



Chemical Engineering Thermodynamics

Experimental measurement and thermodynamic modeling of binary and ternary solid–liquid phase equilibrium for the systems formed by L-arabinose, D-xylose and water[☆]

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ABSTRACT

Solid–liquid phase equilibrium data for binary (L-arabinose–water) and (D-xylose–water) systems at temperatures from (269.85–298.05) K and ternary (L-arabinose–D-xylose–water) system at temperatures of 273.85 K, 278.85 K and 284.45 K were measured at atmospheric pressure. The ternary phase diagrams of the systems were constructed on the base of the measured solubility. Two pure solid phases were formed at given temperatures, including pure L-arabinose and pure D-xylose, which were confirmed and determined by the method of Schreinemakers' wet residue. At the same temperature, the crystallization region of L-arabinose was larger than D-xylose's. The acquired solubility data were then correlated using the NRTL model, Wilson model and Xu model. The calculated solubility with the three models agreed well with the experimental values.

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1. Introduction

Research of hemicellulose is significant subject concerning the exploitation and the utilization of biomass resources. The hemicellulose can be used to produce several kinds of monosaccharide by dilute acid hydrolysis, enzymatic hydrolysis or other methods [1–3]. Due to the huge quantity and wide distribution, agricultural straw has been well studied. The hemicellulose in agricultural straw is hydrolyzed, mainly generating xylose and arabinose. Xylose can be put into producing xylitol, furfural, and other chemical products [4,5], while arabinose can be used to produce pharmaceutical intermediates of antiviral drugs [6], as a result of which, the separation and the purification of xylose and arabinose are of cardinal significance.

The method of crystallization separation is widely applied in the separation of the solid mixture. Crystallization separation is operated on account of solid–liquid equilibria data; therefore, the solid–liquid equilibria data of D-xylose–L-arabinose–water system is of great importance for the separation of D-xylose and L-arabinose. More studies about the ternary systems, formed by sugar and mixture solvent, have been reported in the literature [7,8]; nevertheless, studies about the

systems formed by two kinds of solid and water are common in water–salt system [9,10], and are rarely in water–sugar system as well. In this paper, the solubility of D-xylose and L-arabinose in water at different temperatures was determined by the refraction index method. The phase diagrams for D-xylose–L-arabinose–water are investigated by using the method of Schreinemakers' wet residue [11]. The experimental data were correlated with NRTL model [12], Wilson model [13], as well as Xu model [14].

2. Experimental

2.1. Materials

D-Xylose and L-arabinose were purchased from Shandong Longlive Bio-Technology Co., Ltd. (China). Redistilled deionized water was produced in our lab. The information of materials is listed in Table 1 in detail.

2.2. Apparatus and procedure of measurement

The solubility of pure D-xylose and L-arabinose in water was determined respectively by the refraction index (RI) analysis with an Abbe Refractometer (WAY-2S) at 298.15 K which was purchased from Shanghai Precision & Scientific Instrument Co., Ltd. China. The method

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Table 1

Sources and purity of the materials employed

Materials	Mass fraction purity/%	Sources	Analytical method	Density/kg·m ⁻³
D-Xylose	99.5	Shandong Longlive Bio-Technology Co., Ltd. (China)	HPLC ^①	1525 ^②
L-Arabinose	99.3	Shandong Longlive Bio-Technology Co., Ltd. (China)	HPLC ^①	1585 ^③

^① High-performance liquid chromatography.^② Taken from literature [15].^③ Taken from literature [16].

of isothermal saturation [17] was employed to control the ternary phase equilibria. Schreinemakers' wet residue method was employed to confirm the equilibrium composition of the solid. A standard digital refrigerated circulating bath (SD07R-20-A12E, Polyscience, America) was employed to keep the temperature of the system, which was offered by Polyscience Co., Ltd. America. An analytical balance (BSA124S-CW) was employed to govern the mass of the solute, solvent, equilibrium liquid and equilibrium wet solid, which was purchased from Sartorius Scientific Instruments Co., Ltd. China.

For the binary systems of D-xylose–water and L-arabinose–water, the experimental saturated solutions were prepared in a three-necked flask by adding excess D-xylose or L-arabinose into water. The concentration of D-xylose or L-arabinose at equilibrium in water at the different temperatures was controlled by the measurement of the refraction index (RI). The curve for D-xylose or L-arabinose mass percent as a function of the refraction index and D-xylose or L-arabinose solubility as a function of temperature was adjusted by the least square method [18]. With regard to ternary system of D-xylose–L-arabinose–water, the initial solution was prepared as a mixture of an excessive D-xylose and L-arabinose in the water, and the relevant amounts were chosen by changing the D-xylose/L-arabinose ratio from 0 to 1, and from 1 to 0 respectively. The liquor was stirred by an electric stirring at a constant temperature for no less than 40 h. The solution was extracted from the three-necked flask at 2 h interval using a plastic syringe with a 0.22 μm pore syringe filter precooled in standard digital refrigerated circulating bath and then analyzed by an Abbe Refractometer. The system was considered to achieve balance when the RI of the upper liquor was constant. And the compositions of the upper liquor and the wet solid were analyzed by HPLC (L-2000, Hitachi Limited, Japan) with a refractive index detector using an Aminex HPX-87P column (300 mm × 7.8 mm, Bio-Rad, America). The mobile phase was water, while the flow rate was 0.40 mL·min⁻¹. The column temperature was 358.15 K, and the temperature of the refractive index detector was 308.15 K. Compositions of various equilibrium liquor and wet solid were acquired by changing the ratio of D-xylose and L-arabinose. In this work, every experimental point was measured at least three times, and it is expressed by the average value at the same time. The relative standard uncertainty of the measured values based on the error analysis was less than 2.0% in mass fraction.

2.3. Melting properties of D-xylose and L-arabinose

The fusion enthalpy (ΔH_m) and the melting temperature (T_m) for D-xylose together with the L-arabinose, were determined with differential scanning calorimetry (Diamond DSC, PerkinElmer, America) under a nitrogen atmosphere [19,20]. About 2.0 mg samples were put in a closed DSC pan. The temperature was ranging from 293.15 to 573.15 K, and the heating rate was 5 K·min⁻¹. The standard uncertainty for melting temperature and fusion enthalpy is estimated to be 0.2 K and 2%, respectively.

3. Solid–Liquid Phase Equilibrium Modeling

In different models, the assumption for the standard state has diverse definitions. In the Xu model, the assumption for the standard state is put forward considering the solute in water as molecules. Under the conditions that the concentration of the solute is close to solubility, activity $a_i = m_i \times \gamma_i$ (m_i is molality, γ_i is activity coefficient) is close to 1 [14]. In the Wilson model and NRTL model, γ_i tends to 1 when the concentration of the solute tends to 0. And the equation for solid–liquid phase equilibrium is expressed as Eq. (1) on the basis of the activity coefficient [21,22].

$$\ln x_i = \frac{\Delta H_m}{R} \left(\frac{1}{T_m} - \frac{1}{T} \right) - \ln \gamma_i \quad (1)$$

where ΔH_m is the molar melting enthalpy, T_m is the melting temperature.

3.1. Xu model

Xu et al. [14] brought forward a new model, considering the solute in water as molecules, which is described as Eq. (2).

$$\ln \gamma_i = E_i + \sum_{j \neq i} (F_{i,j} m_j + G_{i,j} m_j^{0.5}) \quad (2)$$

$$E_i = pa_{i-1}T + pa_{i-2}T^{0.5} + pa_{i-3}/T \quad (3)$$

$$F_{i,j} = pb_{i-j}T + pc_{i-j}T^{k_i} \quad (4)$$

$$G_{i,j} = pd_{i-j}T + pe_{i-j}T^{k_i} \quad (5)$$

where k_i is the temperature parameter and which is taken as 0.5, pb_{i-j} , pc_{i-j} , pd_{i-j} and pe_{i-j} are solute–solute parameters, while pa_{i-1} , pa_{i-2} and pa_{i-3} are water–solute parameters [14].

3.2. Wilson model

The Wilson model [13] described the activity coefficient as Eq. (6).

$$\ln \gamma_i = - \ln \left(\sum_{j=1}^m x_j \Lambda_{ij} \right) + 1 - \sum_{k=1}^m \frac{x_k \Lambda_{ki}}{\sum_{j=1}^m x_j \Lambda_{kj}} \quad (6)$$

$$\Lambda_{ij} = \frac{v_j}{v_i} \exp \left(- \frac{\Delta \lambda_{ij}}{RT} \right) \quad (7)$$

where Λ_{ij} , Λ_{kj} and Λ_{ki} are the Wilson parameters. v_i is the molar volume of the component i . $\Delta \lambda_{ij}$ is the adjustable parameter which relates to the interaction energy.

3.3. NRTL model

The NRTL model [12] described the activity coefficient as Eq. (8).

$$\ln \gamma_i = \frac{\sum_{j=1}^m \tau_{ji} x_j G_{ji}}{\sum_{k=1}^m x_k G_{ki}} + \sum_{j=1}^m \frac{x_j G_{ij}}{\sum_{k=1}^m x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_{r=1}^m \tau_{rj} x_r G_{rj}}{\sum_{k=1}^m x_k G_{kj}} \right) \quad (8)$$

$$G_{ji} = \exp(-\alpha_{ji} \tau_{ji}) \quad (9)$$

$$\tau_{ji} = \frac{\Delta g_{ji}}{RT} \quad (10)$$

where $\tau_{ij} \neq \tau_{ji}$, $\tau_{ii} = 0$, and Δg_{ji} are constants which can be gained by regression from the experimental solubility data. No-random parameter $\alpha_{ij} = \alpha_{ji}$ is taken as 0.21.

4. Results and Discussion

4.1. Melting properties of D-xylose and L-arabinose

The values of T_m and melting enthalpy (ΔH_m) of D-xylose and L-arabinose are shown in Table 2. There is a little deviation in the T_m and melting enthalpy with the literatures in Table 2. The different measurement methods, the purity of D-xylose and L-arabinose, the diverse experimental environment or other factors may lead to deviations [23]. In this study, extrapolated onset value as T_m was adopted.

Table 2

The values of T_m and melting enthalpy of D-xylose and L-arabinose

Sources	Compound	T_m/K			$\Delta H_m/kJ \cdot mol^{-1}$
		Onset value	Extrapolated onset value	Peak value	
This work	D-Xylose	417.53	424.95	431.48	36.48
Roos' report ^①	D-Xylose	416.15	–	430.15	31.68
This work	L-Arabinose	418.90	431.59	436.39	39.56
Raemy's report ^②	L-Arabinose	408.15	–	428.15	39.03
Hou's report ^③	L-Arabinose	–	–	440.25	–

^① Taken from literature [24].

^② Taken from literature [25].

^③ Taken from literature [26].

4.2. Binary systems of D-xylose–water and L-arabinose–water

Experimental and calculated values of mass fraction solubility of pure D-xylose and L-arabinose in water are shown in Table 3. All the data points are average values belonging to three experimental measurements. The experimental mass fraction solubility of D-xylose in water at 298.05 K was 0.5523, while Gong *et al.* [27] found that the experimental mass fraction solubility of D-xylose in this same system at 298.2 K was 0.5680. The result is largely similar to the literature value.

From Table 3, we can know that the solubilities of D-xylose and L-arabinose in water increase with the temperature increasing. The solubility of D-xylose in water is larger than that of L-arabinose. D-Xylose and L-arabinose are isomers. The solubility of binary systems of D-xylose–water and L-arabinose–water is not the same owing to the different molecular structure that is shown in Fig. 1. The adjacent hydroxyl easily forms an intramolecular hydrogen bond. The ability to form intramolecular hydrogen bonds for L-arabinose is stronger than D-xylose, which is against the dissolution of L-arabinose in water. Furthermore, it is easier for D-xylose to form intermolecular hydrogen bonds with water than L-arabinose, which is conducive to the dissolution of D-xylose.

Table 3

Experimental and calculated values of mass fraction solubility for the binary systems of D-xylose–water and L-arabinose–water at different temperatures under atmospheric pressure^①

T/K	D-Xylose				T/K	L-Arabinose			
	Experimental values/%	Calculated values/%				Experimental values/%	Calculated values/%		
		Wilson	NRTL	Xu			Wilson	NRTL	Xu
269.85	40.91	40.67	41.00	40.75	270.05	29.47	28.21	29.94	29.77
273.85	42.78	43.41	42.98	43.02	273.90	31.26	30.44	31.43	31.61
278.85	45.76	45.71	45.63	45.78	278.85	34.16	32.66	33.33	33.95
283.35	48.21	47.96	47.98	48.17	283.75	36.21	36.02	35.71	36.22
284.45	48.73	48.60	48.55	48.74	284.45	36.38	36.69	36.11	36.54
287.75	50.49	50.19	50.28	50.42	288.75	38.26	39.57	38.32	38.48
293.00	53.06	52.88	53.04	52.98	293.55	40.55	42.48	40.83	40.57
298.05	55.23	55.78	55.74	55.32	298.05	42.61	45.33	43.33	42.47
RAD		0.0106	0.0071	0.0019			0.0511	0.0169	0.0053

^① The standard uncertainty of T is $u(T) = 0.02$ K. The standard uncertainty of the solubility measurement is $u(w) = 0.02$.

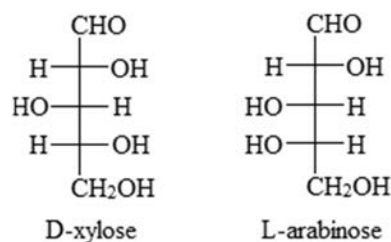


Fig. 1. Molecular structure of D-xylose and L-arabinose.

4.3. Ternary system of D-xylose–L-arabinose–water

According to the solubility of D-xylose and L-arabinose in water (Table 3), the higher the temperature, the greater the solubility. On the contrary, the lower the temperature, the smaller the solubility, so the more conducive to the crystallization of the material in solution. The study of the solid–liquid equilibrium system formed by D-xylose, L-arabinose and water at low temperatures (273.85, 278.85 and 284.45 K) can provide the theoretical basis for the crystallization separation of D-xylose and L-arabinose.

The solid–liquid phase equilibrium data at atmospheric pressure for the ternary system of D-xylose–L-arabinose–water at the temperatures of (273.85, 278.85 and 284.45) K are presented in Tables 4–6, respectively. Ternary phase diagrams are constructed according to the compositions of the liquid phase and solid phase, shown in Figs. 2–4 respectively.

S_a , S_b and S_c stand for the solubility of D-xylose in water at 273.85 K, 278.85 K, 284.45 K respectively. And S^*_a , S^*_b and S^*_c stand for the solubility of L-arabinose in water at the different temperatures. What is more, the points C_a , C_b and C_c stand for co-saturated ones of D-xylose and L-arabinose in the ternary system at different temperatures.

At different temperatures, S_aC_a , S_bC_b , S_cC_c , $S^*_aC_a$, $S^*_bC_b$ and $S^*_cC_c$ are the crystalline curves of pure solid of D-xylose, and L-arabinose in Figs. 2–4, respectively.

Composition points of equilibrium liquor, together with its corresponding equilibrium wet solid are connected along the curves S_aC_a , S_bC_b or S_cC_c . Moreover, extend the lines towards to the vertical axis, the intersection point of these lines is approximately the pure solid-phase component for D-xylose. Composition points of equilibrium liquor and its corresponding equilibrium wet solid are connected along the curves $S^*_aC_a$, $S^*_bC_b$ or $S^*_cC_c$. And then extend the lines towards to abscissa axis, the intersection point of these lines is approximately the pure solid-phase component for L-arabinose.

In Figs. 2–4, I_a , I_b and I_c are crystallization regions of D-xylose. II_a , II_b , and II_c are crystallization regions of L-arabinose. III_a , III_b and III_c are crystalline zones of D-xylose and L-arabinose mixture. IV_a , IV_b and IV_c are unsaturated regions.

Table 4
Experimental and calculated values of mass fraction solubility for the ternary system of D-xylose–L-arabinose–water at 273.85 K under atmospheric pressure^①

Experimental values/%			Calculated values/%					
Liquid phase		Solid phase	Wilson		NRTL		Xu	
D-Xylose	L-Arabinose		D-Xylose	L-Arabinose	D-Xylose	L-Arabinose	D-Xylose	L-Arabinose
42.78	0.00	D-X	43.41	–	42.98	–	43.02	–
41.03	3.03	D-X	41.61	–	41.01	–	41.13	–
39.19	6.85	D-X	38.97	–	38.58	–	38.89	–
36.77	10.59	D-X	37.47	–	36.10	–	36.77	–
35.10	13.85	D-X	35.66	–	34.01	–	34.91	–
32.91	17.69	D-X + L-a	34.02	17.60	31.51	18.69	32.78	17.74
25.85	20.25	L-a	–	20.15	–	21.52	–	20.03
19.33	22.41	L-a	–	23.15	–	24.32	–	22.31
12.41	24.78	L-a	–	26.62	–	27.23	–	24.91
5.12	28.05	L-a	–	29.50	–	29.88	–	28.01
0.00	31.54	L-a	–	30.44	–	31.43	–	31.59
RAD			0.0248		0.0405		0.0061	

^① D-X, D-xylose; L-a, L-arabinose. The standard uncertainty of T is $u(T) = 0.02$ K. The standard uncertainty of the solubility measurement is $u(w) = 0.02$.

Table 5
Experimental and calculated values of mass fraction solubility for the ternary system of D-xylose–L-arabinose–water at 278.85 K under atmospheric pressure^①

Experimental values/%			Calculated values/%					
Liquid phase		Solid phase	Wilson		NRTL		Xu	
D-Xylose	L-Arabinose		D-Xylose	L-Arabinose	D-Xylose	L-Arabinose	D-Xylose	L-Arabinose
45.76	0.00	D-X	45.71	–	45.63	–	45.78	–
44.62	1.44	D-X	45.28	–	44.65	–	44.82	–
43.20	4.52	D-X	42.85	–	42.66	–	42.98	–
41.64	7.06	D-X	41.55	–	40.99	–	41.51	–
37.98	12.67	D-X	39.29	–	37.28	–	38.39	–
36.90	15.30	D-X	37.39	–	35.59	–	36.86	–
34.67	19.08	D-X + L-a	35.81	18.69	33.11	18.97	34.78	19.23
32.83	19.50	L-a	–	19.70	–	19.95	–	19.89
26.40	21.85	L-a	–	22.29	–	22.73	–	22.10
20.36	23.91	L-a	–	25.30	–	25.49	–	24.29
14.56	26.22	L-a	–	27.98	–	27.94	–	26.48
8.51	28.75	L-a	–	30.88	–	30.48	–	28.96
4.44	31.29	L-a	–	31.73	–	31.81	–	30.81
0.00	34.16	L-a	–	32.66	–	33.33	–	33.95
RAD			0.0277		0.0288		0.0087	

^① D-X, D-xylose; L-a, L-arabinose. The standard uncertainty of T is $u(T) = 0.02$ K. The standard uncertainty of the solubility measurement is $u(w) = 0.02$.

Table 6
Experimental and calculated values of mass fraction solubility for the ternary system of D-xylose–L-arabinose–water at 284.45 K under atmospheric pressure^①

Experimental values/%			Calculated values/%					
Liquid phase		Solid phase	Wilson		NRTL		Xu	
D-Xylose	L-Arabinose		D-Xylose	L-Arabinose	D-Xylose	L-Arabinose	D-Xylose	L-Arabinose
48.73	0.00	D-X	48.60	–	48.55	–	48.74	–
45.26	6.20	D-X	44.51	–	44.42	–	44.99	–
42.24	11.08	D-X	42.06	–	41.19	–	42.28	–
39.63	16.30	D-X	38.77	–	37.71	–	39.35	–
36.81	20.82	D-X + L-a	37.06	19.46	34.76	19.03	36.94	20.83
29.96	23.35	L-a	–	22.26	–	22.20	–	23.29
25.03	25.20	L-a	–	24.52	–	24.54	–	25.11
18.17	27.88	L-a	–	27.93	–	27.81	–	27.74
10.88	30.89	L-a	–	31.73	–	31.25	–	30.69
0.00	36.38	L-a	–	36.69	–	36.11	–	36.54
RAD			0.0208		0.0305		0.0044	

^① D-X, D-xylose; L-a, L-arabinose. The standard uncertainty of T is $u(T) = 0.02$ K. The standard uncertainty of the solubility measurement is $u(w) = 0.02$.

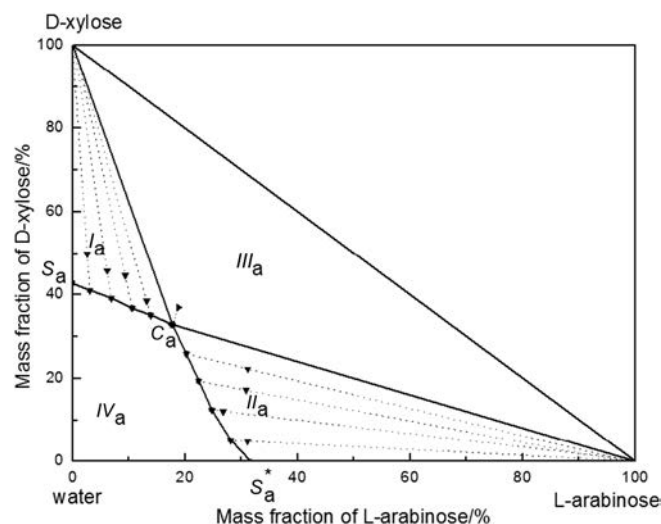


Fig. 2. Ternary phase diagram for system of D-xylose-L-arabinose-water at 273.85 K. I_a , crystalline zone of D-xylose; II_a , crystalline zone of L-arabinose; III_a , crystalline zone of D-xylose and L-arabinose mixture; IV_a , unsaturated zone; S_a , solubility of D-xylose in water at 273.85 K; S_a^* , solubility of L-arabinose in water at 273.85 K; C_a , co-saturated point of D-xylose and L-arabinose; ■, composition of equilibrium liquor; ▼, composition of equilibrium wet solid.

From Figs. 2–4 it can be seen that the unsaturated region increases along with temperature increasing ($IV_c > IV_b > IV_a$). The solubility of D-xylose and L-arabinose of the co-saturated composition points increases with temperature increasing. At the same temperature, the crystallization regions of L-arabinose are larger than D-xylose. The crystalline fields of D-xylose and L-arabinose in the solid-liquid phase equilibrium increase as the temperature decreases.

4.4. Correlations and calculations of solid-liquid phase equilibrium

The Wilson model, NRTL model and Xu model are employed to correlate the binary solid-liquid phase equilibrium systems of D-xylose-water and L-arabinose-water, as well as the ternary solid-liquid phase equilibrium system of D-xylose-L-arabinose-water at

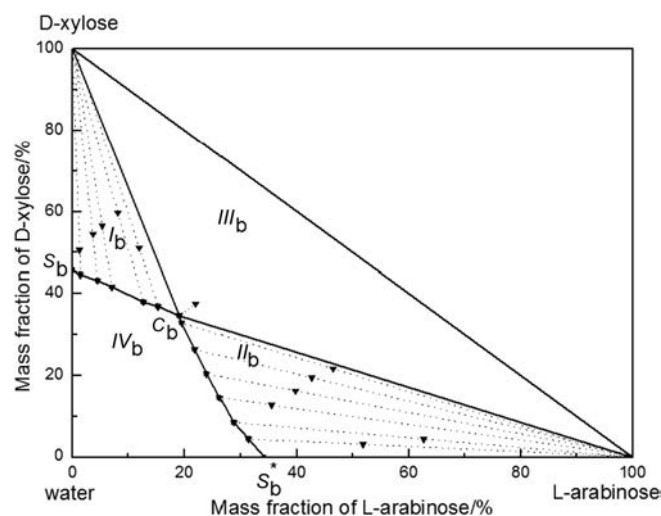


Fig. 3. Ternary phase diagram for system of D-xylose-L-arabinose-water at 278.85 K. I_b , crystalline zone of D-xylose; II_b , crystalline zone of L-arabinose; III_b , crystalline zone of D-xylose and L-arabinose mixture; IV_b , unsaturated zone; S_b , solubility of D-xylose in water at 278.85 K; S_b^* , solubility of L-arabinose in water at 278.85 K; C_b , co-saturated point of D-xylose and L-arabinose; ■, composition of equilibrium liquor; ▼, composition of equilibrium wet solid.

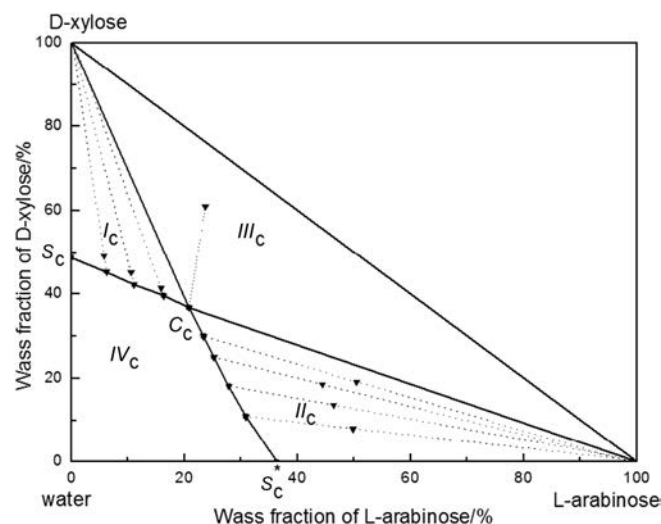


Fig. 4. Ternary phase diagram for system of D-xylose-L-arabinose-water at 284.45 K. I_c , crystalline zone of D-xylose; II_c , crystalline zone of L-arabinose; III_c , crystalline zone of D-xylose and L-arabinose mixture; IV_c , unsaturated zone; S_c , solubility of D-xylose in water at 284.45 K; S_c^* , solubility of L-arabinose in water at 284.45 K; C_c , co-saturated point of D-xylose and L-arabinose; ■, composition of equilibrium liquor; ▼, composition of equilibrium wet solid.

different temperatures. Binary interaction parameters of D-xylose-water and L-arabinose-water can be acquired by the regression method according to the measured solubility of binary systems formed by D-xylose + water or L-arabinose + water.

The binary interaction parameters for the two binary systems are listed in Tables 7 and 8 together with the root-mean-square deviations (RMSD) which is described Eq. (11):

$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^N (w_i^c - w_i)^2}{N}} \quad (11)$$

where N is the number of data points, w_i represents the experimental mass fraction solubility values, w_i^c represents the mass fraction solubility calculated.

The relative average deviation (RAD) is also applied to estimate the thermodynamic models, which is described as Eq. (12).

$$\text{RAD} = \frac{1}{N} \sum_{i=1}^N \left| \frac{w_i - w_i^c}{w_i} \right| \quad (12)$$

The calculated solubility of D-xylose in water and L-arabinose in water at different temperatures according to the model parameters, and the RAD values are calculated and presented in Table 3. The values of RAD are not more than 0.0511. In general, the three models provide better results for the two binary systems.

The values for binary interaction parameters of D-xylose-L-arabinose and the RMSD values are acquired and also shown in Tables 7 and 8 according to the binary interaction parameters of D-xylose-water and L-arabinose-water, and the solubility data of the ternary system of D-xylose-L-arabinose-water at different temperatures. The calculated mass fraction solubility of the ternary system of D-xylose-L-arabinose-water at different temperatures is shown in Tables 4–6. The values of RAD of mass fraction solubility calculated using the Xu model, Wilson model and NRTL model according to the experimental values of D-xylose-L-arabinose-water are all not more than 0.0405 at temperatures of 273.85 K, 278.85 K and 284.45 K. In Tables 7 and 8, the RMSD values for the Wilson model, NRTL model and Xu model are 0.910×10^{-2} , 1.15×10^{-2} and 0.241×10^{-2} , respectively. In accordance with the analysis of RAD values and RMSD values of the three models, it can be seen that the three models all supply satisfying results

Table 7

The regressed binary interaction parameters of the NRTL model and Wilson model for the ternary D-xylose–L-arabinose–water system

Parameter	<i>i</i>	<i>j</i>	Wilson		RMSD $\times 10^{-2}$	NRTL		RMSD $\times 10^{-2}$
			$\Delta\lambda_{ij} \times 10^3$	$\Delta\lambda_{ji} \times 10^3$		$\Delta g_{ij} \times 10^3$	$\Delta g_{ji} \times 10^5$	
Sugar–water	Xylose	Water	−4.623	−0.292	0.348	−9.325	0.135	0.239
	Arabinose	Water	1.957	−1.203	1.480	−9.498	0.200	0.482
Sugar–sugar	Xylose	Arabinose	−5.409	−1.839	0.910	−5.927	5.215	1.150

Table 8

The regressed binary interaction parameters of the Xu model for the ternary D-xylose + L-arabinose + water system

<i>i</i>	<i>j</i>	Sugar–water parameters			RMSD $\times 10^{-2}$	Sugar–sugar parameters			RMSD $\times 10^{-2}$
		$Pa_{i-1} \times 10^{-2}$	Pa_{i-2}	$Pa_{i-3} \times 10^3$		$Pb_{i-j} \times 10^{-4}$	$Pc_{i-j} \times 10^{-2}$	$Pd_{i-j} \times 10^{-3}$	$Pe_{i-j} \times 10^{-1}$
Xylose	Arabinose	2.819	−0.939	1.701	0.115	−58.660	9.986	0.852	−0.133
Arabinose	Xylose	3.449	−1.050	1.863	0.213	0.502	−0.160	−9.762	1.700

for the ternary system. As a consequence, the Wilson model, NRTL model and Xu model can all be employed to correlate and evaluate the ternary D-xylose–L-arabinose–water system at different temperatures.

5. Conclusions

Solid–liquid equilibria data for binary (L-arabinose–water) system and (D-xylose–water) systems at temperatures from 269.85 to 298.05 K and ternary (L-arabinose–D-xylose–water) system at temperatures of 273.85 K, 278.85 K and 284.45 K were measured at atmospheric pressure. Based on the measured solubility, three ternary phase diagrams were constructed. For the ternary system of L-arabinose–D-xylose–water, the pure solids were determined by Schreinemakers' wet residue method. The solubility of D-xylose and L-arabinose in water increases along with the temperature increasing. The co-saturated composition points move upward with the temperature increasing. The crystallization region of L-arabinose was larger than that of D-xylose at each temperature.

The obtained solubility data in water were correlated and evaluated using the NRTL model, Wilson model, and Xu model. The interaction parameters for L-arabinose–D-xylose were acquired. The calculated solubility using the three models agreed well with the experimental ones at given temperatures.

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