Supporting Information

Determination and Correlation of the Solubility of Monosodium fumarate in Different Neat and Binary Solvent Systems

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1. Determination of Solid-liquid Equilibrium Time

The solid-liquid equilibrium time is of great important in the solubility measurement process. To determine a suitable equilibrium time, a randomly selected experimental point in the mixed solvent of water + ethanol (the mole fraction of ethanol was 0.500) at T = 303.15 K was selected. The experiment was carried out by the gravimetric method at the dissolution time ranging from 10 to 300 min. The obtained solubility data of monosodium fumarate at different dissolution time were listed in Table S1. The results indicated that 60 min was enough for establishing the solid-liquid equilibrium.

2. Experimental Method Verification

In order to verify the reliability and accuracy of the method, the solubility data of xylitol in ethanol from 293.15 to 333.15 K and maltitol in water + ethanol system from 298.15 to 323.15 K were determined respectively, and the results were listed in Tables S2 and S3. It can be seen that the obtained experimental results were similar to the data reported in the literatures,[1, 2] and the ARD were 2.299 % for xylitol and 5.052 % for maltitol. On the basis of the above verifications, the gravimetric method utilized in this work was feasible to determine the monosodium fumarate solubility.

Table captions:

Table S1. Solubility Data of Monosodium Fumarate in Water + Ethanol (Mole Fraction of Ethanol x_2 = 0.500) Binary Solvent System at Temperature T = 303.15 K and Pressure P = 0.1 MPa at Different Dissolution Time[a]

Table S2. Comparisons of the Experimental Mole Fraction Solubility (x_1) of Xylitol in Ethanol from 293.15 to 333.15 K (P = 0.1 MPa) and the Data Reported in the Literature (x_1^{ref})[a]

Table S3. Comparisons of the Experimental Mole Fraction Solubility (x_1) of Maltitol in Water + Ethanol Binary Solvent System (Mole Fraction of Water x_2 = 0.5229) from 298.15 to 323.15 K (P = 0.1 MPa) and the Data Reported in the Literature (x_1^{ref})[a]

Figure captions:

Figure S1. Apelblat-Jouyban-Acree model fitting plot of ln(x_1) versus T (from 283.15 to 323.15 K) and x_2 (from 0.000 to 1.000) for monosodium fumarate solubility in the full range in water + methanol.

Figure S2. Apelblat-Jouyban-Acree model fitting plot of ln(x_1) versus T (from 283.15 to 323.15 K) and x_2 (from 0.000 to 1.000) for monosodium fumarate solubility in the full range in water + ethanol.

Figure S3. Apelblat-Jouyban-Acree model fitting plot of ln(x_1) versus T (from 283.15 to 323.15 K) and x_2 (from 0.000 to 1.000) for monosodium fumarate solubility in the full range in water + 2-propanol.

Figure S4. Apelblat-Jouyban-Acree model fitting plot of ln(x_1) versus T (from 283.15 to 323.15 K) and x_2 (from 0.000 to 1.000) for monosodium fumarate solubility in the full range in water + acetone.

Table S1. Solubility Data of Monosodium Fumarate in Water + Ethanol (Mole Fraction of Ethanol x_2 = 0.500) Binary Solvent System at Temperature T = 303.15 K and Pressure P = 0.1 MPa at Different Dissolution Time[a]

Time/min	10	20	30	60	90
10^3x_1	1.345	1.362	1.366	1.374	1.374
Time/min	120	180	240	300	
10^3x_1	1.374	1.374	1.375	1.375	

[a]The standard uncertainty of temperature $u(T)$ = 0.05 K; the relative standard uncertainty of pressure $u_r(p)$ = 0.05; the relative standard uncertainty of the mole fraction solubility $u_r(x_1)$ = 0.15.

Table S2. Comparisons of the Experimental Mole Fraction Solubility (x_1) of Xylitol in Ethanol from 293.15 to 333.15 K (P = 0.1 MPa) and the Data Reported in the Literature (x_1^{ref})[a]

T/K	10^3x_1	$10^3x_1^{ref}$	10^2RD[b]	10^2ARD[c]
293.15	1.707	1.728	1.212	2.299
298.15	2.412	2.419	0.294	
303.15	3.072	3.091	0.610	
308.15	3.896	3.974	1.995	
313.15	5.037	5.224	3.704	
318.15	6.785	7.090	4.491	
323.15	9.690	9.657	0.344	
328.15	13.452	13.150	2.244	
333.15	16.871	17.850	5.801	

[a]The standard uncertainty of temperature $u(T)$ = 0.05 K; the relative standard uncertainty of pressure $u_r(p)$ = 0.05; the relative standard uncertainty of the mole fraction solubility $u_r(x_1)$ = 0.15. [b]RD is the relative deviation between the experimental solubility data and the literature data. [c]ARD is the average relative deviation between the experimental solubility data and the literature data.

Table S3. Comparisons of the Experimental Mole Fraction Solubility (x_1) of Maltitol in Water + Ethanol Binary Solvent System (Mole Fraction of Water x_2 = 0.5229) from 298.15 to 323.15 K (P = 0.1 MPa) and the Data Reported in the Literature (x_1^{ref})[a]

T/K	10^3x_1	$10^3x_1^{ref}$	RD[b]	ARD[c]
298.15	4.980	4.794	3.732	5.052
303.15	5.923	5.793	2.187	
308.15	8.042	7.646	4.927	
313.15	10.796	10.093	6.513	
318.15	15.369	16.091	4.695	
323.15	20.209	21.878	8.258	

[a]The standard uncertainty of temperature $u(T)$ = 0.05 K; the relative standard uncertainty of pressure $u_r(p)$ = 0.05; the relative standard uncertainty of the mole fraction solubility $u_r(x_1)$ = 0.15. [b]RD is the relative deviation between the experimental solubility data in this work and the literature data. [c]ARD is the average relative deviation between the experimental solubility data and the literature data.

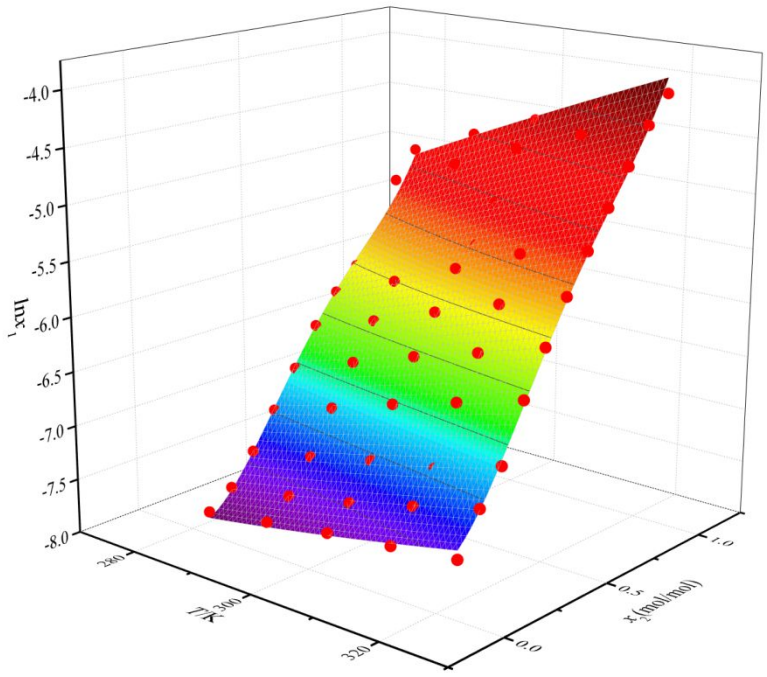
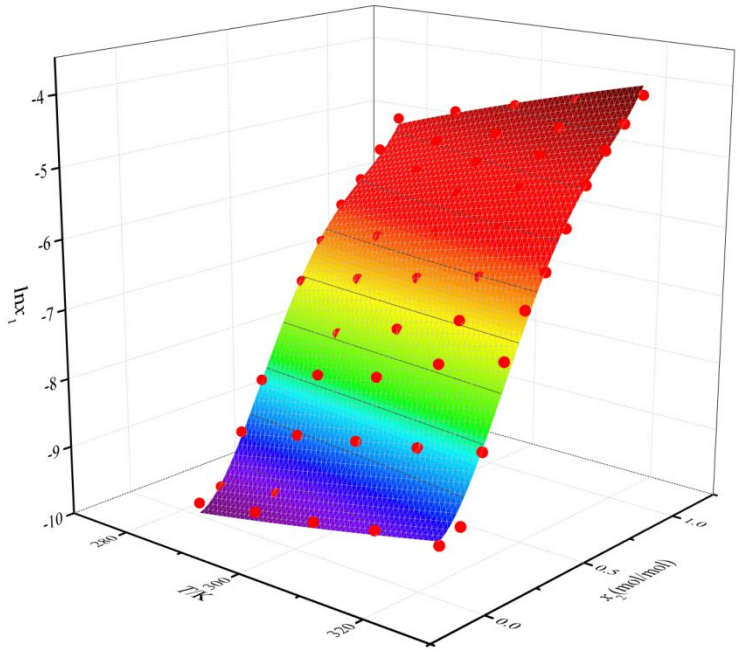


Figure S1. Apelblat-Jouyban-Acree model fitting plot of ln(x_1) versus T (from 283.15 to 323.15 K) and x_2 (from 0.000 to 1.000) for monosodium fumarate solubility in the full range in water + methanol.



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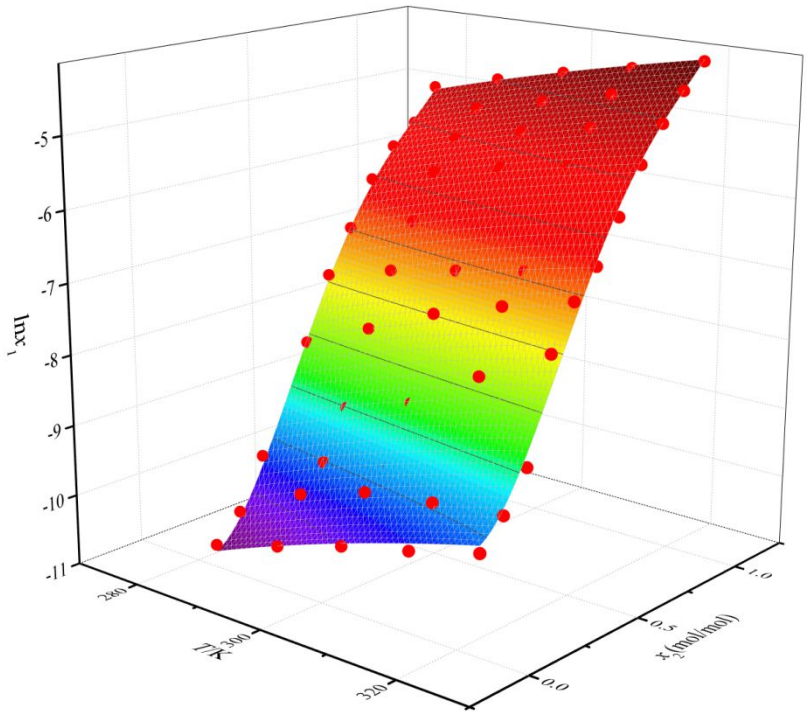

Figure S3. Apelblat-Jouyban-Acree model fitting plot of ln(x_1) versus T (from 283.15 to 323.15 K) and x_2 (from 0.000 to 1.000) for monosodium fumarate solubility in the full range in water + 2-propanol.

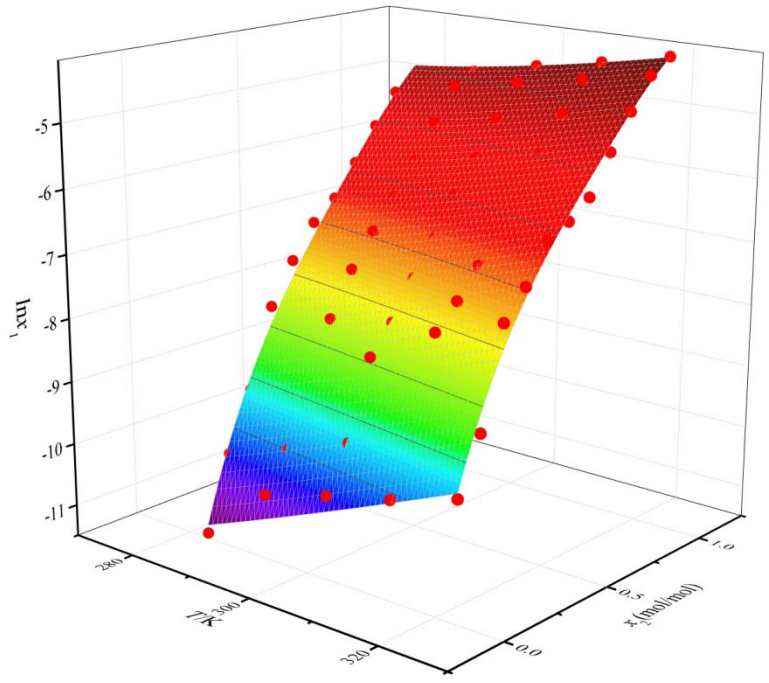

Figure S4. Apelblat-Jouyban-Acree model fitting plot of ln(x_1) versus T (from 283.15 to 323.15 K) and x_2 (from 0.000 to 1.000) for monosodium fumarate solubility in the full range in water + acetone.

References

(1) Li, Z.; Zhang, T.; Huang, C.; Wang, H.; Yu, B.; Gong, J. Measurement and correlation of the solubility of maltitol in different pure solvents, methanol–water mixtures, and ethanol–water mixtures. *J. Chem. Eng. Data* **2016**, 61, 1065-1070.
(2) Wang, S.; Li, Q.-S.; Li, Z.; Su, M.-G. Solubility of xylitol in ethanol, acetone, N,N-dimethylformamide, 1-butanol, 1-pentanol, toluene, 2-propanol, and water. *J. Chem. Eng. Data* **2007**, 52, 186-188.