

Modeling of water activity, oxygen solubility and density of sugar and sugar alcohol solutions

Peijun Ji^a, Wei Feng^{b,*}, Tianwei Tan^b, Danxing Zheng^a

^a College of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029, China

^b College of Life Science and Technology, Beijing University of Chemical Technology, Beijing 100029, China

Received 6 September 2006; received in revised form 6 October 2006; accepted 3 December 2006

Abstract

Water activity, oxygen solubility and density of aqueous solutions of sugar and sugar alcohols have been modeled with the statistical associating fluid theory (SAFT). The modeling is accomplished by extending the previously developed method to determine the SAFT parameters for sugar and sugar alcohols. For the aqueous solutions of sorbitol/water, xylitol/water, mannitol/water, xylitol/sorbitol/water and xylitol/mannitol/water, the water activity has been predicted. The solubilities of oxygen in water and in aqueous solutions of glucose/water, fructose/water, sucrose/water, maltose/water and mannitol/water have been modeled. The density predictions for mannitol/sucrose/water, mannitol/sorbitol/water and mannitol/sorbitol/sucrose/water have been carried out. All the modeling results show that, by using the previously developed method to determine the SAFT parameters, the SAFT model has been able to model the water activity, oxygen solubility and density with very good accuracy, and the SAFT model can be taken as a suitable tool for describing sugar and sugar containing solutions.

© 2007 Elsevier Ltd. All rights reserved.

Keywords: Sugar; Sugar alcohol; Water activity; Oxygen solubility; Density; SAFT

1. Introduction

Aqueous solutions of sugars and sugar alcohols are of practical importance in food chemistry and technology, and the sugar industry (Gros & Dussap, 2003; Starzak & Mathlouthi, 2006). Sugar alcohols like xylitol, mannitol, and sorbitol are used in many processed foods, such as hard candies, cookies, chewing gums, and soft-drinks because they have little effect on blood sugar levels. In the design of equipment and processes for producing products from raw materials, reliable data on the equilibrium properties of materials, for example, water activity, oxygen solubility, and density of multicomponent solutions, are required. Due to the difficulty of measurement, the availability of experimental data is limited, and cannot satisfy the engineering demand. It is necessary to develop a prac-

tical method to estimate physical properties of aqueous solutions involving various sugars and sugar alcohols.

Among the thermodynamic models, the statistical associating fluid theory (SAFT) (Chapman, Gubbins, Jackson, & Radosz, 1989; Chapman, Gubbins, Jackson, & Radosz, 1990; Huang & Radosz, 1990) are versatile tools for describing phase behavior and phase equilibrium, and have been applied to a wide variety of fluids (Muller & Gubbins, 2001). In the previous work (Feng, van der Kooi, & De Swaan Arons, 2005), through developing a new method to determine the SAFT parameters for sugars, the SAFT model has been applied to describe the sugar solubility in water and mixed solvents.

This work is emphasized on the application of the SAFT equation of state (Huang & Radosz, 1990) to aqueous solutions of sugars and sugar alcohols. The water activity, oxygen solubility, and density of aqueous solutions of sugars and sugar alcohols will be described by the SAFT model through extending the previously developed method to

* Corresponding author. Tel.: +86 10 64446249; fax: +86 10 51370732.
E-mail address: fengwei@mail.buct.edu.cn (W. Feng).

Nomenclature

a	Helmholtz energy
D_{ij}	square-well energy constants in Eq. (2)
$g(d)^{\text{hs}}$	hard sphere distribution function
k	Boltzmann constant
k_{ij}	binary interaction parameter in Eq. (11)
m	segment number
M	molarity
N_{AV}	Avogadro's number
N^{ass}	number of association sites on a molecule
P	pressure
R	gas constant
t	temperature (°C)
T	temperature (K)
u/k	temperature-dependent dispersion energy of interaction between segments (K)
u^0/k	temperature-independent dispersion energy of interaction between segments (K)
V	molar volume (cm ³ /mol)
v^0	temperature-dependent segment volume (cm ³ /mol)
v^{00}	temperature-independent segment volume (cm ³ /mol)
X^A	mole fraction of molecules not bonded at site A

Greek symbols

κ^{AB}	volume of interaction between sites A and B
Δ^{AB}	strength interaction between sites A and B
ε^{AB}/k	association energy interaction between sites A and B
η	reduced density
ρ	density
τ	constant, $\sqrt{2\pi}/6$
μ_i	chemical potential of component i
μ_i^0	chemical potential of component i at standard state
α	α phase
β	β phase

Superscripts

res	residual
seg	segment
assoc	association

Subscripts

c	critical
B	boiling point

determine the SAFT parameters for sugar and sugar alcohols.

2. Revisit of statistical associating fluid theory (SAFT) equation of state

The SAFT equation of state applied is the version of Huang and Radosz (1990). The general expression for the residual Helmholtz energy is given by

$$a^{\text{res}} = a^{\text{seg}} + a^{\text{chain}} + a^{\text{assoc}}, \quad (1)$$

a^{res} is the residual Helmholtz energy, defined as $a^{\text{res}}(T, V, N) = a(T, V, N) - a^{\text{ideal}}(T, V, N)$, where $a(T, V, N)$ and $a^{\text{ideal}}(T, V, N)$ are the total Helmholtz energy per mole and the ideal gas Helmholtz energy per mole at the same temperature and density.

$$\frac{a^{\text{seg}}}{RT} = m \left(\frac{4\eta - 3\eta^2}{(1 - \eta)^2} + \sum_i \sum_j D_{ij} \left[\frac{u}{kT} \right]^i \left[\frac{\eta}{\tau} \right]^j \right), \quad (2)$$

a^{seg} represents segment–segment interactions, i.e., hard sphere and mean-field interactions. D_{ij} is the square-well energy constants, η reduced density, m segment number, u/k temperature-dependent dispersion energy of interaction between segments, R gas constant, τ constant ($\sqrt{2\pi}/6$), T temperature.

$$\frac{a^{\text{chain}}}{RT} = (1 - m) \ln \frac{1 - 0.5\eta}{(1 - \eta)^3}, \quad (3)$$

a^{chain} is due to the presence of covalent chain-forming bonds among the segments.

$$\frac{a^{\text{assoc}}}{RT} \sum_A \left[\ln X^A - \frac{X^A}{2} \right] + \frac{1}{2} N^{\text{ass}}, \quad (4)$$

a^{assoc} accounts for site-site specific interactions among the segments, for example, hydrogen-bonding interactions. X^A is the mole fraction of molecules not bonded at site A , N^{ass} number of association sites on a molecule.

The mole fraction of molecules not bonded at site A is expressed as

$$X^A = \left[1 + N_{\text{AV}} \sum_B \rho X^B \Delta^{AB} \right]^{-1}, \quad (5)$$

where N_{AV} is Avogadro's number, ρ density, and Δ^{AB} , the association strength, is expressed as

$$\Delta^{AB} = g(d)^{\text{hs}} [\exp(\varepsilon^{AB}/kT) - 1] (\sigma^3 \kappa^{AB}), \quad (6)$$

$g(d)^{\text{hs}}$ is hard sphere distribution function, $g(d)^{\text{hs}} = (1 - 0.5\eta)/(1 - \eta)^3$, ε^{AB}/k association energy interaction between sites A and B , κ^{AB} volume of interaction between sites A and B , σ Lennard-Jones segment diameter calculated by $\sigma = (6\tau v^{00}/\pi N_{\text{AV}})^{1/3}$, and v^{00} the segment volume.

For the explanation of association site, the detailed description for alcohols as an example by Huang and Radosz (1991) is cited here “each hydroxylic group (OH) in alkanols, in principle, has three association sites, labeled A and B on oxygen and C on hydrogen. The association

strength Δ due to the like, oxygen–oxygen or hydrogen–hydrogen (AA , AB , BB , and CC) interactions is assumed to be equal to zero. The only non-zero Δ is due to the unlike (AC and BC) interactions, which are considered to be equivalent”.

In the above expressions, the reduced density is calculated by

$$\eta = \tau \rho m v^{00} \left[1 - C \exp \left[\frac{-3u^0}{kT} \right] \right]^3, \quad (7)$$

where, $v^{00}(1 - C \exp(-3u^0/kT))^3$ is the segment molar volume in a close-packed arrangement, which is based on the work of Chen and Kreglewski (1977), and the integration constant C is set to 0.12. The temperature-dependent dispersion energy of interaction between segments, u/k , is expressed as

$$\frac{u}{k} = \frac{u^0}{k} \left[1 + \frac{e}{kT} \right], \quad (8)$$

where e/k is a constant that was related to Pitzer’s acentric factor and the critical temperature (Chen & Kreglewski, 1977; Kreglewski, 1984) for various molecules. As the energy parameter is for segments, $e/k = 10$ for all the molecules. But for oxygen, according to Chen and Kreglewski (1977, 1984), $e/k = 0$.

For each fluid, three parameters are needed for a non-associating component, segment number, m , segment volume, v^{00} , and segment–segment interaction energy, u^0/k . And two additional parameters are needed for an associating component, the association energy ε^{AB}/k and volume κ^{AB} .

For mixtures, the following mixing rule (Huang & Radosz, 1991) is used

$$\frac{u}{k} = \frac{\sum_i \sum_j X_i X_j m_i m_j \left[\frac{u_{ij}}{kT} \right] (v^0)_{ij}}{\sum_i \sum_j X_i X_j m_i m_j (v^0)_{ij}}, \quad (9)$$

where

$$(v^0)_{ij} = \left[\frac{1}{2} \left[(v^0)_i^{1/3} + (v^0)_j^{1/3} \right] \right]^3, \quad (10)$$

$$\frac{u_{ij}}{k} = (1 - k_{ij}) \left(\frac{u_i}{k} \frac{u_j}{k} \right)^{1/2}. \quad (11)$$

Water activity can be calculated by

$$a_i = \exp \left(\frac{\mu_i - \mu_i^0}{RT} \right). \quad (12)$$

Phase equilibrium calculation can be carried out by applying Eq. (13):

$$\mu_i^\alpha = \mu_i^\beta. \quad (13)$$

3. Determination of the SAFT parameters for sugar and sugar alcohols

The parameters of the SAFT model are generally determined using the data of saturated vapor pressure and liquid

density (Huang & Radosz, 1990). However, this approach cannot be applied to sugars and sugar alcohols, as this kind of data cannot be obtained for sugars and sugar alcohols. In this work, the new method (Feng et al., 2005) previously developed is extended to determine the SAFT parameters for sugars and sugar alcohols. Here, we again give a description of parameter determination.

For describing sugars and sugar alcohols, five parameters are required by the SAFT model. There are three steps for the parameter determination. First, both the parameters segment volume v^{00} and association volume κ^{AB} are set to a value, the parameters of m , u^0/k , and ε^{AB}/k are taken as the three variables in Eqs. (14)–(16) (the three equations are expressed by the SAFT model), which are the pressure at the critical temperature T_C , the first derivative of pressure with respect to density at T_C , P_C and V_C , the second derivative of pressure with respect to density at T_C , P_C and V_C , respectively. By making use of the critical properties of temperature, pressure and volume, the three equations can be solved, and then the parameters of m , u^0/k , and ε^{AB}/k are determined. Second, with the five parameters (three of them are determined mentioned above), the SAFT model is used to calculate normal boiling temperature. If the normal boiling temperature is calculated correctly, then we say the early value given to the parameter κ^{AB} is the correct one. Otherwise, κ^{AB} is adjusted to a new value, and the above procedures (first and second steps) are repeated until the normal boiling temperature is calculated correctly. Third, with the above five parameters (four of them have been obtained through the determination steps) the SAFT model is used to calculate density of sugar or sugar alcohol at room temperature and atmospheric pressure. If the density is calculated with a small deviation from the crystal density of the sugar or sugar alcohol at room temperature (the crystal density is taken as a reference density of the sugar or sugar alcohol assumed to be in an amorphous state at room temperature), then the early value given to the parameter v^{00} is the correct one. Otherwise, the parameter v^{00} is set to a new value, and the procedures of parameter determination mentioned above are repeated. In this way, the five parameters of the SAFT model are determined finally.

$$P|_{T_C} = P_C, \quad (14)$$

$$\left[\frac{\partial P}{\partial \rho} \right]_{T_C} = 0, \quad (15)$$

$$\left[\frac{\partial^2 P}{\partial \rho^2} \right]_{T_C} = 0. \quad (16)$$

For sugars and sugar alcohols, critical temperature, pressure, and density, as well as the normal boiling temperature are estimated using Joback’s modification of Lydersen’s method (Reid, Prausnitz, & Poling, 1987), as shown in Eqs. (17)–(20).

$$T_C = T_B \left[0.584 + 0.965 \sum \Delta T - \left(\sum \Delta T \right)^2 \right]^{-1}, \quad (17)$$

$$P_C = \left[0.113 + 0.0032n_A - \sum \Delta P \right]^{-2}, \quad (18)$$

$$V_C = 17.5 + \sum \Delta V, \quad (19)$$

$$T_B = 198 + \sum \Delta b. \quad (20)$$

How to calculate ΔT , ΔP , ΔV and Δb has been described in detail elsewhere (Reid et al., 1987).

On the basis of the group contribution method the molecular structure information, the critical properties of temperature, pressure, and volume as well the normal boiling temperatures have been estimated and the values are listed in Table 1. Using the method of parameter determination described above, the SAFT parameters for sugar and sugar alcohols have been determined and are listed in Table 2.

4. Prediction of water activity of aqueous solutions of sugar alcohols

With the SAFT model, the prediction of water activity is carried out using the SAFT parameters of individual components listed in Table 2. For binary aqueous solutions mannitol/water, sorbitol/water, and xylitol/water, the predicted water activity has been shown in Figs. 1–3, respectively. Figs. 4 and 5 present the predicted water activity of ternary aqueous solutions xylitol/sorbitol/water and xylitol/mannitol/water, respectively.

Table 1
Critical properties and normal boiling points

Substance	T_C (K)	P_C (bar)	V_C (cm ³ mol ⁻¹)	T_b (K)
Sucrose	1309.79	46.26	782.5	1030.18
Mannitol	698.80	46.40	479.5	568.15 ^a
Xylitol	759.66	48.97	407.5	620.03
Sorbitol ^b	868.00	46.40	483.0	704.00

^a From the web <<https://fscimage.fishersci.com>>.

^b From Daubert and Danner (1989).

Table 2
The parameters of the SAFT equation

Substance	m	u/k (K)	v^{00} (cm ³ /mol)	ε^{AB} (K)	κ^{AB}	N^{ass}
Fructose ^a	5.026	215.67	12.0	7867	0.00025	4
Glucose ^a	5.238	199.18	12.0	7654	0.0007	4
Sucrose ^b	2.583	206.054	55.0	7297.70	0.0055	6
Mannitol ^b	4.872	178.400	14.0	5022	0.001	6
Sorbitol ^b	4.096	189.526	16.0	0.0014	7295.76	4
Xylitol ^b	5.160	168.173	10.0	0.0009	6841.89	4
Water ^a	1.165	194.29	8.0	3229	0.052	3
Oxygen ^b	1.362	124.94	11.19	0	0	0

N^{ass} is number of association sites. For fructose, glucose, sorbitol, mannitol and xylitol, the four association sites are distributed on two OH groups, each has one site on oxygen and one site on hydrogen; for sucrose, the six association sites are distributed on three OH groups, each has one site on oxygen and one site on hydrogen; for water, two sites on oxygen and one site on hydrogen.

^a From Feng et al. (2005).

^b This work.

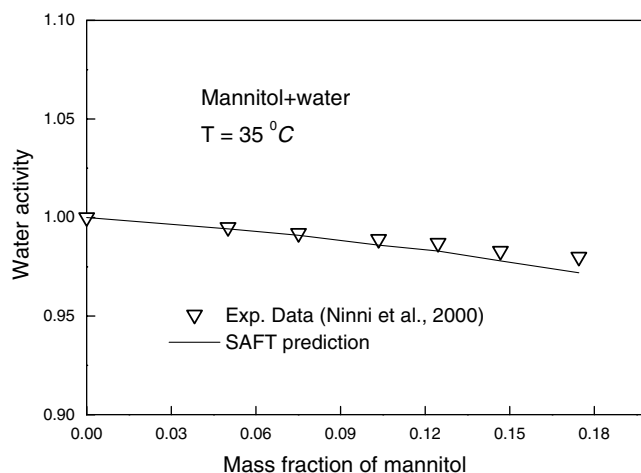


Fig. 1. Water activity of mannitol/water. The solid line is predicted by SAFT. (See above-mentioned references for further information.)

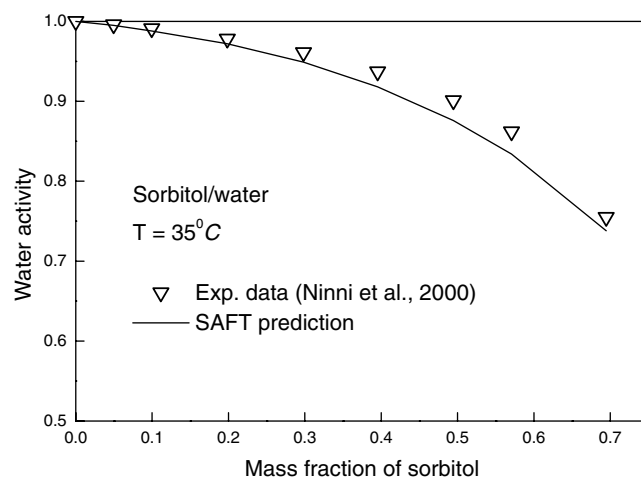


Fig. 2. Water activity of sorbitol/water. The solid line is predicted by SAFT.

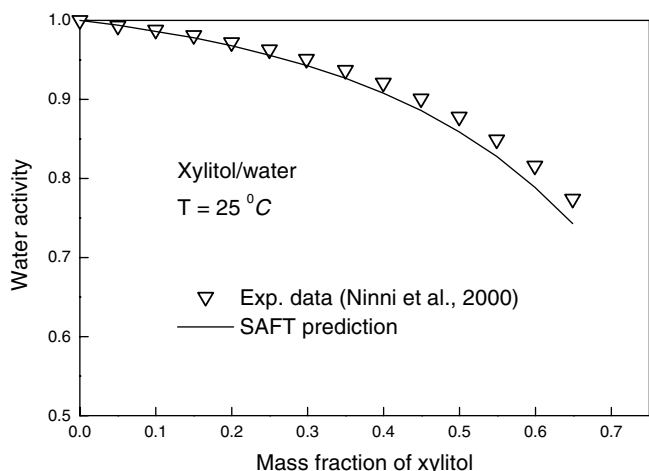


Fig. 3. Water activity of xylitol/water. The solid line is predicted by SAFT.

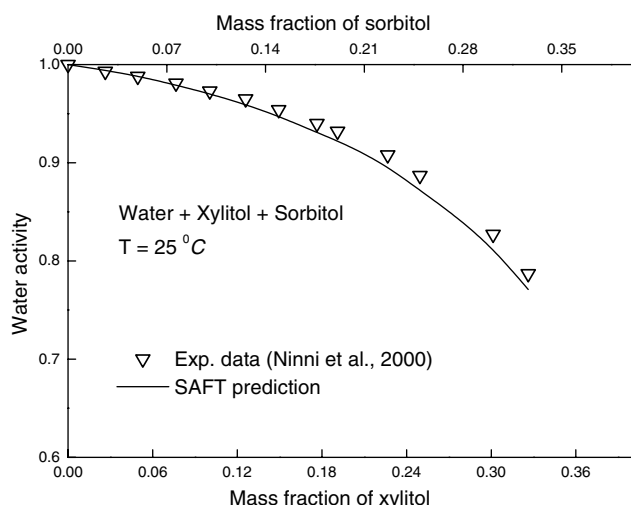


Fig. 4. Water activity of xylitol/sorbitol/water. The solid line is predicted by SAFT.

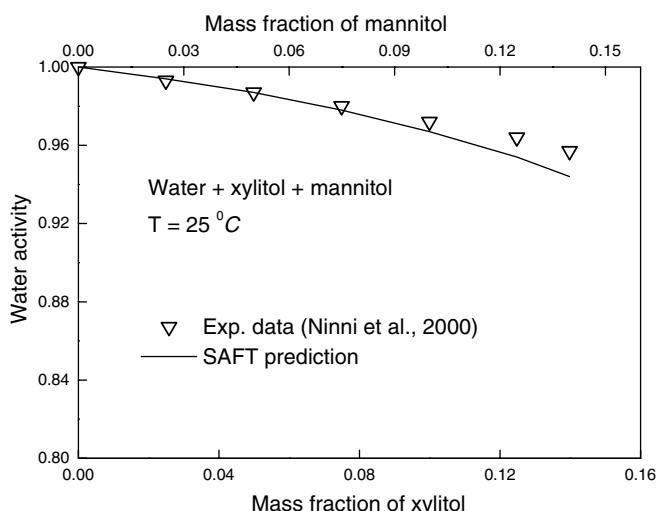


Fig. 5. Water activity of xylitol/mannitol/water. The solid line is predicted by SAFT.

5. Modeling of oxygen solubility in pure water and in aqueous solutions

5.1. Oxygen solubility in pure water

For oxygen, the SAFT parameters are determined based on the data of saturated liquid density and vapor pressure (Daubert & Danner, 1989). The obtained parameters are listed in Table 2. The saturated liquid density and vapor pressure are reproduced very well as shown in Figs. 6 and 7, respectively. The average relative deviation of the calculation of the saturated liquid density is 1.35%, and that of the saturated vapor pressure 2.01%.

Fig. 8 presents the oxygen solubility in pure water at atmospheric pressure and in the temperature range of 0–40 °C, the line showing good agreement with the data is correlated by the SAFT model. A temperature-dependent function of binary interaction parameter is needed.

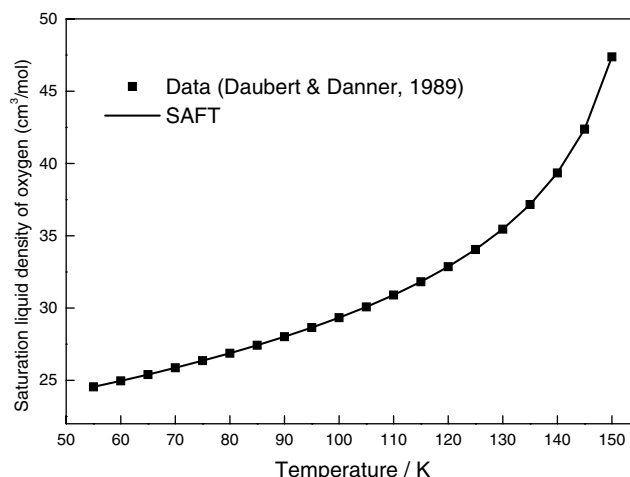


Fig. 6. Reproducing the data of saturated liquid density of oxygen by SAFT.

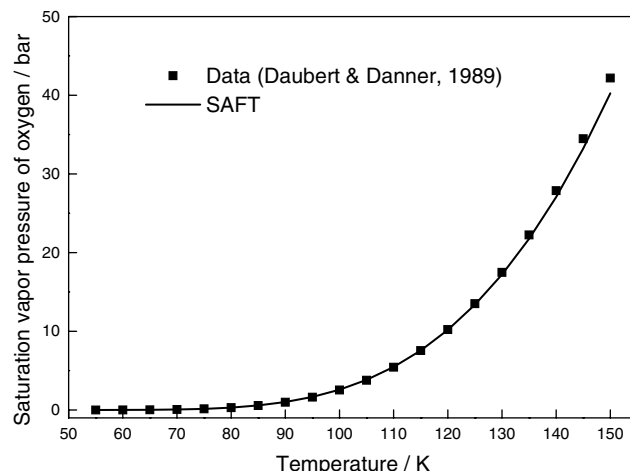


Fig. 7. Reproducing the data of saturated vapor pressure of oxygen by SAFT.

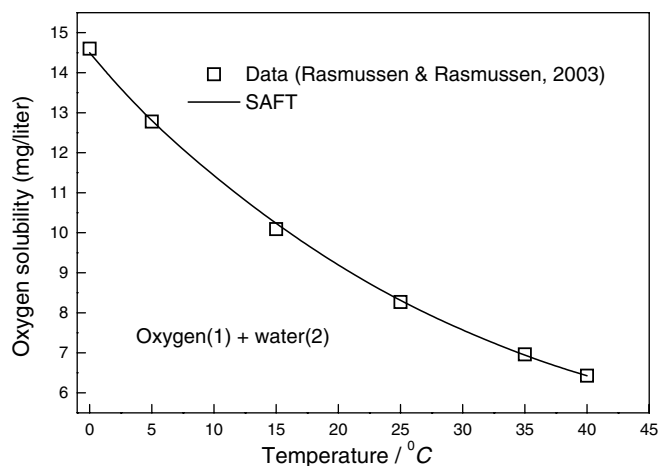


Fig. 8. Oxygen solubility in water. The line is correlated by SAFT. The binary interaction parameter function $k_{12} = 0.29317 + 4.457 \times 10^{-3}T$ ($^{\circ}\text{C}$) is used. (See above-mentioned references for further information.)

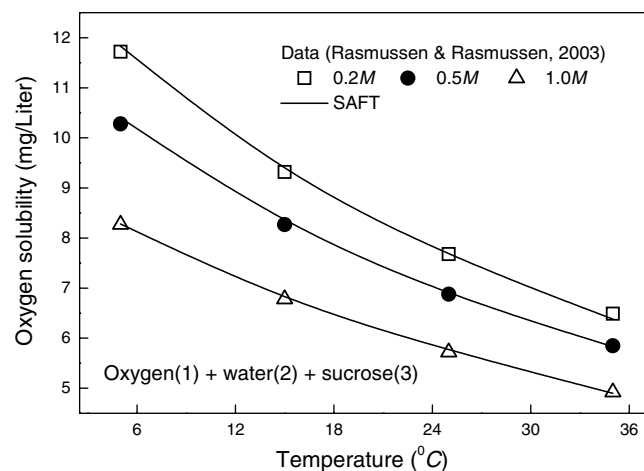


Fig. 11. Oxygen solubility in the aqueous solution of sucrose/water. The lines are calculated by SAFT. The binary interaction parameter functions $k_{12} = 0.29317 + 4.457 \times 10^{-3}T$ ($^{\circ}\text{C}$) and $k_{13} = 0.49 + 0.22M$ are used. M is the molarity of sucrose.

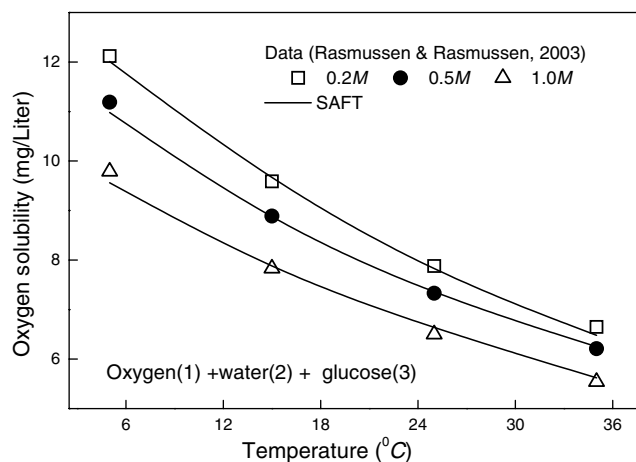


Fig. 9. Oxygen solubility in the aqueous solution of glucose/water. The lines are calculated by SAFT. The binary interaction parameter function $k_{12} = 0.29317 + 4.457 \times 10^{-3}T$ ($^{\circ}\text{C}$) and the binary interaction parameter $k_{13} = -0.4$ are used. M is the molarity of glucose.

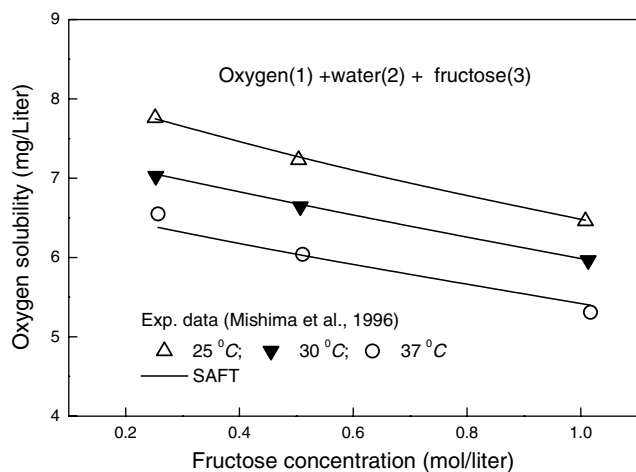


Fig. 10. Oxygen solubility in the aqueous solution of fructose/water. The lines are calculated by SAFT. The binary interaction parameter function $k_{12} = 0.29317 + 4.457 \times 10^{-3}T$ ($^{\circ}\text{C}$) and the binary interaction parameter $k_{13} = 0.7$ are used. (See above-mentioned references for further information.)

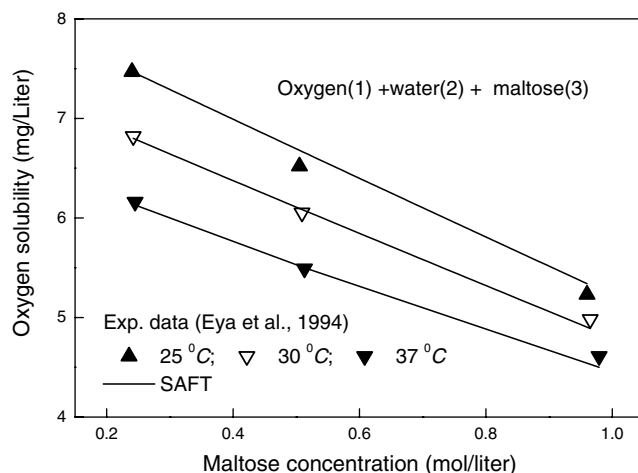


Fig. 12. Oxygen solubility in the aqueous solution of maltose/water. The lines are calculated by SAFT. The binary interaction parameter functions $k_{12} = 0.29317 + 4.457 \times 10^{-3}T$ ($^{\circ}\text{C}$) and $k_{13} = 0.3555 + 0.1632M$ are used. M is the molarity of maltose. (See above-mentioned references for further information.)

5.2. Oxygen solubility in aqueous solutions of sugars and sugar alcohols

Compared to in water, the oxygen solubility in aqueous solutions of sugars is decreased with sugar concentration and temperature. As shown in Figs. 9–12, in the temperature range of 5–37 $^{\circ}\text{C}$ and sugar-concentration range of 0.2 M–1.0 M, the data of oxygen solubility have been reproduced well by the SAFT model. When carrying on the modeling, the function of binary interaction parameter for oxygen/water obtained in Fig. 8 is applied throughout. For oxygen/water/glucose and oxygen/water/fructose, the binary interaction parameters $k_{13} = -0.4$ between oxygen and glucose and $k_{13} = 0.7$ between oxygen and fructose are needed; for oxygen/water/sucrose and oxygen/water/maltose, the sugar-concentration-dependent functions of binary interaction parameter between oxygen and sugars

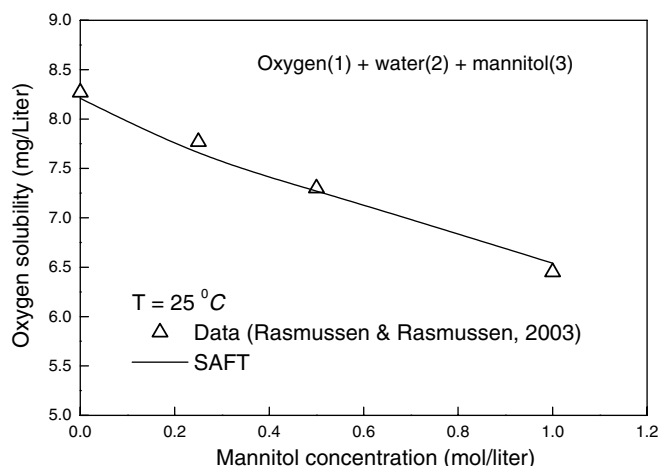


Fig. 13. Oxygen solubility in the aqueous solution of mannitol/water. The lines are calculated by SAFT. The binary interaction parameter function $k_{12} = 0.29317 + 4.457 \times 10^{-3}T$ ($^{\circ}\text{C}$) and the binary interaction parameter $k_{13} = 0.75$ are used.

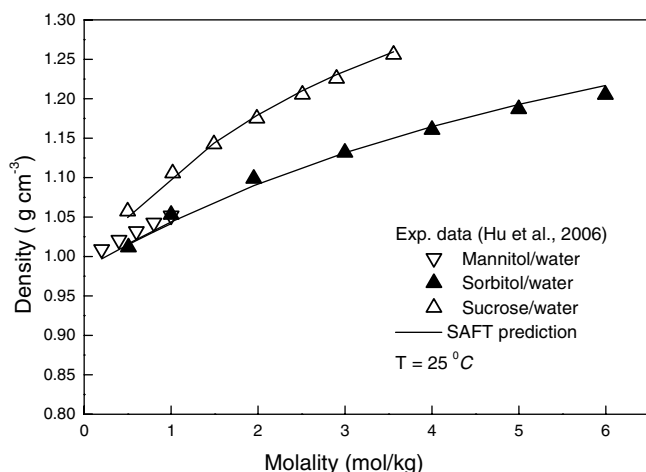


Fig. 14. Density of mannitol/water, sorbitol/water and sucrose/water at 25 $^{\circ}\text{C}$. The lines are predicted by SAFT.

are used. Fig. 13 presents the calculations of oxygen solubility in the aqueous solution of mannitol at 25 $^{\circ}\text{C}$, like in aqueous solutions of sugars, the function of binary interaction parameter for oxygen/water is applied, and the binary interaction parameter $k_{13} = 0.75$ between oxygen and mannitol is used.

6. Prediction of density of aqueous solutions of sugar and sugar alcohol

Fig. 14 presents the results of density prediction of mannitol/water, sorbitol/water and sucrose/water at 25 $^{\circ}\text{C}$. The lines are predicted by SAFT, which are in good agreement with the experimental data. Table 3 lists the results of density prediction of mannitol/sucrose/water, the largest relative deviation of density prediction is 1.12%, and the average relative deviation is 0.72%. The density of mannitol/sorbitol/water is also predicted well, as shown in Table 4, with an average relative deviation

Table 3
Density prediction by the SAFT model for mannitol + sucrose + water at 25 $^{\circ}\text{C}$

Molality (mol/kg)		Density (g/cm^3)		Relative deviation (%)
Mannitol	Sucrose	Experimental ^a	Predicted	
0.1008	0.0499	1.00912	0.99779	1.12
0.1285	0.0608	1.01251	1.00098	1.14
0.1208	0.25021	1.03525	1.02556	0.94
0.1588	0.30601	1.04337	1.03457	0.84
0.3186	0.15891	1.03483	1.02493	0.96
0.2589	0.25021	1.04204	1.03308	0.86
0.3016	0.30601	1.05017	1.04209	0.77
0.4218	0.19851	1.04446	1.03544	0.86
0.5104	0.11671	1.04006	1.03010	0.96
0.3895	0.23721	1.04704	1.03843	0.82
0.2643	0.36191	1.05434	1.04677	0.72
0.1344	0.49121	1.06197	1.05514	0.64
0.3186	0.42681	1.06348	1.05692	0.62
0.6731	0.15061	1.05192	1.04278	0.87
0.5157	0.30781	1.06040	1.05313	0.69
0.3513	0.47191	1.06933	1.06351	0.54
0.1797	0.64321	1.07873	1.07390	0.45
0.8748	0.19121	1.06356	1.05749	0.57
0.6731	0.39261	1.07383	1.07000	0.36
0.4601	0.60371	1.08480	1.08241	0.22
0.2371	0.82711	1.09669	1.09497	0.16

^a Hu et al. (2006).

tion of 0.71% and the largest relative deviation of 1.02%. For the quaternary aqueous solution of mannitol/sorbitol/sucrose/water, the results of density prediction are presented in Table 5, and the largest relative deviation is 0.76%, the average relative deviation is 0.59%.

Table 4
Density prediction by the SAFT model for mannitol + sorbitol + water at 25 $^{\circ}\text{C}$

Molality (mol/kg)		Density (g/cm^3)		Relative deviation (%)
Mannitol	Sucrose	Experimental ^a	Predicted	
0.0809	0.0605	0.98964	0.99343	-0.38
0.1012	0.1528	0.99452	1.00055	-0.61
0.1528	0.1482	1.00215	1.00336	-0.12
0.2028	0.1989	1.01076	1.00943	0.13
0.2582	0.2619	1.02050	1.01640	0.40
0.3061	0.3106	1.02821	1.02194	0.61
0.1254	0.5001	1.02558	1.02288	0.26
0.2511	0.3750	1.02686	1.02262	0.41
0.3766	0.2500	1.02980	1.02235	0.72
0.5020	0.1251	1.03162	1.02208	0.93
0.3570	0.3617	1.03550	1.02767	0.76
0.6593	0.1660	1.04362	1.03293	1.02
0.4944	0.3317	1.04351	1.03337	0.97
0.3302	0.4967	1.04295	1.03380	0.88
0.1652	0.6625	1.04100	1.03422	0.65
0.4219	0.4360	1.04493	1.03529	0.93
0.6398	0.3036	1.04802	1.03945	0.82
0.4263	0.5314	1.05094	1.04071	0.97
0.8528	0.1330	1.05156	1.04124	0.98
0.7060	0.2861	1.05105	1.04192	0.87
0.5018	0.5022	1.05362	1.04302	1.01
0.9008	0.1252	1.05208	1.04327	0.84
0.8588	0.2055	1.05491	1.04540	0.90
0.2133	0.8513	1.05682	1.04689	0.94

^a Hu et al. (2006).

Table 5
Density prediction by the SAFT model for mannitol + sorbitol + sucrose + water at 25 °C

Molality (mol/kg)			Density (g/cm ³)		Relative deviation (%)
Mannitol	Sorbitol	Sucrose	Experimental ^a	Predicted	
0.6857	0.2856	0.1099	1.06110	1.05366	0.70
0.3269	0.2167	0.4327	1.07396	1.06879	0.48
0.5848	0.1821	0.1330	1.05489	1.04591	0.85
0.2826	0.1588	0.3858	1.06485	1.05866	0.58
0.1865	0.3728	0.2367	1.05391	1.04797	0.56
0.4281	0.1316	0.2138	1.05276	1.04475	0.76
0.3660	0.1381	0.1886	1.04652	1.03889	0.73
0.1986	0.1512	0.2898	1.04898	1.04301	0.57
0.2558	0.2356	0.1114	1.03481	1.02898	0.56
0.2269	0.2167	0.1081	1.03095	1.02591	0.49
0.1848	0.1821	0.1410	1.03026	1.02577	0.44
0.1519	0.1889	0.1232	1.02528	1.02207	0.31

^a Hu et al. (2006).

7. Conclusions

The previously developed method has been extended to determine the SAFT parameters for sugars and sugar alcohols, which makes the SAFT model capable of modeling water activity, oxygen solubility and density of aqueous solutions of sugars and sugar alcohols, and very good accuracy has been obtained. There are some advantages of applying the SAFT model to such type of solutions. The SAFT model can be applied to both vapor and liquid phases when modeling the oxygen solubility in the aqueous solutions, avoiding the model inconsistency caused by using activity coefficient models, such as UNIFAC and UNIQUAC. On the other hand, the SAFT equation of state can be easily applied to calculate the density of multicomponent aqueous solutions of sugars and sugar alcohols. This can overcome the problem of using empirical models for density calculation, empirical models are generally very difficult or impossible to be applied to multicomponent aqueous solutions. All the results obtained show that for aqueous solutions of sugar and sugar alcohols, the SAFT model can be taken as a suitable model to estimate the equilibrium properties and carry out density calculation.

Acknowledgements

This work was supported by The National Science Foundation of China (Grant Nos. 20676014, 20676009, 20576013 and 50576001).

References

- Chapman, W. G., Gubbins, K. E., Jackson, G., & Radosz, M. (1989). SAFT: Equation-of-state solution model for associating fluids. *Fluid Phase Equilibria*, *52*, 31–38.
- Chapman, W. G., Gubbins, K. E., Jackson, G., & Radosz, M. (1990). New reference equation of state for associating liquids. *Industrial and Engineering Chemistry Research*, *29*, 1709–1721.
- Chen, S. S., & Kreglewski, A. (1977). *Berichte Der Bunsen-Gesellschaft-Physical Chemistry Chemical Physics*, *81*, 1048.
- Daubert, T. E., & Danner, R. P. (1989). *Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation*. New York: Hemisphere.
- Eya, H., Mishima, K., Nagatani, M., Iwai, Y., & Arai, Y. (1994). Measurement and correlation of solubilities of oxygen in aqueous solutions containing glucose sucrose and maltose. *Fluid Phase Equilibria*, *97*, 201–209.
- Feng, W., van der Kooi, H., & De Swaan Arons, J. (2005). Application of the SAFT equation of state to biomass fast pyrolysis liquid. *Chemical Engineering Science*, *60*, 617–624.
- Gros, J.-B., & Dussap, C. G. (2003). Estimation of equilibrium properties in formulation or processing of liquid foods. *Food Chemistry*, *82*, 41–49.
- Huang, H. S., & Radosz, M. (1990). Equation of state for small, large, polydisperse, and associating molecules. *Industrial and Engineering Chemistry Research*, *29*, 2284–2294.
- Huang, H. S., & Radosz, M. (1991). Equation of state for small, large, polydisperse, and associating molecules: extension to fluid mixtures. *Industrial and Engineering Chemistry Research*, *30*, 1994–2005.
- Hu, Y., Zhang, Z.-X., Zhang, Y.-H., Fan, S.-S., & Liang, D.-Q. (2006). Viscosity and density of the nonelectrolyte system mannitol + sorbitol + sucrose + H₂O and its binary and ternary subsystems at 298.15 K. *Journal of Chemical Engineering Data*, *51*, 438–442.
- Mishima, K., Matsuo, N., Kawakami, A., Komorita, N., Nagatani, M., & Ouchi, M. (1996). Measurement and correlation of solubilities of oxygen in aqueous solutions containing galactose and fructose. *Fluid Phase Equilibria*, *118*, 221–226.
- Kreglewski, A. (1984). *Equilibrium Properties of Fluids and Fluid Mixtures; The Texas Engineering Experiment Station (TEES) Monograph Series*. College Station: Texas A&M University Press.
- Muller, E. A., & Gubbins, K. E. (2001). Molecular-based equations of state for associating fluids: a review of SAFT and related approaches. *Industrial and Engineering Chemistry Research*, *40*, 2193–2211.
- Ninni, L., Camargo, M. S., & Meirelles, A. J. A. (2000). Water activity in polyol systems. *Journal of Chemical Engineering Data*, *45*, 654–660.
- Rasmussen, H. N., & Rasmussen, U. F. (2003). Oxygen solubilities of media used in electrochemical respiration measurements. *Analytical Biochemistry*, *319*, 105–113.
- Reid, R. C., Prausnitz, J. M., & Poling, B. E. (1987). *The Properties of Gases and Liquids*. New York: McGraw-Hill.
- Starzak, M., & Mathlouthi, M. (2006). Temperature dependence of water activity in aqueous solutions of sucrose. *Food Chemistry*, *96*, 346–370.