.01149	0.00413	0.98438	0.4969	0.4271	0.0760

4 ^a Standard uncertainties (u) are $u(T) = 0.1$ K, $u(p) = 1$ kPa, $u(w_1^I) = 0.00026$, $u(w_2^I) = 0.00007$, $u(w_3^I)$
5 $= 0.00027$, $u(w_1^{II}) = 0.0033$, $u(w_2^{II}) = 0.0025$, $u(w_3^{II}) = 0.0041$.

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1 **TABLE 3**

2 (Liquid + liquid) equilibrium data in mass fraction for ternary system { 2-pentanone (1) + *m*-cresol (2)
3 + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa.^a

Aqueous phase			Organic phase		
w_1^I	w_2^I	w_3^I	w_1^{II}	w_2^{II}	w_3^{II}
$T = 298.15$ K					
0.03910	0.00026	0.96064	0.8659	0.0941	0.0400
0.03295	0.00059	0.96646	0.7788	0.1752	0.0460
0.02827	0.00096	0.97077	0.7096	0.2392	0.0512
0.02558	0.00126	0.97316	0.6650	0.2806	0.0544
0.02205	0.00183	0.97612	0.6102	0.3311	0.0587
0.01863	0.00246	0.97891	0.5590	0.3788	0.0622
0.01639	0.00327	0.98034	0.5196	0.4160	0.0644
$T = 323.15$ K					
0.02975	0.00033	0.96992	0.8634	0.0872	0.0494
0.02488	0.00067	0.97445	0.7835	0.1620	0.0545
0.02165	0.00111	0.97724	0.7084	0.2315	0.0601
0.01887	0.00159	0.97954	0.6568	0.2785	0.0647
0.01715	0.00202	0.98083	0.6239	0.3089	0.0672
0.01457	0.00307	0.98236	0.5559	0.3718	0.0723
0.01222	0.00437	0.98341	0.4908	0.4323	0.0769

4 ^a Standard uncertainties (u) are $u(T) = 0.1$ K, $u(p) = 1$ kPa, $u(w_1^I) = 0.00026$, $u(w_2^I) = 0.00007$, $u(w_3^I)$
5 $= 0.00027$, $u(w_1^{II}) = 0.0033$, $u(w_2^{II}) = 0.0025$, $u(w_3^{II}) = 0.0041$.

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1 **TABLE 4**

2 (Liquid + liquid) equilibrium data in mass fraction for ternary system { 2-pentanone (1) + *p*-cresol (2)
3 + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa.^a

Aqueous phase			Organic phase		
w_1^I	w_2^I	w_3^I	w_1^{II}	w_2^{II}	w_3^{II}
$T = 298.15$ K					
0.03958	0.00030	0.96012	0.8619	0.0977	0.0404
0.03142	0.00063	0.96795	0.7787	0.1745	0.0468
0.02617	0.00098	0.97285	0.7067	0.2408	0.0525
0.02263	0.00140	0.97597	0.6502	0.2922	0.0576
0.01973	0.00179	0.97848	0.6003	0.3381	0.0616
0.01828	0.00233	0.97939	0.5470	0.3878	0.0652
0.01532	0.00298	0.98170	0.4982	0.4332	0.0686
$T = 323.15$ K					
0.02871	0.00036	0.97093	0.8589	0.0914	0.0497
0.02393	0.00073	0.97534	0.7719	0.1715	0.0566
0.01975	0.00118	0.97907	0.6996	0.2376	0.0628
0.01709	0.00169	0.98122	0.6297	0.3019	0.0684
0.01532	0.00237	0.98231	0.5630	0.3634	0.0736
0.01266	0.00315	0.98419	0.4992	0.4226	0.0782
0.01031	0.00371	0.98598	0.4646	0.4536	0.0818

4 ^a Standard uncertainties (u) are $u(T) = 0.1$ K, $u(p) = 1$ kPa, $u(w_1^I) = 0.00026$, $u(w_2^I) = 0.00007$, $u(w_3^I)$
5 $= 0.00027$, $u(w_1^{II}) = 0.0033$, $u(w_2^{II}) = 0.0025$, $u(w_3^{II}) = 0.0041$.

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1 **TABLE 5**

2 Distribution coefficients (D) and separation factors (S) for the ternary systems {2-pentanone (1) +
 3 o -cresol, m -cresol, or p -cresol (2) + water (3)} at $T = (298.15, 323.15)$ K.

$T = 298.15$ K		$T = 323.15$ K	
D	S	D	S
<i>2-Pentanone (1) + o-cresol (2) + water (3)</i>			
355.22	8698.48	296.43	6071.97
326.80	6944.10	275.00	5044.49
291.10	5512.53	223.62	3741.05
234.14	4038.82	181.42	2740.11
189.51	3079.61	147.15	2094.88
164.11	2570.03	130.10	1781.33
131.75	1930.18	103.41	1339.46
<i>2-Pentanone (1) + m-cresol (2) + water (3)</i>			
361.92	8691.94	264.24	5188.14
296.95	6238.90	241.79	4323.18
249.17	4724.29	208.56	3391.21
222.70	3983.85	175.16	2651.83
180.93	3008.66	152.92	2231.98
153.98	2423.41	121.11	1645.52
127.22	1936.58	98.92	1265.06
<i>2-Pentanone (1) + p-cresol (2) + water (3)</i>			
325.67	7739.58	253.89	4959.93
276.98	5728.78	234.93	4048.38
245.71	4553.20	201.36	3139.20
208.71	3536.44	178.64	2562.63
188.88	3000.29	153.33	2046.48
166.44	2500.11	134.16	1688.46
145.37	2080.30	122.26	1473.72

1 **TABLE 6**

2 Othmer-Tobias and Hand equation parameters, a , b , and regression coefficients, R^2 for the studied
 3 systems {2-pentanone (1) + *o*-cresol, *m*-cresol, or *p*-cresol (2) + water (3)}.

T/K	Othmer-Tobias equation			Hand equation		
	a_1	b_1	R^2	a_2	b_2	R^2
<i>2-Pentanone (1) + o-cresol (2) + water (3)</i>						
298.15	-10.3377	-2.6573	0.9896	4.6874	0.8333	0.9846
323.15	-12.7271	-3.0977	0.9772	4.3671	0.8114	0.9901
<i>2-Pentanone (1) + m-cresol (2) + water (3)</i>						
298.15	-9.4014	-2.4035	0.9743	4.3917	0.7980	0.9950
323.15	-12.0898	-2.9600	0.9930	4.4115	0.8280	0.9911
<i>2-Pentanone (1) + p-cresol (2) + water (3)</i>						
298.15	-9.0857	-2.2882	0.9956	5.0635	0.8948	0.9993
323.15	-11.1528	-2.6858	0.9828	5.2881	0.9488	0.9990

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1 **TABLE 7**

2 The UNIQUAC structural parameters (r and q) for pure components.

Component	r	q
Water	0.9200	1.400
<i>o</i> -cresol	4.2867	3.248
<i>m</i> -cresol	4.2867	3.248
<i>p</i> -cresol	4.2867	3.248
2-pentanone	3.9223	3.416

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1 **TABLE 8**

2 The NRTL and UNIQUAC binary interaction parameters for the studied ternary systems.

<i>T/K</i>	NRTL					UNIQUAC			
	<i>i-j</i>	<i>b_{ij}/K</i>	<i>b_{ji}/K</i>	<i>α_{ij}</i>	<i>rmsd/%</i>	<i>i-j</i>	<i>a_{ij}/K</i>	<i>a_{ji}/K</i>	<i>rmsd/%</i>
<i>{2-Pentanone (1) + o-cresol (2) + water (3)}</i>									
298.15	1-2	-1098.54	-92.96	0.3	0.310	1-2	500.12	-159.60	0.367
	1-3	146.81	1291.26	0.2		1-3	-405.60	-74.45	
	2-3	-173.10	1346.31	0.2		2-3	10.08	-98.74	
323.15	1-2	-1138.04	-69.83	0.3	0.195	1-2	625.88	-240.72	0.237
	1-3	92.79	1545.88	0.2		1-3	-344.21	-134.12	
	2-3	-231.36	1466.48	0.2		2-3	42.83	-60.38	
<i>{2-Pentanone (1) + m-cresol (2) + water (3)}</i>									
298.15	1-2	-1071.45	-142.18	0.3	0.099	1-2	489.84	-117.77	0.140
	1-3	148.21	1286.11	0.2		1-3	-410.00	-72.25	
	2-3	-174.66	1321.30	0.2		2-3	16.21	-89.54	
323.15	1-2	-1206.00	-40.40	0.3	0.245	1-2	773.03	-377.36	0.265
	1-3	82.80	1547.49	0.2		1-3	-333.39	-135.59	
	2-3	-226.90	1389.57	0.2		2-3	20.63	64.55	
<i>{2-Pentanone (1) + p-cresol (2) + water (3)}</i>									
298.15	1-2	-1012.54	-26.38	0.3	0.320	1-2	940.08	-1122.18	0.331
	1-3	148.14	1306.43	0.2		1-3	-388.68	-82.51	
	2-3	-201.71	1490.99	0.2		2-3	-63.58	238.64	
323.15	1-2	-1157.04	213.96	0.3	0.258	1-2	654.77	-1138.74	0.184
	1-3	78.70	1569.87	0.2		1-3	-319.71	-145.47	
	2-3	-251.93	1642.60	0.2		2-3	-10.30	-108.19	

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2 **FIGURE 1.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
3 system {2-pentanone (1) + *o*-cresol (2) + water (3)} at $T = 298.15$ K and $p = 101.3$ kPa: (■-■)
4 experimental data, (Δ---Δ) NRTL model, and (×...×) UNIQUAC model.

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6 **FIGURE 2.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
7 system {2-pentanone (1) + *o*-cresol (2) + water (3)} at $T = 323.15$ K and $p = 101.3$ kPa: (■-■)
8 experimental data, (Δ---Δ) NRTL model, and (×...×) UNIQUAC model.

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2 **FIGURE 3.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
3 system {2-pentanone (1) + *m*-cresol (2) + water (3)} at $T = 298.15$ K and $p = 101.3$ kPa: (■-■)
4 experimental data, (Δ---Δ) NRTL model, and (×...×) UNIQUAC model.

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6 **FIGURE 4.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
7 system {2-pentanone (1) + *m*-cresol (2) + water (3)} at $T = 323.15$ K and $p = 101.3$ kPa: (■-■)
8 experimental data, (Δ---Δ) NRTL model, and (×...×) UNIQUAC model.

1

2 **FIGURE 5.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
3 system {2-pentanone (1) + *p*-cresol (2) + water (3)} at $T = 298.15$ K and $p = 101.3$ kPa: (■-■)
4 experimental data, (Δ---Δ) NRTL model, and (×····×) UNIQUAC model.

5

6 **FIGURE 6.** Experimental and calculated (liquid + liquid) equilibrium data in mass fraction for ternary
7 system {2-pentanone (1) + *p*-cresol (2) + water (3)} at $T = 323.15$ K and $p = 101.3$ kPa: (■-■)
8 experimental data, (Δ---Δ) NRTL model, and (×····×) UNIQUAC model.

1

2 **FIGURE 7.** Distribution coefficient of cresol plotted versus mass fraction of cresol in the aqueous
3 phase at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa: (■) *o*-cresol, at $T = 298.15$ K, (□) *o*-cresol, at $T =$
4 323.15 K, (●) *m*-cresol, at $T = 298.15$ K, (○) *m*-cresol, at $T = 323.15$ K, (▲) *p*-cresol, at $T = 298.15$ K,
5 (△) *p*-cresol, at $T = 323.15$ K.

6

7 **FIGURE 8.** Separation factor of cresol plotted versus mass fraction of cresol in the aqueous phase at T
8 $= (298.15, 323.15)$ K and $p = 101.3$ kPa: (■) *o*-cresol, at $T = 298.15$ K, (□) *o*-cresol, at $T = 323.15$ K,
9 (●) *m*-cresol, at $T = 298.15$ K, (○) *m*-cresol, at $T = 323.15$ K, (▲) *p*-cresol, at $T = 298.15$ K, (△)
10 *p*-cresol, at $T = 323.15$ K.

1

2 **FIGURE 9.** Othmer-Tobias plots for the ternary systems {2-pentanone (1) + *o*-cresol, *m*-cresol, or

3 *p*-cresol (2) + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa: (■) *o*-cresol, at $T = 298.15$ K, (□)

4 *o*-cresol, at $T = 323.15$ K, (●) *m*-cresol, at $T = 298.15$ K, (○) *m*-cresol, at $T = 323.15$ K, (▲) *p*-cresol, at

5 $T = 298.15$ K, (Δ) *p*-cresol, at $T = 323.15$ K.

6

7 **FIGURE 10.** Hand plots for the ternary systems {2-pentanone (1) + *o*-cresol, *m*-cresol, or *p*-cresol (2)

8 + water (3)} at $T = (298.15, 323.15)$ K and $p = 101.3$ kPa: (■) *o*-cresol, at $T = 298.15$ K, (□) *o*-cresol, at

9 $T = 323.15$ K, (●) *m*-cresol, at $T = 298.15$ K, (○) *m*-cresol, at $T = 323.15$ K, (▲) *p*-cresol, at $T = 298.15$

10 K, (Δ) *p*-cresol, at $T = 323.15$ K