Liquid-liquid Equilibrium for the Ternary Systems of Solvent+ m/o/p-Cresol+Water: Thermodynamic Modeling

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Abstract

In this study, NRTL and UNIQUAC thermodynamic models were used to predict the composition of ternary mixtures of solvents+ m/o/p-cresol+ water in organic and aqueous phases. Various solvents are used for the separation of cresols from water. In this study, methyl propyl ketone, methyl isopropyl ketone, methyl butyl ketone, and methyl isobutyl ketone solvents were investigated. Intermolecular interaction parameters were considered to be a function of temperature. The binary interaction parameters of water and cresols (m, o, or p) in the presence of each type of solvent were considered to be the same. Also, regardless of the type of cresol (m, o, or p), the parameters of binary interaction between water and each solvent were considered to be the same. The results proved the accuracy of the presented models, though the parameters of binary interaction parameters were considered to be the same. The root mean square deviation for NRTL and UNIQUAC models was 0.0086 and 0.0089, respectively.

Keywords

Cresol;
NRTL;
Organic solvent;
Thermodynamic models;
UNIQUAC.

1. Introduction

Coal gasification has been an important alternative method for producing energy from coal in the past decades. Coal contains some impurities, like sulfur, nitrogen, and trace elements which are removed through coal gasification. Furthermore, other gases obtained from coal combustion (e.g. CO_2 and H_2) are used for producing liquid gas (LG), fuel cells, and manufactured plastics [1]. However, a considerable amount of phenolic-compounds is produced in the process, which is the most important disadvantage of this technology. Environmental organizations have imposed strict rules on these harmful materials because they negatively affect human health and the ecosystem. The European Union (EU) has developed rules stating that phenolic-compounds should be <0.0005 mg/L in drinking water [2]. Although these materials have destructive effects on the environment, they are valuable compounds used in disinfectants, sol-

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vents, cleaners, motor oil additives, flavorings, herbicides, surfactants, and dyes [2-5].

Hence, it is really necessary to separate phenolic-compounds, especially cresols which are among the most important phenolic derivatives. While coal gasification is the major source of cresols, they can be also obtained from polymeric resin production companies, chemical industry, oil refineries, coking plants, petrochemical, and pharmaceutical plants [2, 4, 6 and 7].

Cresols are removed from wastewater via destructive and non-destructive processes. In the destructive method, cresols are inverted into other compounds through incineration, chemical oxidation, thermal decomposition, and anaerobic biodegradation [8-10]. However, each of these processes have some limitations. For example, thermal decomposition works in high concentrations of cresols, but it consumes high energy and it is only used in a small scale. Moreover, biodegradation treats wastewater in low concentrations of cresols (< 3000 mg/L) without any salt [2].

Cresols are also separated from wastewater in a non-destructive method which uses liquid-liquid extraction, membrane adsorption, ion exchange, and mixed processes, including liquid-liquid extraction and adsorption [7, 11].

Because of the high selectivity, mild process condition, low cost, and its ability to separate cresols even in high concentrations, liquid-liquid extraction is an appropriate method for treating wastewater [2, 4, 7 and 12]. It has three steps: solving extraction, recovery, and stripping [12]. This process operates based on the interaction between cresols and solvents [2].

Researchers reported a high capacity and selectivity for cresol extraction when using polar organic solvent and reversible chemical complexation [7]. Common solvents that significantly remove cresols from wastewater are benzene, ethyl benzene, ethyl acetate, isopropyl acetate, *n*-butyl acetate, *n*-hexyl acetate, toluene, diisopropyl ether, hexane, methyl isobutyl ketone, 2-metoxy-2-methyl propane, methyl butyl ketone, isopropyl ketone, and 2-pentanone [3, 4, 6 and 12-17].

This study was conducted on the measured liquid-liquid equilibrium systems of organic solvent+ m/o/p-cresol+ water which were obtained from different studies in the literature [1, 12, 14 and 15]. Organic solvents contain various ketone compounds. NRTL (non-random two liquid) and UNIQUAC (UNIversal QUAsi Chemical) thermodynamic models were utilized to study these data. Intermolecular interaction parameters for different models were considered to be a function of temperature. In this study, the amount of intermolecular interaction parameters between each two molecules, irrespective of the other molecule, was obtained and considered to be constant. In other words, the intermolecular interaction parameters for the two molecules of water and m/o/p-cresol were obtained, regardless of the type of the solvent used. Nevertheless, the results indicate the high accuracy of the presented models.

2. Materials and Methods

2.1. Equilibrium data for ketone-based solvents + m/o/p-cresol+ water ternary systems

Various solvents are used to separate m-cresol, o-cresol, and p-cresol from water. This study investigated the ketone-based solvents and their separation capabilities. Experimental data were collected from four different references [1, 12, 14, and 15]. The collected data were about the liquid-liquid equilibrium of ternary systems of solvent (1) + cresol (2) + water (3). The solvents used for the separation of m/o/p-cresol were methyl propyl ketone [1], methyl isopropyl ketone [15], methyl butyl ketone [12], and methyl isobutyl ketone [14]. The total number of data on the mentioned systems was 240, which covered a temperature range of 298.15-353.15 K.

2.2. Thermodynamic models

In this study, NRTL [18] and UNIQUAC [19] thermodynamic models were used to calculate the activity coefficients of components. Experimental data obtained from different studies [1, 12, 14, and 15] covered various temperatures. Therefore, the intermolecular interaction parameters were considered as a function of temperature.

2.2.1. NRTL model

Equation 1 was used to calculate the activity coefficient of component using NRTL model.

$$\gamma_i = \exp\left(\frac{\frac{G_{ji}\sum_j x_j\tau_{ji}}{\sum_l x_l G_{li}} + \sum_j \frac{x_j G_{ij}\left(\tau_{ij} - \frac{\sum_r x_r\tau_{rj}G_{rj}}{\sum_l x_l G_{li}}\right)}{\sum_l x_l G_{li}}}\right) \quad (1)$$

where i, j and, k are representative of each component. γ_i is the activity coefficient of component i; x is the molar fraction; τ_{ij} and τ_{ji} are the intermolecular interaction between the molecules i and j which are calculated as follows:

$$\tau_{ij} = \frac{\Delta g_{ij}}{RT} = A_{ij} + \frac{B_{ij}}{T} \quad (2)$$

$$\left(\tau_{ij} \neq \tau_{ji} \text{ and } \tau_{ii} = 0\right)$$

where A_{ij} and B_{ij} are binary interaction parameters and T is absolute temperature. Moreover, we have:

$$G_{ij} = \exp\left(-\alpha_{ij}\tau_{ij}\right) \quad (3)$$

$$(\alpha_{ij} = \alpha_{ji} \text{ and } \alpha_{ii} = 0)$$

where α_{ij} is non-random parameter which is equal to 0.2 here [18].

2.2.2. UNIQUAC model

Equation 4 was used to calculate the activity coefficient of components using the UNIQUAC model:

$$\gamma_i = \frac{\frac{\phi_i}{x_i}\left(\frac{\theta_i}{\phi_i}\right)^{\frac{zq_i}{2}} \exp\left[l_i - \frac{\phi_i}{x_i}\sum_j x_j l_j - q_i'\left(1 - \sum_j \frac{\theta_j'\tau_{ij}}{\sum_k \theta_k'\tau_{kj}}\right)\right]}{\left(\sum_j \theta_j'\tau_{ji}\right)^{q_i'}} \quad (4)$$

Table 1. Parameters r_i, q_i and q_i' in the studied systems

Component	r_i	q_i	q_i'
methyl propyl ketone	3.9223	3.416	3.416
methyl isopropyl ketone	3.9223	3.416	3.416
methyl butyl ketone	4.5967	3.956	3.956
methyl isobutyl ketone	4.5967	3.956	3.956
m-cresol	4.2687	3.248	3.248
o-cresol	4.2687	3.248	3.248
p-cresol	4.2687	3.248	3.248
water	0.9200	1.400	1.000

where i, j and k are representative of each component; γ_i is the activity coefficient of component i; x is the molar fraction; z is the number of coordinations (equal to 10); τ_{ij} and τ_{ji} are the intermolecular interaction between the molecules i and j, which are calculating as follows:

$$\tau_{ij} = \exp\left(-\frac{a_{ij}}{R}\right) = \exp\left(A_{ij} + \frac{B_{ij}}{T}\right)$$

$$\left(\tau_{ij} \neq \tau_{ji} \text{ and } \tau_{ii} = 0\right) \quad (5)$$

where A_{ij} and B_{ij} are binary interaction parameters and T is absolute temperature. In addition, ϕ_i is the volume fraction of the component i, θ_i is the surface fraction of the component i, θ_i' is the interaction surface fraction of the component i, r_i is the volume of the molecule i, q_i is the surface of the molecule i, q_i' is the molecular interaction surface (for non-water and light non-alcoholic component $q_i = q_i'$), and l_i is a compound parameter of r_i, q_i, and z. Equations 6 to 9 were used to calculate the values of l_i, ϕ_i, θ_i and θ_i' [19]. The values of r_i, q_i and q_i' for the organic solvents, m/o/p-cresol and water, are presented in Table 1.

$$l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1) \quad (6)$$

$$\phi_i = \frac{r_i x_i}{\sum_j r_j x_j} \quad (7)$$

$$\theta_i = \frac{q_i x_i}{\sum_j q_j x_j} \quad (8)$$

$$\theta_i' = \frac{q_i' x_i}{\sum_j q_j' x_j} \quad (9)$$

2.3. Liquid-liquid equilibrium: Calculations and estimation of parameters

The binary interaction parameters of NRTL and UNIQUAC thermodynamic models are determined through optimization. For this purpose, the objective function (Equation 10) was minimized. This function represents the mean square difference of the measured and calculated (using the presented models) mass fractions for all the components in organic and aqueous phases:

$$OF = 100 \times \frac{1}{3D}\sum_{j=1}^{D}\sum_{i=1}^{3}\left(\left(w_{ij}^{aq.,exp} - w_{ij}^{aq.,calc}\right)^2 + \left(w_{ij}^{O,exp} - w_{ij}^{O,calc}\right)^2\right) \quad (10)$$

Furthermore, the root mean square deviation ($RMSD$) was used to compare the accuracy of the examined models, which is shown in Equation 11:

$$RMSD = \left(\frac{1}{3D}\sum_{j=1}^{D}\sum_{i=1}^{3}\left(\left(w_{ij}^{aq.,exp} - w_{ij}^{aq.,calc}\right)^2 + \left(w_{ij}^{O,exp} - w_{ij}^{O,calc}\right)^2\right)\right)^{1/2} \quad (11)$$

where D is the total number of lines in the reference databases; i and j subscripts are the components of tie lines; and exp. and calc. are measured and calculated components, respectively. In addition, aq. and O are used for aqueous and organic phases, respectively.

2.4. Equilibrium calculation procedure

In equilibrium condition, the chemical potentials (fugacity) of the components in the two phases are equal, so:

$$w_i^{aq.}\gamma_i^{aq.}\left(w_1^{aq.}, w_2^{aq.}, w_3^{aq.}\right) = w_i^{O}\gamma_i^{O}\left(w_1^{O}, w_2^{O}, w_3^{O}\right); i = 1,2,3 \quad (12)$$

$$K_i = \frac{\gamma_i^{aq.}}{\gamma_i^{O}} = \frac{w_i^{O}}{w_i^{aq.}} \; ; i = 1,2,3 \quad (13)$$

where K_i is the equilibrium constant between two organic and aqueous phases for the i component; i is equal to 1, 2, and 3 for the solvent, cresol, and water, respectively.

The mass fractions of the components in the aqueous and organic phases were obtained using

$$w_i^{aq.} = \frac{Z_i}{1+(K_i-1)O} \text{ and } \quad w_i^{O} = K_i w_i^{aq.} \; ; \; i = 1,2,3 \quad (14)$$

the following equation:

where O is the mass of the solvent-rich phase. Moreover, Z_i is the mass fraction of i component in the feed. Taking into consideration $\sum w_i^{aq.} = 1$ and $\sum w_i^{O} = 1$, and $\sum w_i^{aq.} - \sum w_i^{O} = 0$, we have:

$$\sum_{i=1}^{3}\frac{Z_i(K_i-1)}{1+(K_i-1)O} = 0 \quad (15)$$

Genetic algorithm toolbox of MATLAB 7.8.0 software was employed for calculations of the proposed models. The equilibrium calculation procedure was as follows:

1. Input $\{Z_i\}$ and T.
2. Guess initial values for $\{w_i^{aq.}\}$ and $\{w_i^{O}\}$.
3. Guess intermolecular interaction parameters (A_{ij} and B_{ij}).
4. Calculate activity coefficients and K values of each components.
5. Solve equation (15) to find O.
6. Update $\{w_i^{aq.}\}$ and $\{w_i^{O}\}$ using equation (14).
7. If OF $<$ ε go to next step else go to step 3.
8. Display results.

2.5 Distribution coefficient and selectivity

Distribution coefficient and selectivity are the two important factors for choosing the solvent in the liquid-liquid extraction process. These factors are defined as:

$$K_2 = \frac{w_2^{O}}{w_2^{aq.}} \quad (16)$$

$$\beta = \frac{K_2}{K_3} = \frac{w_2^{O}/w_2^{aq.}}{w_3^{O}/w_3^{aq.}} \quad (17)$$

where K_2 and β are the distribution coefficient and selectivity, respectively. Subscripts 2 and 3 are representing cresols and water, respectively. The value of β must always be higher than one. Also, the distribution coefficient should have a high value (less solvent is needed).

3. Results and Discussion

3.1. Intermolecular interaction parameters

Of all the experimental data described in the Materials and Methods section, 70% were used to determine the intermolecular interaction parameters of the presented models. Using the algo-

rithm presented in Section 2.4 (equilibrium calculation procedure), intermolecular interaction parameters were obtained for NRTL and UNIQUAC thermodynamic models. Tables 2 and 3 show the intermolecular interactions of different molecules obtained using NRTL and UNIQUAC thermodynamic models, respectively. As presented in these tables, the parameters of interaction between water molecule and ketone organic solvents (methyl propyl ketone, methyl isopropyl ketone, methyl butyl ketone, and methyl isobutyl ketone) were considered to be the same for all the systems. These values were set regardless of the type of cresol (m, o, and p). Moreover, the values of the parameters of interaction between m/o/p-cresol and water were determined regardless of the type of organic solvents. The value of the objective function (Equation 10) obtained for the ternary systems including organic solvent+ m/o/p-cresol+ water using NRTL and UNIQUAC were 0.0074 and 0.0079, respectively. Therefore, the accuracy of the models were as follows: NRTL>UNIQUAC.

3.2. Comparison of models

After determining the intermolecular interaction parameters using the presented thermodynamic models, the models were applied to all the data in the database and the accuracy of each thermodynamic model was determined. Table 4 shows the root mean square deviation of ternary systems of organic solvent+ m/o/p-cresol+ water for different models. In addition, Table 5 indicates the values of *RMSD* for these mixtures, irrespective of the temperature.

Furthermore, in these tables (Tables 4 and 5), the distribution coefficients and selectivity are presented for different solvents. As shown in Table 5, according to the previous studies, the selectivity of the ketone-based solvents for the extraction of all types of cresol (m/o/p) is as follows:
methyl butyl ketone> methyl propyl ketone> methyl isopropyl ketone> methyl isobutyl keton

These results are more clearly shown in Fig. 1. Concerning the distribution coefficient, the trend is different from that of the selectivity. In other words, the distribution of cresols in the organic phase is at the maximum level when using methyl isobutyl ketone solvent and is at the minimum level when using methyl butyl ketone solvent. As presented in Table 4, with increasing the temperature, the selectivity and distribution coefficient decrease. In other words, the separation of cresols from water by means of ketone-based organic solvents is more efficient at lower temperatures.

Table 2. Parameters of NRTL intermolecular interaction between solvents+ m/o/p-cresol+ water

Component		Binary interaction parameter			
i	j	A_{ij}	B_{ij} (K)	A_{ji}	B_{ji} (K)
methyl propyl ketone	m-cresol	1.1470	1.6734	-0.8695	5.9322
	o-cresol	-0.3061	3.5917	0.0179	4.7481
	p-cresol	-0.4992	0.3989	0.7831	1.1070
	water	-2.0787	4.3425	-0.8693	-1.1390
methyl isopropyl ketone	m-cresol	-0.2687	0.4966	0.8653	-1.2170
	o-cresol	-1.5400	4.5735	1.7286	0.6822
	p-cresol	0.6072	3.1074	-0.4834	5.3375
	water	-1.8508	-2.0618	-1.0876	1.1618
methyl butyl ketone	m-cresol	-0.0342	0.3298	-0.2679	4.1002
	o-cresol	-1.0635	0.3899	0.0055	-1.5196
	p-cresol	-0.6427	-0.0791	0.0884	2.5296
	water	-2.6012	-4.4635	-0.7787	-2.8135
methyl isobutyl ketone	m-cresol	-1.5385	-0.3012	0.7000	-3.4453
	o-cresol	-2.3137	-2.5755	1.4645	-0.0083
	p-cresol	-2.0680	-1.6953	1.2349	3.3040
	water	-3.3427	-12.0988	2.6589	-3.6786
water	m-cresol	-0.6144	-0.0627	-1.5039	1.6185
	o-cresol	-0.2480	-4.9489	-2.0936	2.1087
	p-cresol	-0.8372	-3.7154	-1.5216	4.8399

Table 3. Parameters of UNIQUAC intermolecular interaction between solvents+ m/o/p-cresol+ water

Component		Binary interaction parameter			
i	*j*	A_{ij}	B_{ij} (K)	A_{ji}	B_{ji} (K)
methyl propyl ketone	m-cresol	0.4324	6.2935	0.3090	0.0467
	o-cresol	0.2576	-0.6025	-0.2001	1.2750
	p-cresol	1.7827	3.3802	0.1599	-0.4802
	water	1.6835	-0.8358	1.0700	8.7673
methyl isopropyl ketone	m-cresol	0.7533	0.5525	-1.4942	-3.1770
	o-cresol	-1.3910	0.8379	1.2592	2.5453
	p-cresol	1.9121	2.4908	-1.1471	0.5938
	water	-1.3519	-5.4740	1.7314	10.6009
methyl butyl ketone	m-cresol	0.0703	6.1263	0.3194	-1.2307
	o-cresol	0.3125	1.0619	-0.5301	-0.7032
	p-cresol	1.5243	-2.2783	0.0563	-0.4395
	water	0.2360	-1.6616	1.4918	5.1040
methyl isobutyl ketone	m-cresol	0.6357	7.1945	-0.1035	-1.4111
	o-cresol	-0.0040	-5.9316	0.3457	2.6990
	p-cresol	1.9967	-3.3021	-0.7968	1.9872
	water	0.6164	6.7477	0.7936	3.3856
water	m-cresol	1.0266	2.4761	1.6116	-5.5327
	o-cresol	1.0503	3.0160	1.1623	3.7951
	p-cresol	0.9876	0.7465	2.5814	-3.6653

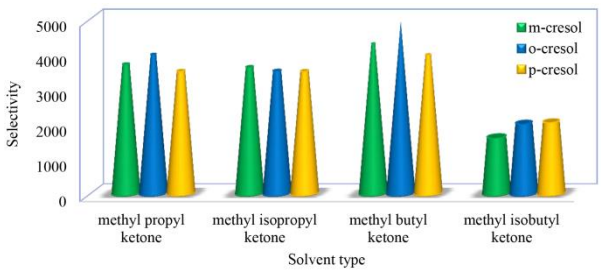

Figure 1. Selectivity of ketone-based solvents for the extraction of m/o/p-cresol

Fig. 2 presents the accuracy of NRTL and UNIQUAC thermodynamic models in predicting the composition of components in organic and aqueous phases (Figures 2-a, 2-b, and 2-c are for m-cresol, o-cresol, and p–cresol, respectively). Using NRTL and UNIQUAC models the RSMD values for systems containing organic solvent+ m/o/p-cresol+ water were obtained which were 0.0086 and 0.0089, respectively. Obviously, the accuracy of the thermodynamic models are as follows: NRTL>UNIQUAC.

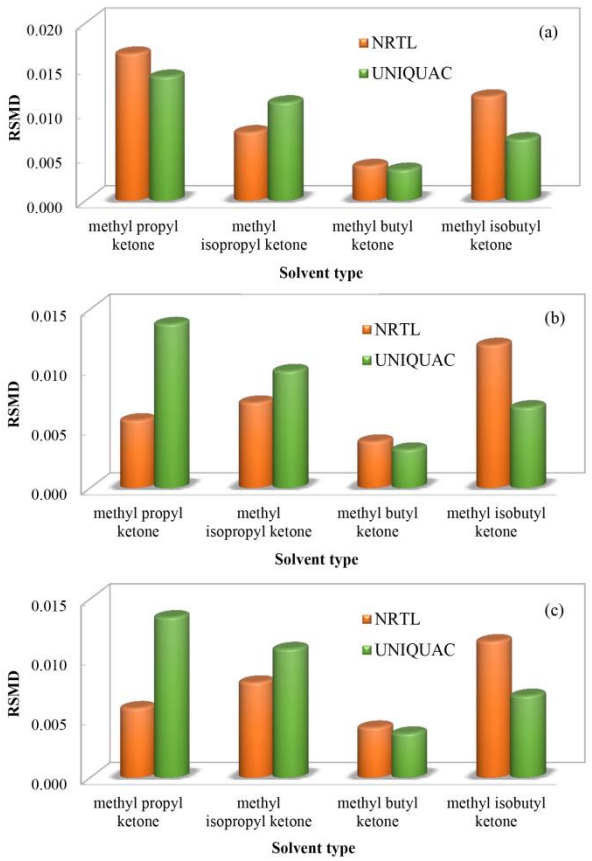

Figure 2. RSMD of thermodynamic models to predict the components composition in organic and aqueous phases; a) m-cresol, b) o-cresol, c) p-cresol

Table 4. Liquid-liquid equilibrium data of the systems of solvents+ m/o/p-cresol+ water and the accuracy of NRTL and UNIQUAC models at different temperatures

No.	System	T (K)	NDP	RSMD		K_2	β	Reference
				NRTL	UNIQUAC			
1	methyl propyl ketone + m-cresol + water	298.15	7	0.0066	0.0156	227.55	4429.66	[1]
2		323.15	7	0.0053	0.0121	180.39	2956.70	[1]
3	methyl isopropyl ketone + m-cresol + water	298.15	9	0.0082	0.0128	228.38	4073.43	[15]
4		313.15	9	0.0073	0.0091	195.56	3150.49	[15]
5	methyl butyl ketone + m-cresol + water	298.15	9	0.0040	0.0036	199.97	4982.09	[12]
6		313.15	9	0.0039	0.0034	176.96	3566.69	[12]
7	methyl isobutyl ketone + m-cresol + water	333.15	10	0.0117	0.0081	576.75	1940.74	[14]
8		343.15	10	0.0108	0.0039	521.60	1611.94	[14]
9		353.15	10	0.0127	0.0080	444.55	1312.29	[14]
10	methyl propyl ketone + o-cresol + water	298.15	7	0.0063	0.0156	241.80	4681.96	[1]
11		323.15	7	0.0049	0.0117	193.88	3259.04	[1]
12	methyl isopropyl ketone + o-cresol + water	298.15	9	0.0077	0.0111	212.33	3784.12	[15]
13		313.15	9	0.0066	0.0083	192.15	3227.59	[15]
14	methyl butyl ketone + o-cresol + water	298.15	9	0.0043	0.0035	241.74	5817.22	[12]
15		313.15	9	0.0035	0.0029	232.56	3714.12	[12]
16	methyl isobutyl ketone + o-cresol + water	333.15	10	0.0123	0.0084	715.31	2214.19	[14]
17		343.15	10	0.0106	0.0039	710.78	2211.74	[14]
18		353.15	10	0.0130	0.0072	573.81	1628.29	[14]
19	methyl propyl ketone + p-cresol + water	298.15	7	0.0064	0.0151	222.54	4162.67	[1]
20		323.15	7	0.0052	0.0115	182.65	2845.54	[1]
21	methyl isopropyl ketone + p-cresol + water	298.15	9	0.0083	0.0120	217.41	3804.39	[15]
22		313.15	9	0.0076	0.0094	199.10	3201.10	[15]
23	methyl butyl ketone + p-cresol + water	298.15	9	0.0039	0.0037	206.43	4798.08	[12]
24		313.15	9	0.0045	0.0037	174.79	3127.07	[12]
25	methyl isobutyl ketone + p-cresol + water	333.15	10	0.0117	0.0074	745.25	2347.01	[14]
26		343.15	10	0.0104	0.0044	681.19	2031.87	[14]
27		353.15	10	0.0121	0.0082	623.31	1804.80	[14]

Table 5. Liquid-liquid equilibrium data of the systems of solvents+ m/o/p-cresol+ water and the accuracy of different models

System	T (K)	NDP	RSMD		K_2	β
			NRTL	UNIQUAC		
methyl propyl ketone + m-cresol + water	298.15-323.15	14	0.0166	0.0140	203.97	3693.18
methyl isopropyl ketone + m-cresol + water	298.15-313.15	18	0.0077	0.0111	211.97	3611.96
methyl butyl ketone + m-cresol + water	298.15-313.15	18	0.0039	0.0035	188.47	4274.39
methyl isobutyl ketone + m-cresol + water	333.15-353.15	30	0.0118	0.0069	514.30	1621.66
methyl propyl ketone + o-cresol + water	298.15-323.15	14	0.0057	0.0138	217.84	3970.50
methyl isopropyl ketone + o-cresol + water	298.15-313.15	18	0.0072	0.0098	202.24	3505.85
methyl butyl ketone + o-cresol + water	298.15-313.15	18	0.0039	0.0032	223.65	4925.87
methyl isobutyl ketone + o-cresol + water	333.15-353.15	30	0.0120	0.0068	666.63	2018.08
methyl propyl ketone + p-cresol + water	298.15-323.15	14	0.0058	0.0135	202.60	3504.11
methyl isopropyl ketone + p-cresol + water	298.15-313.15	18	0.0080	0.0108	208.25	3502.75
methyl butyl ketone + p-cresol + water	298.15-313.15	18	0.0042	0.0037	190.61	3962.57
methyl isobutyl ketone + p-cresol + water	333.15-353.15	30	0.0114	0.0069	683.25	2061.23
Total	298.15-353.15	240	0.0086	0.0089		

4. Conclusion

Phenolic compounds, such as m/o/p-cresol are water contaminants. Different organic solvents are used to separate them from water. In this study, NRTL and UNIQUAC thermodynamic models were used to predict the behavior of ternary systems of solvent+ m/o/p-cresol + water (using experimental data obtained from previous studies in the literatures). In order to improve the accuracy of the models, intermolecular interaction parameters were considered as a function of temperature. The results show that the NRTL model is more accurate than UNIQUAC model. Moreover, comparing the various ketone-based organic solvents, it was found that methyl butyl ketone has a higher level of selectivity than the other solvents. In addition, the solvents have better distribution coefficient and selectivity at lower temperatures.

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