Supporting Information

Measurement and Correlation for Solubility of L-Alanine in Pure and Binary Solvents at Temperatures from 283.15 to 323.15 K

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1. Determination of solid-liquid equilibrium time

In order to determine the appropriate equilibrium time, a randomly experimental point in the binary water + methanol solvent system (the mole fraction of water was 0.500) at 303.15 K was selected. The solubility data of L-alanine at the dissolution time ranging from 30 to 300 min were measured by gravimetrical method, and listed in Table S1. The results illustrated that 180 min was enough for establishing the solid-liquid equilibrium.

2. Experimental method verification

To verify the reliability and accuracy of the methods used in this experiment, the solubility data of maltitol (in water + ethanol solvent system at x_1 = 0.5229 from 298.15 to 323.15 K) and xylitol (in ethanol solvent from 293.23 to 333.22 K) were determined in this work. The comparisons between the measured experimental data and the corresponding values in literatures[1, 2] were shown in Table S2 and Table S3. As can be seen from Table S2 and Table S3, the experimental data were basically consistent with the data reported in the literatures. Therefore, the gravimetrical method used in our work can be applied to the determination of the solubility of L-alanine.

3. Comparisons between the solubility data of L-alanine in this work and the data reported in the literatures

The solubility data of L-alanine in pure water and the mixed solvent systems (water + methanol, water + ethanol, water + 2-propanol and water + 1-propanol) measured in this work and the values reported in the literatures were tabulated in Tables S4 – S5 and plotted in Figures S1 – S9, respectively and the corresponding ARD values were 6.739 %, 11.207 %, 17.777 %, 122.031 %, 93.045 %, 11.802 %, 29.063 %, 15.943%, and 16.188%. The L-alanine solubility calculated by Apelblat-Jouyban-Acree model was generally consistent with the literature data except for that at pure ethanol from Needham's work[3], and at x_1 = 0.001 in water + 2-propanol (1-propanol) solvent systems from Orella and Kirman's work[4].

Table captions:

Table S1. Solubility data of L-alanine at 303.15 K in the binary water + methanol solvent system (x_1 = 0.500) at different dissolution time

Table S2. Comparisons between experimental solubility (x_A^{exp}) of maltitol in water + ethanol solvent system (x_1 = 0.5229) at different temperatures under atmospheric pressure and the data reported in the literature (x_A^r) [a]

Table S3. Comparisons between experimental solubility (x_A^{exp}) of xylitol in pure ethanol at different temperatures under atmospheric pressure and the data reported in the literature (x_A^r) [a]

Table S4. Comparisons between the solubility data of L-alanine (x_A^{cal})[a] in pure water at different temperatures in this work and the data reported in the literatures (x_A^r)

Table S5. Comparisons between the solubility data of L-alanine (x_A^{cal})[a] in four binary solvent systems (water + methanol, water + ethanol, water + 2-propanol, and water + 1-propanol) at T = 298.15 K in this work and the data reported in the literatures (x_A^r)

Figure captions:

Figure S1. Comparisons between the solubility data of L-alanine (x_A^{cal}) in pure water in this work and the data reported in the literatures (x_A^{r})

Figure S2. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + methanol binary solvent system at 298.15 K in this work and the data from Gekko's work in 1981 (x_A^{r})

Figure S3. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + ethanol binary solvent system at 298.15 K in this work and the data reported in Bowden's work (x_A^{r})

Figure S4. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + 2-propanol binary solvent system at 298.15 K in this work and the data reported in Orella and Kirman's work (x_A^{r})

Figure S5. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + 1-propanol binary solvent system at 298.15 K in this work and the data reported in Orella and Kirman's work (x_A^{r})

Figure S6. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + methanol binary solvent system at 298.15 K in this work and the data reported in Needham's work (x_A^{r})

Figure S7. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + ethanol binary solvent system at 298.15 K in this work and the data reported in Needham's work (x_A^{r})

Figure S8. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + 1-propanol binary solvent system at 298.15 K in this work and the data reported in Needham's work (x_A^{r})

Figure S9. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + 2-propanol binary solvent system at 298.15 K in this work and the data reported in Needham's work (x_A^{r})

Figure S10. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water + methanol from 283.15 to 323.15 K (p = 0.1 MPa)

Figure S11. Experimental mole fraction solubility of L-alanine in the binary mixed

solvent of water+ ethanol from 283.15 to 323.15 K (p = 0.1 MPa)

Figure S12. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water + 1-propanol from 283.15 to 323.15 K (p = 0.1 MPa)

Figure S13. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water + 2-propanol from 283.15 to 323.15 K (p = 0.1 MPa)

Figure S14. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water + acetone from 283.15 to 323.15 K (p = 0.1 MPa)

Table S1. Solubility data of L-alanine at 303.15 K in the binary water + methanol solvent system (x_1 = 0.500) at different dissolution time

Time/min	10	20	30	60	90
10^3x_A	3.127	3.137	3.132	3.143	3.135
Time/min	120	180	240	300	
10^3x_A	3.146	3.141	3.148	3.145	

Table S2. Comparisons between experimental solubility (x_A^{exp}) of maltitol in water + ethanol solvent system (x_1 = 0.5229) at different temperatures under atmospheric pressure and the data reported in the literature (x_A^r) [a]

T/K	$10^3x_A^{exp}$	$10^3x_A^r$	RD/%[b]	ARD/%[c]
298.15	4.862	4.794	1.425	9.589
303.15	6.171	5.793	6.525	
308.15	7.911	7.646	3.463	
313.15	10.131	10.093	0.379	
318.15	12.497	16.091	22.336	
323.15	16.757	21.878	23.408	

[a]The standard uncertainty of temperature $u(T)$ = 0.05 K, the relative uncertainty of pressure $u_r(P)$ = 0.05 and the relative uncertainty of the mole fraction solubility $u_r(x_A)$ = 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 between experimental solubility (x_A^{exp}) of xylitol in pure ethanol at different temperatures under atmospheric pressure and the data reported in the literature (x_A^r) [a]

T/K	$10^3x_A^{exp}$	$10^3x_A^r$	RD/%[b]	ARD/%[c]
293.23	1.866	1.728	7.992	5.139
298.28	2.475	2.419	2.301	
303.17	3.152	3.091	1.972	
308.21	4.184	3.974	5.277	

313.19	5.343	5.224	2.284
318.29	6.859	7.090	3.252
323.24	9.124	9.657	5.522
328.19	12.023	13.150	8.573
333.22	16.230	17.850	9.074

[a]The standard uncertainty of temperature $u(T)$ = 0.05 K, the relative uncertainty of pressure $u_r(P)$ = 0.05 and the relative uncertainty of the mole fraction solubility $u_r(x_A)$ = 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 S4. Comparisons between the solubility data of L-alanine (x_A^{cal})[a] in pure water at different temperatures in this work and the data reported in the literatures (x_A^{r})

T/K	$10^3x_A^{cal}$	$10^3x_A^{r}$	RD/%[f]	ARD/%[g]
298.15	32.132	33.374[b]	3.723	6.739
303.15	35.213	35.255[b]	0.118	
313.15	42.066	39.503[b]	6.488	
323.15	49.916	43.791[b]	13.986	
333.15	58.861	48.767[b]	20.700	
298.25	32.191	33.718[c]	4.528	
298.15	32.132	33.556[d]	4.244	
298.15	32.132	32.093[e]	0.122	

[a]The solubility data of L-alanine(x_A^{cal}) in water were calculated by the Apelblat-Jouyban-Acree model. [b]The solubility data was reported by Jin and Chao[5]. [c]The solubility data was reported by Nozaki and Tanford[6]. [d]The solubility data was reported by Gekko in 1989[7]. [e]The solubility data was reported by Held and co-workers[8]. [f]RD is the relative deviation between the experimental solubility data and the literature data. [g]ARD is the average relative deviation between the experimental solubility data and the literature data.

Table S5. Comparisons between the solubility data of L-alanine (x_A^{cal})[a] in four binary solvent systems (water + methanol, water + ethanol, water + 2-propanol, and water + 1-propanol) at T = 298.15 K in this work and the data reported in the literatures (x_A^{r})

x_1	$10^3x_A^{cal}$	$10^3x_A^{r}$	RD/%[f]	ARD/%[g]
Water + Methanol[b]				

0.000	0.436	0.454	3.896	11.207
0.359	1.554	2.000	22.280	
0.599	4.659	5.517	15.554	
0.771	10.010	11.307	11.467	
0.900	18.515	20.566	9.971	
1.000	32.132	33.495	4.071	
		Water + Ethanol[c]		
0.000	0.245	0.282	13.316	17.777
0.390	0.845	1.013	16.600	
0.630	2.82	4.204	32.822	
0.793	7.907	7.857	0.634	
0.911	17.114	13.635	25.516	
		Water + 2-Propanol[d]		
0.001	0.156	0.015	938.363	122.031
0.527	1.274	1.100	15.808	5.413
0.690	3.430	3.500	2.000	
0.803	7.272	7.170	1.428	
0.886	12.998	11.900	9.223	
0.951	20.823	21.300	2.240	
0.986	26.874	28.700	6.362	
1.000	32.132	32.400	0.827	
		Water + 1-Propanol[d]		
0.001	0.231	0.030	669.185	93.045
0.529	2.131	1.740	22.473	10.739
0.690	5.460	5.290	3.205	
0.805	10.439	9.840	6.084	
0.889	16.646	14.60	14.017	
0.950	23.413	20.300	15.336	
0.986	28.761	25.400	13.234	
1.000	32.132	32.400	0.827	
		Water + Methanol[e]		
0.000	0.436	0.485	10.106	11.802
0.200	0.779	0.935	16.712	
0.490	2.834	2.916	2.798	
0.692	7.017	5.286	32.744	
0.840	13.766	14.224	3.218	
0.953	24.493	26.518	7.638	
1.000	32.132	29.373	9.394	
		Water + Ethanol[e]		
0.000	0.244	0.117	109.324	29.063
0.265	0.535	0.763	29.928	
0.581	2.135	2.654	19.561	
0.764	6.545	8.565	23.583	
0.883	14.303	15.801	9.483	

0.967	24.242	24.779	2.164	
1.000	32.132	29.373	9.394	
		Water + 1-Propanol[e]		
0.000	0.229	0.150	53.086	15.943
0.316	0.575	0.512	12.276	
0.640	3.992	4.229	5.612	
0.806	10.578	10.339	2.313	
0.906	18.518	15.913	16.369	
0.974	26.776	23.790	12.549	
1.000	32.132	29.373	9.394	
		Water + 2-Propanol[e]		
0.000	0.1555	0.382	59.294	16.188
0.320	0.442	0.346	27.718	
0.644	2.578	2.712	4.933	
0.809	7.584	7.990	5.077	
0.908	15.236	14.659	3.936	
0.974	24.709	23.998	2.961	
1.000	32.132	29.373	9.394	

[a]The solubility data of L-alanine (x_A^{cal}) in three binary solvent systems were calculated by the Apelblat-Jouyban-Acree model. [b]The solubility data was reported by Gekko in 1981[9]. [c]The solubility data was reported by Bowden[10]. [d]The solubility data was reported by Orella and Kirman[4]. [e]The solubility data was reported by Needham[3]. [f]RD is the relative deviation between the experimental solubility data and the literature data. [g]ARD is the average relative deviation between the experimental solubility data and the literature data.

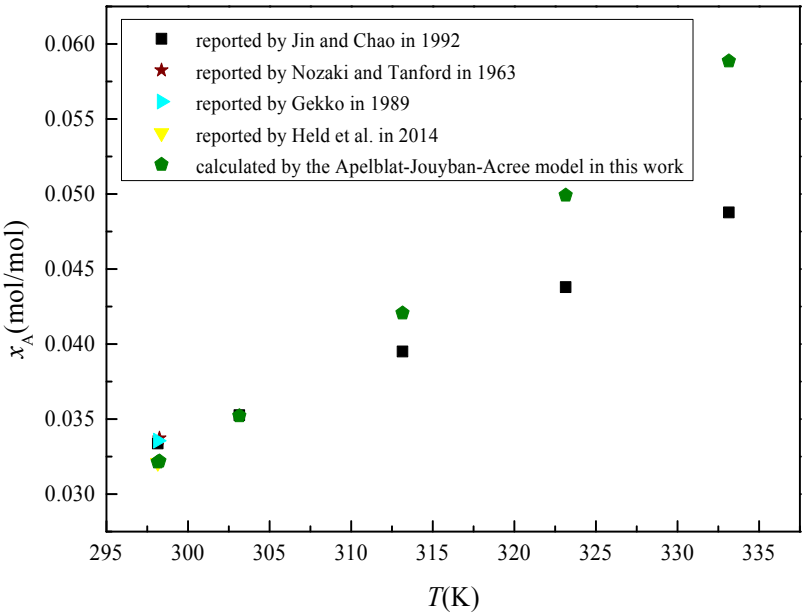

Figure S1. Comparisons between the solubility data of L-alanine (x_A^{cal}) in pure water in this work and the data reported in the literatures (x_A^{r})

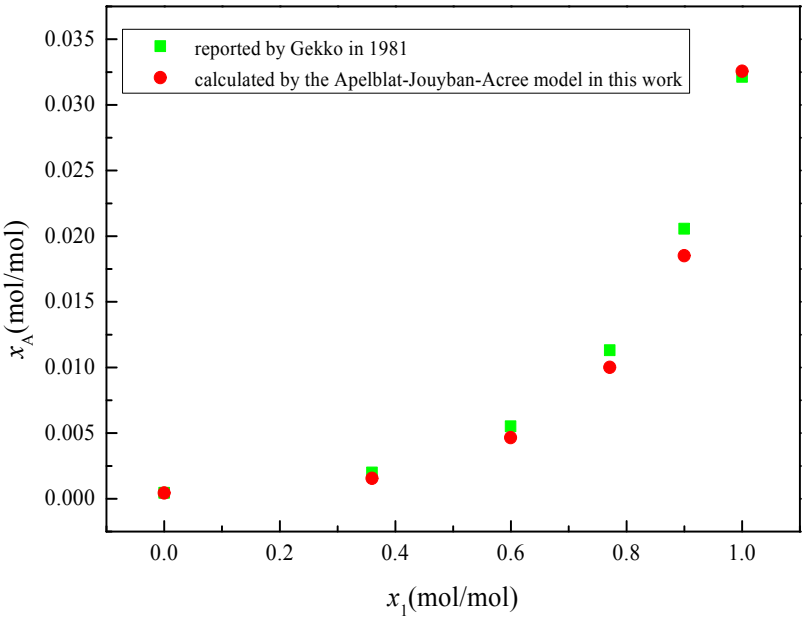

Figure S2. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + methanol binary solvent system at 298.15 K in this work and the data from Gekko's work in 1981 (x_A^{r})

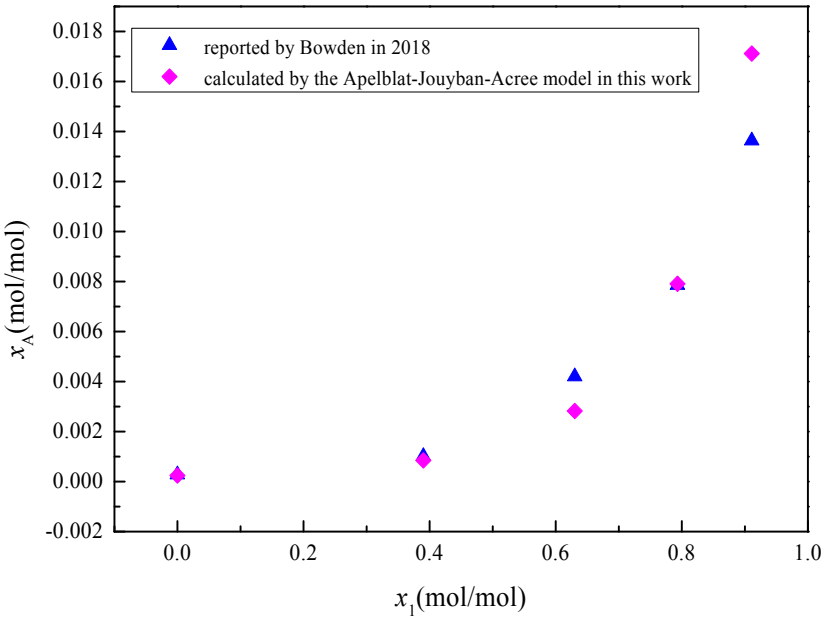

Figure S3. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + ethanol binary solvent system at 298.15 K in this work and the data reported in Bowden's work (x_A^{r})

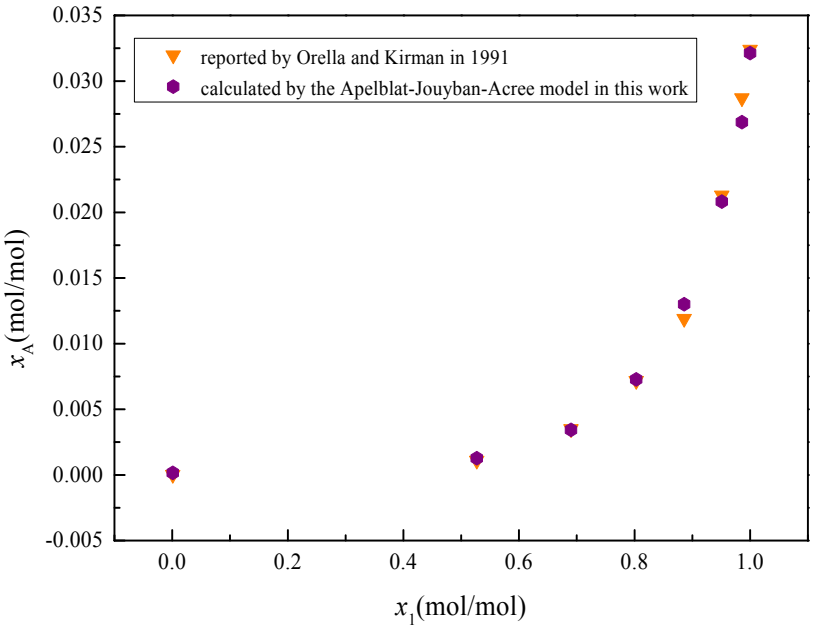

Figure S4. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + 2-propanol binary solvent system at 298.15 K in this work and the data reported in Orella and Kirman's work (x_A^{r})

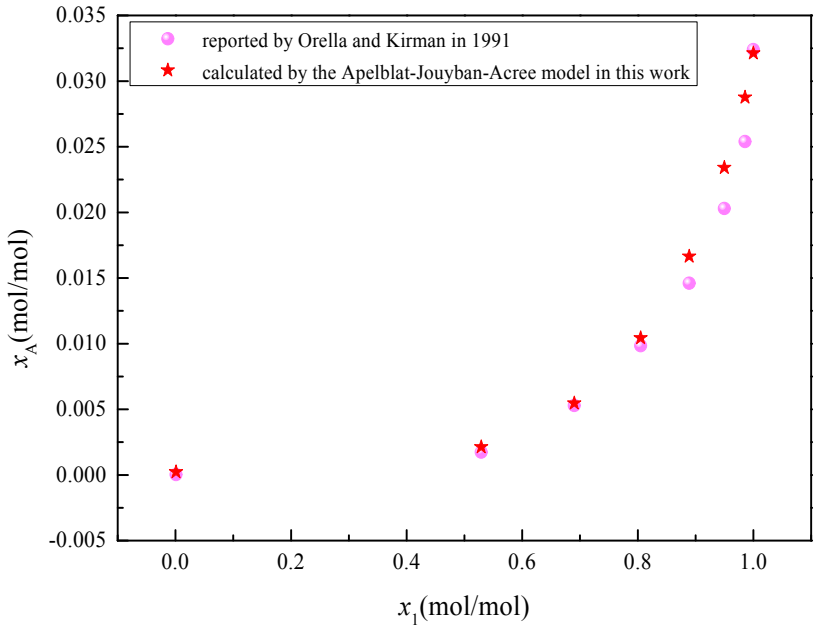

Figure S5. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + 1-propanol binary solvent system at 298.15 K in this work and the data reported in Orella and Kirman's work (x_A^{r})

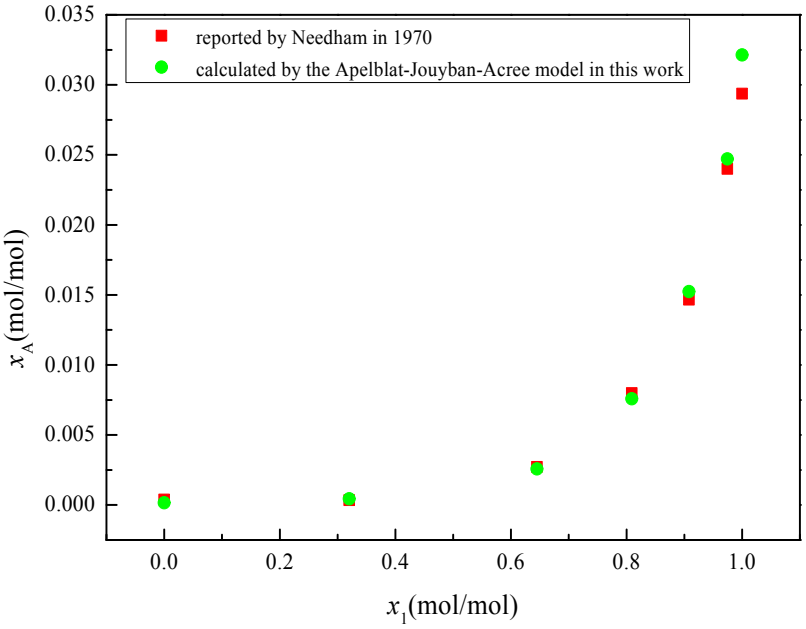

Figure S6. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + methanol binary solvent system at 298.15 K in this work and the data reported in Needham's work (x_A^{r})

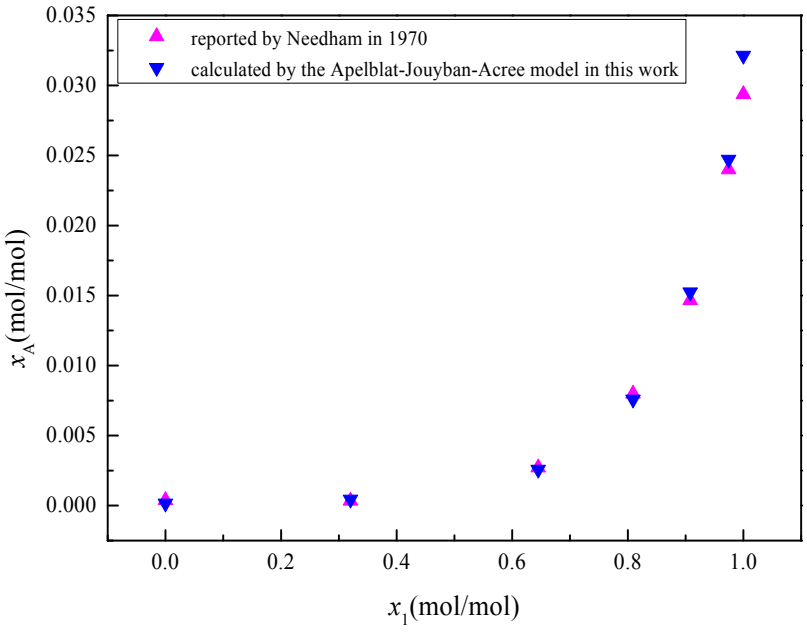

Figure S7. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + ethanol binary solvent system at 298.15 K in this work and the data reported in Needham's work (x_A^r)

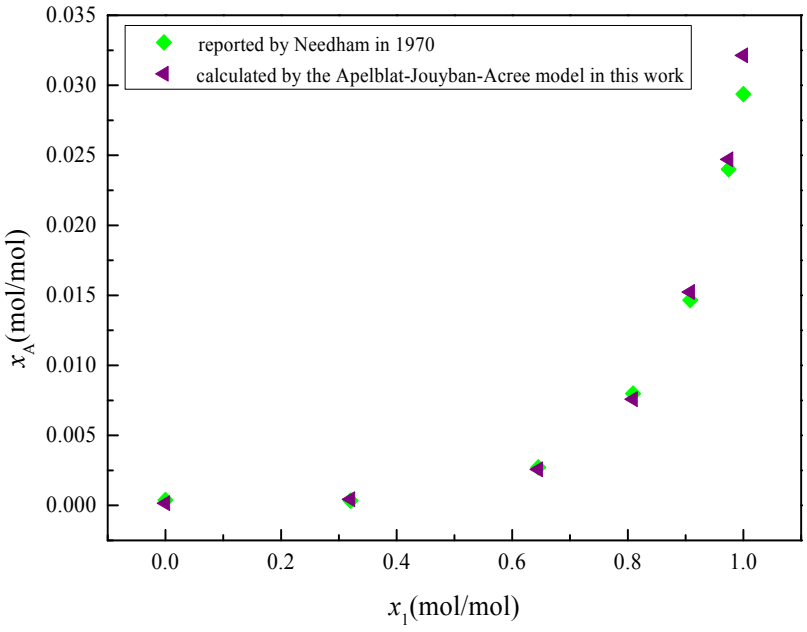

Figure S8. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + 1-propanol binary solvent system at 298.15 K in this work and the data reported in Needham's work (x_A^r)

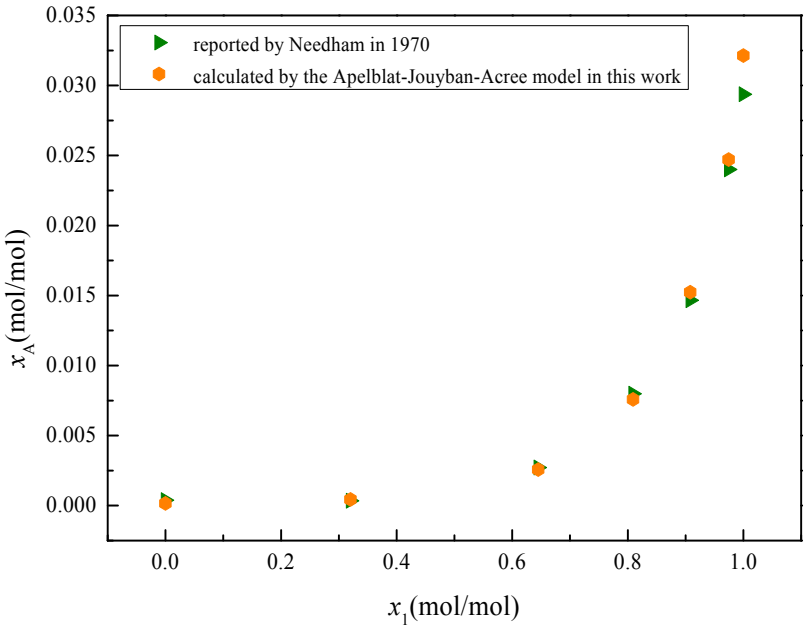

Figure S9. Comparisons between the solubility data of L-alanine (x_A^{cal}) in water + 2-propanol binary solvent system at 298.15 K in this work and the data reported in Needham's work (x_A^{r})

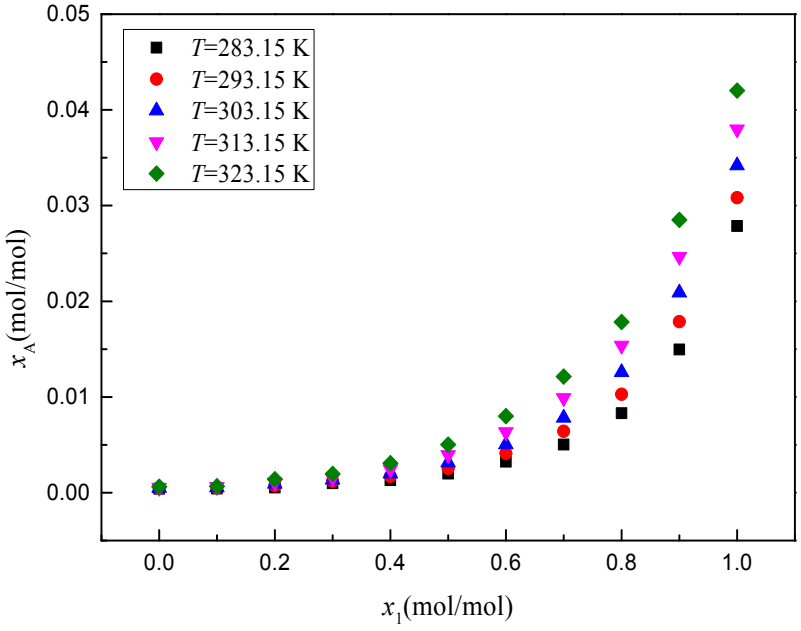

Figure S10. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water + methanol from 283.15 to 323.15 K (p = 0.1 MPa)

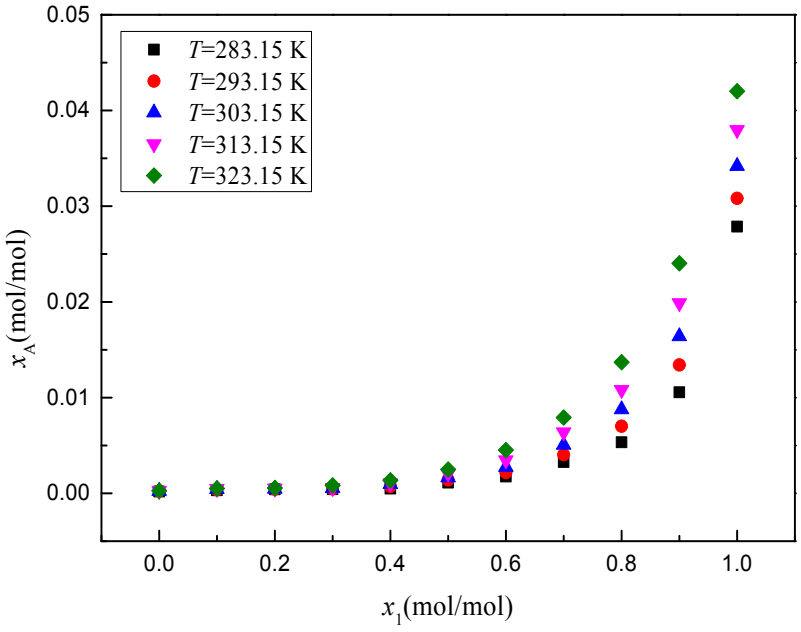

Figure S11. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water+ ethanol from 283.15 to 323.15 K (p = 0.1 MPa)

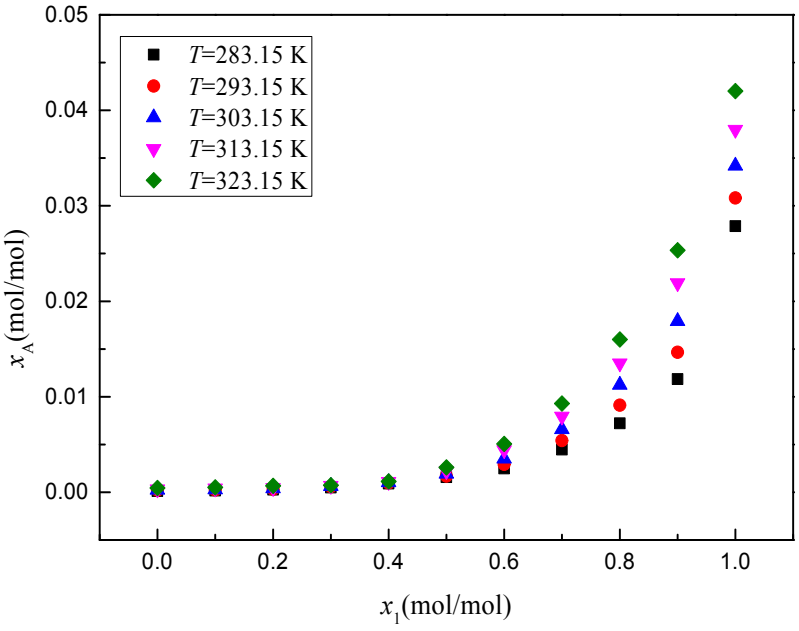

Figure S12. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water + 1-propanol from 283.15 to 323.15 K (p = 0.1 MPa)

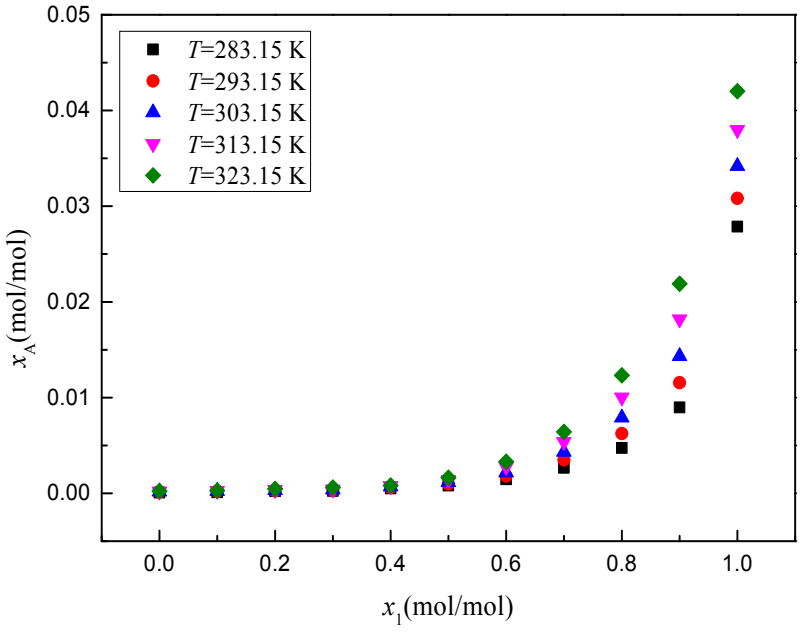

Figure S13. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water + 2-propanol from 283.15 to 323.15 K (p = 0.1 MPa)

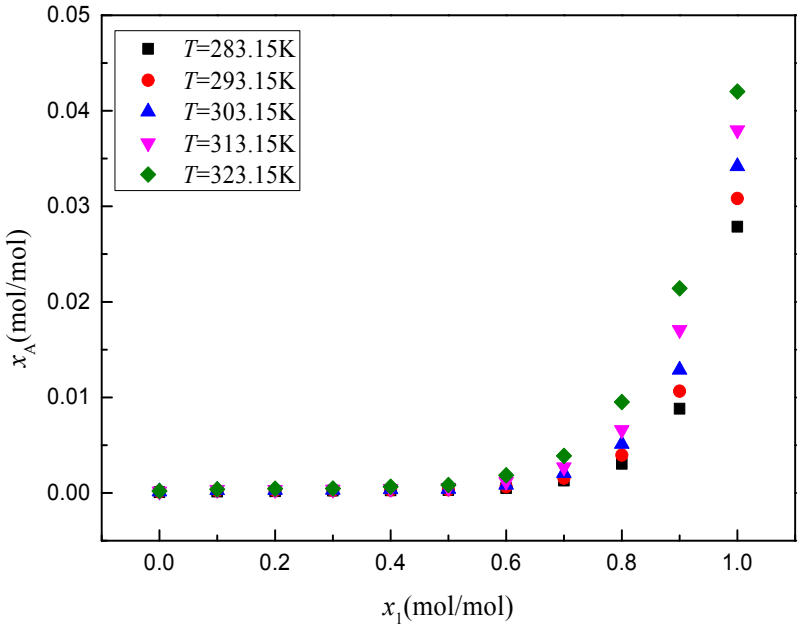

Figure S14. Experimental mole fraction solubility of L-alanine in the binary mixed solvent of water + acetone from 283.15 to 323.15 K (p = 0.1 MPa)

References Section

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