Solubility of Sebacic Acid in Binary Mixtures Containing Alcohols

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The solubilities of sebacic acid in mixed solvents *n*-propanol + water have been measured by a dynamic method using a laser monitoring observation technique over a temperature range (288 to 351) K. A synergistic effect on solubility was found to occur in sebacic acid + *n*-propanol + water mixed systems. To detect the synergistic effect, solubilities of sebacic acid in 14.35 %, 36.97 %, 79.81 %, and 90.00 % mole fraction ethanol aqueous solution were determined to supplement our previous report. A weak synergistic effect was found for sebacic acid + ethanol + water mixed systems. The solid−liquid equilibrium (SLE) data have been fitted using the λh equation, the Wilson equation, and the NRTL equation. The comparison between the experimental and the calculated solubilities for the three models is reasonable, and the root-mean-square deviations for each system range from (0.30 to 1.95) K.

Introduction

Sebacic acid $C_{10}H_{18}O_4$ (CASRN 111-20-6), which is manufactured from the caustic fusion of castor oil, is an important organic intermediate used for synthesis of nylon, alkyd resins, plasticizers, and lubricants, etc.[1−3] The crystallization is an important step in the industrial process of sebacic acid. Solubilities of sebacic acid in various solvents are necessary for design crystallization and other related chemical processes handling sebacic acid. Information on the solubility of sebacic acid is sparse in the literature. Bonhomme[4] reported solubility data of sebacic acid in ethanol + water binary mixtures at 298 K, with trace HCl (10^{-3} N) added to the binary mixtures to prevent ionization of sebacic acid. Tudorovskaya[5] determined solubility data of sebacic acid in water over a temperature range from (346.1 to 386.3) K by the visual polythermal method. Xia[6] published the solubility of sebacic acid in ethanol + water binary mixtures, which were measured by a dynamic method over a temperature range from (288 to 352) K and correlated with the Wilson equation.

The use of mixed solvents showing the phenomenon of enhanced solubility in comparison with that of pure solvents has been the subject of numerous investigations. The occurrence of synergistic effects can be predicted on the basis of the Scatchard−Hildebrand theory.[7] The main condition for the enhanced solubility is that the solubility parameter of the solute is between the two solvents. According to the solubility parameters of solute and solvents, Domanska[8] predicted the system hydrocarbon + cyclohexane + ethanol should reveal a synergistic effect, and Ghanima[9] predicted the system anthracene + toluene + 2-propanol should reveal enhanced solubility; however, a synergistic effect was not observed in the above systems. The synergistic effect has been observed for naphthalene and phenanthrene[10] in hexane + alcohol binary solvents, 2-acetyl-1-naphthol[11] in cyclohexane + ethanol binary solvents, eicosanoic acid[12] in cyclohexane + alcohols, 3,4-dimethylphenol[13] in ester + alcohol binary solvents, as well as *n*-alkanols[14] in cyclohexane + 2-propanol binary solvents. Chen[15] verified its authenticity by experimentally measuring the solubility of terephthalic acid in a mixture of acetic acid and water. Draucker[16] reported a synergistic effect for the 5-fluoroisatin + propanol + nitromethane system. The same phenomenon was also found in the phthalic acid + acetic acid + water system by Wang.[17] Domanska[11] suggested that the systems which tended to reveal the synergistic effect were divided into two groups. The first group comprised solutes with stable intramolecular hydrogen bonds and nonpolar compounds as well as forming stable aggregate solutions. The second group included compounds forming intermolecular hydrogen bonds with the solvent.

The present work is to continue systematic investigations on the solid−liquid equilibrium (SLE) concerning sebacic acid. In this paper, the solubilities of sebacic acid in alcohol + water binary mixtures have been measured by a dynamic method. Measurements were carried out over a range of *n*-propanol mole fraction from 0 to 1, ethanol from 0.1435 to 0.9000, and over a temperature range from (288 to 351) K. The SLE data were correlated with the λh equation, the Wilson equation, and the nonrandom two liquids (NRTL) equation. The model parameters were regressed. The synergistic effect that appeared in this study was discussed.

Experimental Section

Materials. Sebacic acid was purchased from the Hengshui Dongfeng Chemical Co. Ltd., Hebei, China. To obtain sebacic acid with high purity for the experiment, the sebacic acid was recrystallized from ethanol aqueous solutions and stored over silica gel after drying in a dryer at 370 K to remove water and ethanol. After these treatments, the purity of sebacic acid used in the solubility measurements exceeded 99.4 % (HLPC). Enthanol and *n*-propanol had a purity of 99.7 % and 99.8 %, respectively, which were purchased from the Guangfu Chemical Reagents Co., Tianjin, China.

Apparatus and Procedure. Solubilities were determined by the dynamic method using a laser technique.[18] The apparatus and procedure have been described in detail previously.[6] Briefly, a predetermined mixture of a solute and solvent was heated slowly with continuous stirring inside a vessel of (100 to 250) mL. The heating rate would be less than 0.2 K·h^{-1} at a

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Table 1. Solubility Measurements of Sebacic Acid (1) in *n*-Propanol (2) + Water (4) Binary Solvent System

x_1	T^{exptl}/K	x_1	T^{exptl}/K	x_1	T^{exptl}/K
$x_2^0 = 0.2000$					
2.750E-03	295.41	9.450E-03	311.10	2.580E-02	329.28
2.950E-03	296.72	1.084E-02	313.47	3.160E-02	332.94
4.750E-03	300.83	1.229E-02	315.38	3.927E-02	335.80
6.040E-03	303.93	1.431E-02	317.73	4.446E-02	338.32
6.630E-03	305.74	1.789E-02	322.99	5.075E-02	340.50
8.580E-03	309.56	1.968E-02	324.89		
$x_2^0 = 0.\ 4000$					
5.060E-03	291.32	2.593E-02	312.90	7.124E-02	334.72
9.120E-03	294.00	3.018E-02	316.10	7.840E-02	336.74
9.470E-03	295.65	3.420E-02	318.34	8.466E-02	338.24
1.014E-02	295.95	3.838E-02	321.05	9.326E-02	340.76
1.235E-02	299.97	4.275E-02	323.37	1.023E-01	342.77
1.488E-02	302.24	4.951E-02	326.35	1.123E-01	345.12
1.879E-02	307.14	5.590E-02	328.52	1.235E-01	347.84
2.151E-02	309.32	6.435E-02	332.32	1.334E-01	349.77
$x_2^0 = 0.6011$					
9.670E-03	292.05	4.364E-02	316.82	9.363E-02	336.71
1.402E-02	295.65	5.089E-02	320.60	1.055E-01	338.50
1.746E-02	298.75	5.655E-02	322.35	1.171E-01	341.32
2.319E-02	302.96	6.181E-02	325.15	1.294E-01	344.31
2.851E-02	307.59	6.739E-02	327.45	1.427E-01	347.66
3.288E-02	311.08	7.662E-02	331.15		
3.714E-02	314.44	8.673E-02	334.80		
$x_2^0 = 0.8003$					
1.355E-02	292.21	4.338E-02	316.25	9.676E-02	335.43
1.786E-02	297.06	4.846E-02	318.03	1.092E-01	339.05
2.346E-02	301.92	5.555E-02	321.30	1.221E-01	342.15
2.847E-02	305.97	6.137E-02	324.00	1.354E-01	345.00
3.279E-02	309.37	6.812E-02	327.07		
3.623E-02	311.66	8.864E-02	333.29		
$x_2^0 = 1.000$					
9.000E-03	292.00	4.289E-02	318.74	1.086E-01	340.30
1.353E-02	297.66	4.756E-02	321.50	1.096E-01	340.35
1.624E-02	300.34	5.294E-02	323.44	1.180E-01	342.05
2.127E-02	304.99	6.141E-02	327.14	1.333E-01	345.08
2.606E-02	308.87	7.582E-02	331.86	1.425E-01	347.47
3.004E-02	311.80	9.025E-02	336.76	1.548E-01	348.62
3.442E-02	314.56	9.561E-02	337.71		

temperature near the SLE temperature. A laser monitoring system was run to observe the dissolving processes. The temperature at which the solid disappeared and the intensity of the laser beam reached a maximum was taken as the SLE temperature. The precision in the temperature measurements was ± 0.01 K, and the uncertainty of the measured temperature was ± 0.1 K which was calculated from the standard deviations of repeated experimental measurements. Mixtures were prepared by weighing the pure components with an uncertainty of ± 0.0001 g.

To compare the different measurement manner, one static equilibrium experiment was introduced according to the method reported by Wang.[17]

Result and Discussion

The experimental solubilities of sebacic acid in *n*-propanol + water solvent mixtures are summarized in Table 1, where T^{exptl} is the measured temperature; x_1 is the mole fraction solubility; and x_2^0 is mole fraction of *n*-propanol solute-free. Figure 1 shows the plot of x_1 versus temperature at different x_2^0.

As shown in Figure 1, the phenomenon of enhanced solubility of sebacic acid in *n*-propanol + water binary solvents has been observed; that is, 60.11 % and 80.03 % mole fraction of solute-free *n*-propanol + water binary solvents provide enhanced solubility compared to that of pure water and *n*-propanol solvents. At the same temperature, the highest solubility is obtained in 80.03 % mole fraction of solute-free *n*-propanol + water binary solvent. In general, sebacic acid is soluble in *n*-propanol but rather insoluble in water. At low *n*-propanol content, the solubility of sebacic acid increases significantly with x_2^0, but this change becomes faint at high *n*-propanol content.

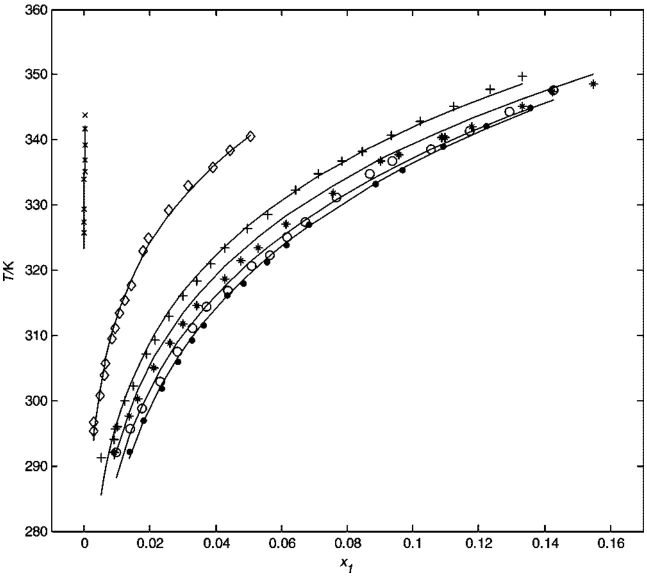

Figure 1. Solubility of sebacic acid in binary *n*-propanol + water solvent mixtures: ×, $x_2^0 = 0$;[6] ◇, $x_2^0 = 0.2000$; +, $x_2^0 = 0.4000$; ○, $x_2^0 = 0.6011$; ●, $x_2^0 = 0.8003$; *, $x_2^0 = 1.000$; —, solubility curve calculated from the λh equation.

One equilibrium method experiment[17] was also applied to determine the solubility of sebacic acid in 40.00 % x_2^0 *n*-propanol + water binary solvent at 295.95 K. The solubility calculated from three measurements is 0.01153. From comparison with the result of the dynamic method, 0.01014, which is listed in Table 1, it is found that the solubilities determined by the dynamic method and the equilibrium method, respectively, have little difference.

The solubilities of sebacic acid in ethanol + water binary mixtures has been measured in our previous report[6] at a mole fraction of ethanol being 0 %, 8.355 %, 28.11 %, 60.99 %, and 100% (mass fraction 0 %, 20 %, 60 %, 80 %, 100 %) binary mixtures. To verify the synergistic effect of sebacic acid in alcohols + water binary solvents, the solubility data of sebacic acid in ethanol + water were supplemented, and the mole fraction of ethanol in the solvent mixtures was 0.1435, 0.3696, 0.7981, and 0.9000. The results are presented in Table 2, where T^{exptl} is the measured temperature; x_1 is the mole fraction solubility; and x_3^0 is mole fraction of ethanol solute-free. Figure 2 shows the plot of x_1 versus temperature at different x_3^0. It can be seen from Figure 2 that a weak synergistic effect was detected in this system, and the solubility−temperature curves for mole fraction of ethanol of 79.81 %, 90.00 %, and 100 % coincided with each other, especially at high temperature. But no solubility in ethanol + water binary mixtures was higher than that in ethanol.

The enhanced solubility in binary solvents, known as the synergistic effect, means that at a particular composition the solvent's power of dissolution becomes much higher than that of their individual components. The Scatchard−Hildebrand theory[7] suggests that when a solid solute is dissolved in a mixture of two carefully selected solvents according to the condition the solubility parameter of the solute has a value intermediate between the values of the solubility parameters of

Table 2. Solubility Measurements of Sebacic Acid (1) in the Ethanol (3) + Water (4) Binary Solvent System

x_1	T^{exptl}/K	x_1	T^{exptl}/K	x_1	T^{exptl}/K
		$x_3^0 = 0.1435$			
6.041E-05	289.30	8.570E-04	313.16	7.287E-03	334.78
9.592E-05	295.54	1.120E-03	317.05	1.039E-02	337.59
1.164E-04	295.59	1.432E-03	319.80	1.431E-02	340.74
2.297E-04	303.14	1.862E-03	322.49	1.790E-02	343.69
3.659E-04	305.49	2.552E-03	325.53	2.065E-02	345.80
4.959E-04	308.31	3.304E-03	327.71	2.572E-02	348.68
6.598E-04	310.34	5.117E-03	330.68	2.892E-02	350.74
		$x_3^0 = 0.3697$			
9.859E-04	288.47	1.131E-02	309.87	4.908E-02	334.33
1.752E-03	290.55	1.445E-02	313.70	5.562E-02	336.44
2.669E-03	292.67	1.567E-02	316.14	6.235E-02	338.74
3.383E-03	296.97	1.975E-02	318.45	6.906E-02	340.33
4.199E-03	298.05	2.411E-02	321.57	7.357E-02	341.96
5.313E-03	300.16	2.939E-02	325.86	8.348E-02	344.16
6.790E-03	303.65	3.071E-02	326.92	9.221E-02	346.04
8.567E-03	306.66	3.621E-02	328.87	1.002E-01	348.01
9.566E-03	309.06	4.242E-02	331.34	1.085E-01	350.08
		$x_3^0 = 0.7981$			
9.400E-03	292.46	4.198E-02	316.01	9.393E-02	335.53
1.451E-02	295.74	5.025E-02	319.91	1.046E-01	337.88
2.024E-02	300.80	5.489E-02	321.52	1.167E-01	340.48
2.476E-02	305.24	6.388E-02	325.39	1.306E-01	344.04
2.975E-02	308.56	7.326E-02	328.73		
3.533E-02	311.91	8.456E-02	332.44		
		$x_3^0 = 0.9000$			
2.702E-02	305.77	3.892E-02	313.76	5.358E-02	321.26

Table 3. λh Model Parameters for Sebacic Acid + Ethanol + Water and Sebacic Acid + *n*-Propanol + Water (Defined by Equation 3)

solvent system	λ	h/K
water + 14.35 mol % ethanol	1.9320	5.5320E+03
water + 36.97 mol % ethanol	2.0417	3.4458E+03
water + 79.81 mol % ethanol	1.1855	4.0661E+03
water + 20.00 mol % *n*-propanol	0.94737	6.5731E+03
water + 40.00 mol % *n*-propanol	1.0866	4.7649E+03
water + 60.11 mol % *n*-propanol	1.0166	4.5584E+03
water + 80.03 mol % *n*-propanol	0.86478	4.9599E+03
n-propanol	1.0767	4.5765E+03

Table 4. Wilson Model Parameters for Sebacic Acid + Ethanol + Water and Sebacic Acid + *n*-Propanol + Water (Defined by Equation 5)

i	j	a_{ij}	a_{ji}	b_{ij}/K	b_{ji}/K
sebacic acid	ethanol	0.46767	−1.2259	−86.148	1453.6
ethanol	water	1.8111	12.600	−510.29	−1466.2
sebacic acid	water	10.799	31.626	−3000.8	−12603
sebacic acid	*n*-propanol	2.4679	−5.0148	−677.16	2461.6
n-propanol	water	0.048479	−6.4192	−3.0622	6913.3

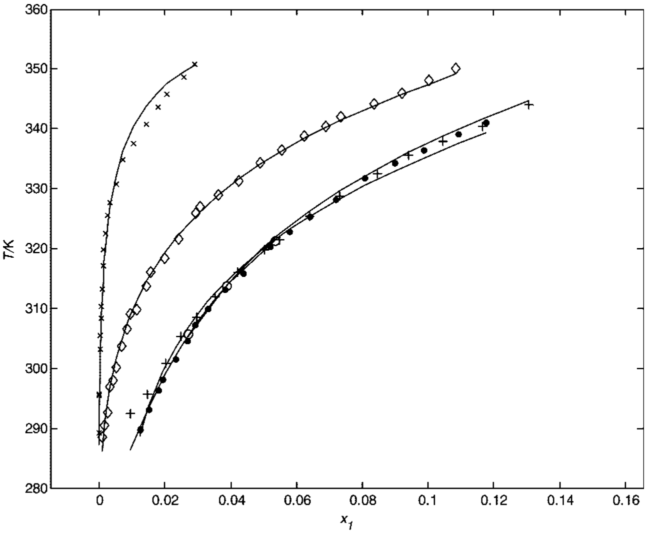

Figure 2. Solubility of sebacic acid in binary ethanol + water solvent mixtures: ×, $x_3^0 = 0.1435$; ◇, $x_3^0 = 0.3697$; +, $x_3^0 = 0.7981$; ○, $x_3^0 = 0.9000$; ●, $x_3^0 = 1.000$;[6] —, solubility curve calculated from the NRTL equation.

the solvents constituting the mixture, and a plot of solubility versus (solute-free) solvent composition should go through a maximum. It follows from the analysis of solubility parameters, sebacic acid $\delta_1 = 20.1$ Mpa$^{1/2}$ which is calculated with the functional group method,[19] *n*-propanol $\delta_2 = 24.3$ Mpa$^{1/2}$,[20] ethanol $\delta_3 = 26.0$ Mpa$^{1/2}$,[20] water $\delta_4 = 47.9$ Mpa$^{1/2}$,[20] that the sebacic acid + *n*-propanol + water system, as well as the sebacic acid + ethanol + water system, should not reveal synergistic effects. However, the experimental results are contrary with this prediction. This result shows that the Scatchard−Hildebrand theory may not be used to predict the synergistic effect for some polar systems. Nevertheless, sebacic acid itself is apt to form dimers by hydrogen bonds, and the binary solvent mixtures are polar mixtures, containing alcohols which can interact with the solute and tend to form intermolecular hydrogen bonds. Our solubility data show that solvent mixtures containing alcohols reveal synergistic effects, so the synergistic effect may be a result of the hydrogen bonds.

SLE can be described by an equation that involves the properties of pure solute, such as enthalpy of fusion, melting point, etc.

$$-\ln x_1\gamma_1 = \frac{\Delta H_{\mathrm{m1}}}{R}\left(\frac{1}{T} - \frac{1}{T_{\mathrm{m1}}}\right) + \frac{\Delta H_{\mathrm{tr1}}}{R}\left(\frac{1}{T} - \frac{1}{T_{\mathrm{tr1}}}\right) - \frac{\Delta Cp_{\mathrm{m1}}}{R}\left(\ln\frac{T}{T_{\mathrm{m1}}} + \frac{T_{\mathrm{m1}}}{T} - 1\right) \quad (1)$$

where T, x_1, γ_1, T_{m1}, ΔH_{m1}, ΔH_{tr1}, T_{tr1}, ΔCp_{m1} stand for equilibrium temperature, mole fraction of solute, activity coefficient, melting temperature, enthalpy of fusion at the melting temperature, enthalpy of solid−solid phase transition, temperature of phase transition, and difference in solute heat capacity between the solid and liquid at the melting temperature, respectively.

The melting temperature and fusion enthalpy of sebacic acid were $T_{\mathrm{m1}} = (405.62 \pm 0.02)$ K and $\Delta H_{\mathrm{m1}} = (45.3 \pm 0.7)$ kJ·mol^{-1} which were determined in our previous paper[6] and agree with the result of Maria.[21] The solid−solid phase transition reported by Maria was not observed in our differential scanning calorimetry measurements and was not included in the solubility calculation. If the contributions of the heat capacities can be neglected, eq 1 becomes[22]

$$-\ln x_1\gamma_1 = \frac{\Delta H_{\mathrm{m1}}}{R}\left(\frac{1}{T} - \frac{1}{T_{\mathrm{m1}}}\right) \quad (2)$$

In this study, the λh equation is used to describe the SLE data. The Wilson equation and the NRTL equation are used to derive the solute activity coefficients γ_1 from the so-called correlation equations that describe the Gibbs excess free energy of mixing G^{E}.

1. The λh Equation. The λh equation was first reported by Buchowski.[23]

$$\ln\left[1 + \frac{\lambda(1 - x_1)}{x_1}\right] = \lambda h\left(\frac{1}{T} - \frac{1}{T_{\mathrm{m1}}}\right) \quad (3)$$

where λ, h are the model parameters which are constants in pure solvents. The λh equation has been successfully used in

Table 5. NRTL Model Parameters for Sebacic Acid + Ethanol + Water and Sebacic Acid + *n*-Propanol + Water (Defined by Equation 7)

i	j	a_{ij}	a_{ji}	b_{ij}/K	b_{ji}/K	$\eta_{ij} = \eta_{ji}$
sebacic acid	ethanol	4.0945	−9.3764	−1821.7	3694.9	0.3
ethanol	water	−9.3183	44.830	3037.4	−12594	
sebacic acid	water	−1.8444	−12.774	255.32	6897.6	
sebacic acid	*n*-propanol	2.9733	−4.1617	−1149.6	1407.0	
n-propanol	water	−19.864	16.577	6623.9	−5377.4	

Table 6. Root-Mean-Square Deviations from the Description by the λh Equation, the Wilson Equation, and the NRTL Equation

solvent system	$\sigma_{\lambda h}$/K	σ_{W}/K	σ_{N}/K
water + 14.35 mol % ethanol	0.98	1.95	0.91
water + 36.97 mol % ethanol	1.86	1.60	1.95
water + 79.81 mol % ethanol	1.38	1.86	0.30
water + 20.00 mol % *n*-propanol	0.98	1.14	1.93
water + 40.00 mol % *n*-propanol	1.40	0.86	1.20
water + 60.11 mol % *n*-propanol	1.31	0.84	0.78
water + 80.03 mol % *n*-propanol	0.46	1.23	0.46
n-propanol	0.64	1.02	0.76

binary solvent systems by treating solvent mixtures as a single component. In this paper, the λh equation remains a two-parameter form in ternary systems. It makes it easy to get high calculation accuracy, but it also results in an impossibility of predicting the solubilities in solvent mixtures using solubilities of the pure solvents.

2. The Wilson Equation. The Wilson equation is used to calculate activity coefficients[24]

$$\ln \gamma_i = 1 - \ln\left(\sum_j^n (\Lambda_{ij}x_j)\right) - \sum_k^n \left(\frac{\Lambda_{ki}x_k}{\sum_j^n (\Lambda_{kj}x_j)}\right) \tag{4}$$

where Λ_{ij} is the model parameter which is expressed by the following empirical equation.[25]

$$\Lambda_{ij} = a_{ij} + b_{ij}/T \tag{5}$$

where a_{ij} and b_{ij} are constants.

3. The NRTL Equation. For the definition of the activity coefficient, the NRTL activity coefficient model[26] was used as

$$\ln \gamma_i = \frac{\sum_j^n \tau_{ji}G_{ji}x_j}{\sum_l^n G_{li}x_l} + \sum_j^n \frac{x_jG_{ij}}{\sum_l^n G_{lj}x_l}\left[\tau_{ij} - \frac{\sum_r^n x_r\tau_{rj}G_{rj}}{\sum_l^n G_{lj}x_l}\right] \tag{6}$$

where G_{ij} and τ_{ij} are NRTL model parameters that need to be experimentally determined by

$$G_{ij} = \exp(-\eta_{ij}\tau_{ij}) \qquad \tau_{ij} = a_{ij} + b_{ij}/T \tag{7}$$

where $\tau_{ij} \neq \tau_{ji}$, $\tau_{ii} = 0$, a_{ij}, and b_{ij} are constants; $\eta_{ij} = \eta_{ji}$ in the optimization process, as Renon and Prausnitz proposed; and η_{ij} was chosen as 0.3.[26]

The coefficients in each model were determined using the Nelder−Mead simplex method. A nonlinear minimization function (Nelder−Mead Simplex) in Matlab (Mathwork, MA) can be employed for the minimization of the objective function, which is the root-mean-square deviation σ between the experimental equilibrium temperature and calculated equilibrium temperature. The σ is defined by

$$\sigma = \left[\sum_{i=1}^N (T^{\mathrm{exptl}} - T)^2/(N-1)\right]^{0.5} \tag{8}$$

where N is number of experimental data points; T^{exptl} is the experimental equilibrium temperature which is listed in Tables 1 and 2; and T is the calculated equilibrium temperature which is calculated from eq 2 to eq 7.

A good description of the experimental curves has been achieved using the λh equation. The values of the model parameters λ, h are listed in Table 3, and the root-mean-square deviations for each solvent system are listed in Table 6, which range from (0.46 to 1.86) K. Table 4 shows the model parameters of the Wilson equation, which are calculated from the experimental data shown in Tables 1 and 2 and in our previous report.[6] The model parameters for the sebacic acid + ethanol + water system have been recalculated because a weak synergistic effect was detected in the present study. The root-mean-square deviations of the Wilson equation for each system are listed in Table 6, which range from (0.84 to 1.95) K. The results calculated by the NRTL equation are listed in Table 5, which are also calculated from the experimental data shown in Tables 1 and 2 and in our previous report.[6] The root-mean-square deviations for each system are listed in Table 6, which range from (0.30 to 1.95) K. These results show that the description of the SLE of the sebacic acid + alcohol + water system with the λh equation, the Wilson equation, and the NRTL equation is reasonable, in which the Wilson equation and the NRTL equation can be used to predict the solubility of sebacic acid in ethanol aqueous solutions and *n*-propanol aqueous solutions. The correlation models and the experimental data obtained in this work can also be utilized as essential information for the synthesis and purification process of sebacic acid.

Conclusions

The solubilities of sebacic acid in a variety of *n*-propanol + water and ethanol + water binary solvents at a temperature range from (288 to 351) K have been measured. A synergistic effect was investigated in the sebacic acid + *n*-propanol + water system. However, only a weak synergistic effect was investigated in the sebacic acid + ethanol + water system. Solubilities tend to be consistent when the mole fraction of ethanol in the solvents was larger than 0.8.

The Scatchard−Hildebrand theory can describe the synergistic effect, but it shows poor consistency with the present experimental results. A synergistic effect exists in the sebacic acid + alcohol + water systems although the solubility parameter of solute is not between those of solvents.

The prediction of solubility by use of the λh equation, the Wilson equation, and the NRTL equation with model parameters obtained through the regression of the solubility data in the binary solvents is satisfactory, and the root-mean-square deviations for each system range from (0.30 to 1.95) K. The NRTL equation provided slightly better results than that given by the λh equation and the Wilson equation. The model parameters of the Wilson equation for the sebacic acid + ethanol + water system were corrected. The Wilson equation and the NRTL equation are also able to correctly predict the solubility of sebacic acid despite revealing the synergistic effect in this study.

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