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Modeling Phase Equilibrium of Common Sugars

Glucose, Fructose, and Sucrose in Mixed Solvents

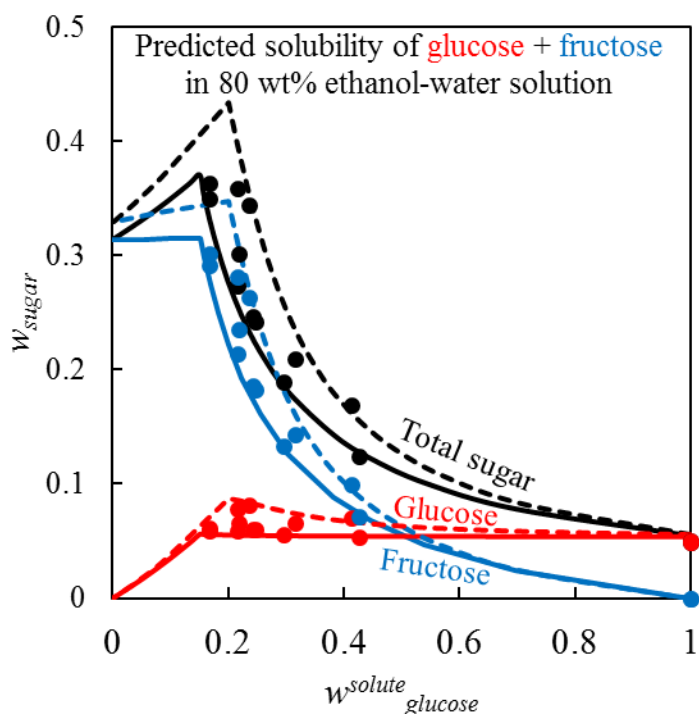
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KEYWORDS: NRTL, Association NRTL, sugar-water-alcohol solubility, phase equilibrium

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ABSTRACT

The industrial processing of sugars and sugar-containing mixtures is gaining widespread use as a form of renewable manufacturing from biomass. To aid in process modeling for design and optimization, a commonly available thermodynamic model is needed that describes the phase equilibrium of these compounds. This work compiles and compares models for solid-liquid and vapor-liquid phase equilibrium from the available data for the representative sugars glucose, fructose, and sucrose in the representative solvents water, methanol, and ethanol, including data for multi-sugar, multi-solvent systems. The Non-random Two liquid (NRTL) model was chosen for these systems because of its widespread use in industry and the availability of parameters for many solvents and co-solutes. The association-NRTL (aNRTL) model was investigated as an improvement for modeling sugars, which may experience a high degree of association due to their many hydroxy groups. Both models accurately capture the data and are able to predict the behavior of multi-sugar systems with only solute-solvent interaction parameters. The aNRTL model shows an improvement over the baseline NRTL model that is most significant for sucrose, the component with the highest association strength, and least significant for fructose, which has the lowest association strength.

INTRODUCTION

The processing of sugars has long been of interest to chemical engineering, but for the most part that interest has been relegated to the food industry.¹ More recently, the processing of biomass into useful chemical precursors has come to the fore as a way to reduce our reliance on nonrenewable resources.² With the rapid expansion of this field, it is necessary to develop a thermodynamic model for industrial processing of these biomass products that can be easily incorporated within the existing process modeling framework.

Many processes that convert biomass to useful products begin with pyrolysis, followed by refining of the resulting bio-oils, vapors and aerosols.³ Sugars are important products of bioprocessing refineries since they can be used to generate products like cellulosic ethanol (EtOH) and bio-based chemicals. Very little deoxygenation occurs during pyrolysis, resulting in bio-oil with elemental composition closely resembling the original biomass.⁴ Bio-oil contains a wide variety of oxygenated functional groups that are highly reactive, promoting esterification, condensation, polymerization, and other reactions that contribute to the instability of bio-oil in storage.⁵

To overcome that problem, it is necessary to submit the products to a series of separation steps to remove reactive contaminants and purify the desired product. Rover et al.⁶ have demonstrated a pyrolysis product refining process that involves several stages manipulating the phase equilibrium of the sugar-rich, high-boiling product referred to as heavy bio-oil. The steps of this process are outlined in **Figure 1**. Of particular interest are the liquid-liquid extraction and crystallization steps, which make use of the differing solubility of the various components in water and other solvents. Development of a thermodynamic model compatible with industrial process simulation is necessary to facilitate the design and optimization of bio-oil refining processes. It is preferable to use one for which the parameters of the other components in bio-oil are already well-defined.

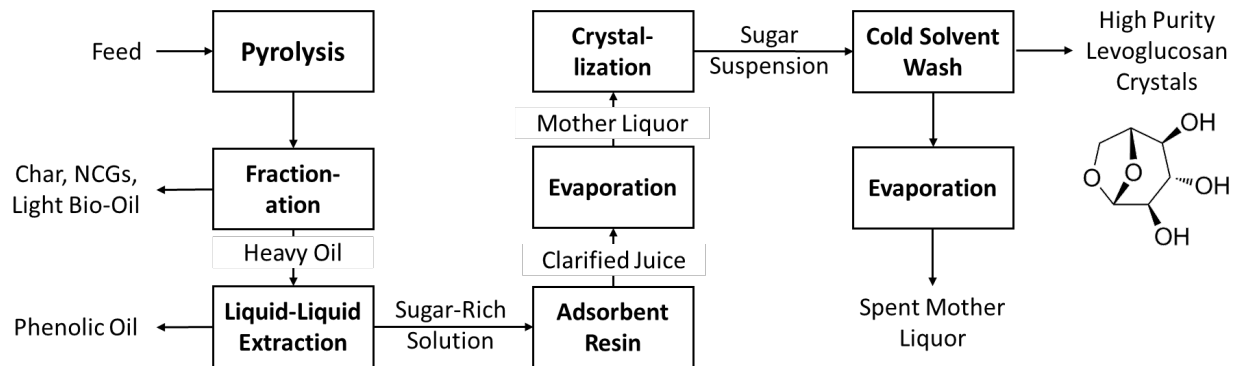


Figure 1: Schematic of a pyrolysis product refining process, adopted from Rover et al.⁶

This work focuses on the phase equilibrium analysis of the three representative sugars glucose, fructose, and sucrose in solvent mixtures of water, methanol (MeOH), and EtOH. At low to moderate pressures, vapor-liquid and solid-liquid equilibrium (VLE and SLE) mostly depend on the activity of the liquid phase. Thus, an activity coefficient model is necessary to describe phase equilibrium in these systems of interest.

Many researchers have proposed activity or osmotic coefficient models for sugars dissolved in water and other solvents. Several sources used their own empirical models, usually in the form of a polynomial series.⁷⁻¹¹ These can be very accurate but tend to fit only the data from which they are derived and are not easily applicable to other conditions or systems. The most common models used are UNIFAC and its derivatives¹²⁻¹⁷ and UNIQUAC and its derivatives^{13, 15, 18-23}. These models tend to be accurate, although those with better fits^{13-18, 20-23} introduce modifications to the original UNIFAC and UNIQUAC models for which there may not be parameters available for extensions to other systems. Once again, most of these models are derived from one or a few sets of data, and so might not reflect the full range of data collected for these systems. For example, Gong et al.¹³ compared predictions by the modified UNIQUAC, S-UNIFAC, and mS-UNIFAC models for glucose, fructose, and sucrose in water-EtOH mixtures. They restricted their data set to solubility only, using their own experimental data and most (but not all) of the solubility data

available at the time.^{15, 21-22, 24} The modified UNIQUAC model performed well, but was restricted to the temperature range of 273.15 to 293.15 K. The accuracy of the model was not investigated for other forms of phase equilibrium, such as VLE.

The Non-random Two-liquid (NRTL) model²⁵ was chosen for this work because of its proven record of dealing with highly nonideal systems and widespread use in the chemical industry. Consequently, most solvents and common co-solutes encountered already have well-defined parameters. Because of the similar chemical nature of sugars, the sugar-sugar interactions in mixed-sugar solutions should be relatively ideal. Therefore, regressing sugar-solvent binary parameters should allow the model to be easily extended to systems with any number of dissolved sugars. The association-NRTL (aNRTL) model²⁶ is an extension of the NRTL model that specifically accounts for associating species, making it particularly well-suited for water, alcohols, and sugars that exhibit high degrees of hydrogen bonding due to an abundance of hydroxyl groups. It introduces two to three new component-specific parameters, increasing the predictive capability of the model without requiring any more data.

PHASE EQUILIBRIUM MODELING

At low to moderate pressures, both VLE and SLE are controlled by the activity of species in the liquid phase. As sugars can be damaged by high temperatures and pressures, an accurate activity coefficient model is the key to modeling separations processes involving these species.

The NRTL model²⁵ calculates the activity coefficient of species i in a mixture, γ_i , as a function of its mole fraction, x_i by the equation:

$$\ln \gamma_i = \frac{\sum_j \tau_{ji} G_{ji} x_j}{\sum_k G_{ki} x_k} + \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right) \quad (1)$$

where

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij}), \quad (2)$$

τ_{ij} is the binary interaction parameter of species i and j , and the non-randomness factor, α_{ij} is fixed at a constant value (usually around 0.3). In this case, the binary interaction parameter is given the temperature dependency:

$$\tau_{ij} = a_{ij} + \frac{b_{ij}}{T} \quad (3)$$

Temperature-dependent NRTL binary interaction parameters for the water and alcohol solvents are included in **Table 1**.

Table 1: Solvent NRTL binary interaction parameters from the Aspen Properties databank.²⁷

Comp. i	Comp. j	a_{ij}	b_{ij}/K	a_{ji}	b_{ji}/K	$a_{ij} = a_{ji}$	$\tau_{ij}(298K)$	$\tau_{ji}(298K)$
Water	EtOH	3.46	-586	-0.80	246	0.3	1.492	0.025
Water	MeOH	2.73	-617	-0.69	173	0.3	0.662	-0.113
MeOH	EtOH	4.71	-1162	-2.31	484	0.3	0.814	-0.690

The NRTL model has been further improved to better describe highly associating systems with the addition of an association term.²⁶ The activity of component i in the aNRTL model is described by the equation:

$$\ln \gamma_i = \ln \gamma_i^{Resid} + \ln \gamma_i^{Comb} + \ln \gamma_i^{Assoc} \quad (4)$$

The residual term, $\ln \gamma_i^{Resid}$, is calculated with the original NRTL equation (Equation 1). The combinatorial term, $\ln \gamma_i^{Comb}$, uses a modified Flory-Huggins expression:²⁸

$$\ln \gamma_i^{Comb} = 1 - \frac{\varphi'_i}{x_i} + \ln \frac{\varphi'_i}{x_i} \quad (5)$$

where φ'_i is the modified volume fraction:

$$\varphi'_i = \frac{r_i^{2/3} x_i}{\sum_j r_j^{2/3} x_j} \quad (6)$$

and r_i is the molecular Van der Waals volume that may be calculated from Bondi's group-contribution method.²⁹ The association term, $\ln \gamma_i^{Assoc}$ was derived by Ferreira et al.^{26, 30} from Wertheim's theory:

$$\ln \gamma_i^{Assoc} = \sum_A v_i^A \left[\ln \left(\frac{X^A}{X_i^A} \right) + \frac{X_i^A - 1}{2} \right] + r_i \sum_A \rho_A \left(\frac{1 - X^A}{2} \right) \quad (7)$$

where:

$$X^A = \frac{1}{1 + \sum_B \rho^B \Delta^{AB} X^B} \quad (8)$$

$$X_i^A = \frac{1}{1 + \sum_B \rho_i^B \Delta^{AB} X_i^B} \quad (9)$$

$$\rho^A = \frac{\sum_j v_j^A x_j}{\sum_j r_j x_j} \quad (10)$$

$$\rho_i^A = \frac{v_i^A}{r_i} \quad (11)$$

Here v_i^A is the number of sites of type A in component i ; X^A and X_i^A are the unbounded site fractions of type A in the solution and in pure component i , respectively; and ρ^A and ρ_i^A are the dimensionless molar density of site type A in the solution and in pure component i . The index B in Equations 8 and 9 refers to the sites which associate with sites of Type A , so the definitions of ρ^B , ρ_i^B , and v_i^B are analogous to those of ρ^A , ρ_i^A , and v_i^A .

In this work, we follow the convention of Hao and Chen³¹ and look at the association strength from hydrogen bonding. The two types of sites are thus labeled A (hydrogen bond Acceptor) and D (hydrogen bond Donor). The dimensionless association strength, Δ^{AD} , can be approximated as a function of the specific association strength parameters, δ^A and δ^D , and a reference association strength, Δ_{ref}^{AD} :

$$\Delta^{AD} = \frac{\delta^A}{\delta_{ref}^A} \frac{\delta^D}{\delta_{ref}^D} \Delta_{ref}^{AD} \quad (12)$$

where the reference association strength parameters, δ_{ref}^A and δ_{ref}^D are both set to 1. The reference association strength is that of the self-association of water, which, according to Mengarelli et al.,³² can be modeled as:

$$\Delta_{ref}^{AD} = \kappa_{ref}^{AD} \left[\exp\left(\frac{\varepsilon_{ref}^{AD}}{kT}\right) - 1 \right] \quad (13)$$

where κ_{ref}^{AD} is the dimensionless characteristic association volume and ε_{ref}^{AD} is the association energy between the reference acceptor and donor sites. For water, their values are $\kappa_{ref}^{AD} = 0.034$ and $\frac{\varepsilon_{ref}^{AD}}{k} = 1960$ K.³¹ The association parameters for the three solvents used in this study were

taken from the literature³¹ and are included in **Table 2**. The residual term parameters were regressed from available experimental data^{27, 33} and are included in **Table 3**.

Table 2: Solvent association parameters.³¹

Solvent	ν_i^A	ν_i^D	δ_i^A	δ_i^D	r_i
Water	2	2	1	1	0.76
MeOH	2	1	1	1	1.43
EtOH	2	1	1	1	2.11

Table 3: Solvent aNRTL residual term parameters regressed from data available in NIST databank.^{27, 33}

Comp. <i>i</i>	Comp. <i>j</i>	a_{ij}	b_{ij}/K	a_{ji}	b_{ji}/K	$a_{ij} = a_{ji}$	$\tau_{ij}(298K)$	$\tau_{ji}(298K)$
Water	EtOH	5.19	-1332	-3.91	1128	0.2	0.72	-0.127
Water	MeOH	1.20		-0.58		0.2	1.20	-0.577
MeOH	EtOH	-10.22	3499	8.92	-3027	0.2	1.52	-1.234

Solubility is modeled with the equation:

$$K_{sp,i} = \frac{\gamma_i x_i^L}{a_i^S} \quad (14)$$

where x_i^L is the mole fraction of species i in the liquid phase and $a_i^S = 1$ is the activity of i in the solid phase. The solubility constant is given the temperature dependence:

$$\ln K_{sp} = a + \frac{b}{T} \quad (15)$$

AVAILABLE EXPERIMENTAL DATA

A thorough examination of the literature found a range of data types including osmotic coefficient (water activity), vapor pressure, boiling point, and solid solubility. The solvents water, MeOH, and EtOH were chosen in order to account for polar and nonpolar interactions as well as varying degrees of association. The availability of data was also considered, so that each sugar is adequately represented in all three solvents. The most comprehensive literature survey and modeling effort for glucose, fructose, and sucrose in these solvents was performed by Peres and Macedo in 1996.²⁰ They continued to update their model with their own experimental data until 2001,¹⁵ but other studies conducted since then have shed further light on these systems. Starzak and Mathlouthi¹¹ performed a very comprehensive literature survey for sucrose-water solutions as part of their modeling efforts, which was used as a starting point for that system in this work. **Table 4**, **Table 5**, and **Table 6** summarize the data, including the data type, temperature range, pressure range, number of data points, and source(s).

The references marked with an asterisk (*) were considered outliers and, therefore, excluded from the regression. Including data from any one of these sources was observed to increase the mean squared error of the associated regression by an order of magnitude. This could have been due to a variety of reasons. The most common justification for excluding a source of solubility data was that it likely included a metastable sugar hydrate, such as glucose·monohydrate ($C_6H_{12}O_6 \cdot H_2O$)³⁴, in the solid phase that was not specified in the solid phase composition. There are a few sources that measure the solubility of glucose^{7, 35-37}, fructose³⁸, and sucrose³⁹ hydrates. These tend to appear at low temperatures and at high water concentrations, and so are not common in the systems studied here. For the purpose of modeling the activity of these sugars in solution, the most common solid phase provides more than sufficient data. For each source excluded, at least two

other data sources of the same type were included, so excluding one data source did not create a gap in model fitting.

The majority of sources do not report uncertainties, so they were assigned based on the variable type. Typical values are 0.1 K for temperature, 0.1 kPa for pressure, 0.005 mole/mass fraction for composition, and 0.005 units for activity coefficient. These standard values were subject to increase by a factor of 2 to 5 in certain cases when the quality of the data was uncertain, or the reported measurements did not have sufficient significant digits. A more thorough discussion of the assignment of standard deviations is included in the Supporting Information.

Table 4: Data for glucose-containing systems.

System	Type^a	<i>T</i>/K	<i>P</i>/kPa^b	Points	Sources
Glucose+Water	Tx	261-433	-	34	[35], [37], [40]*
Glucose+Water	Pxy	298-338	(2.4-25.0)	101	[8],[18],[41]
Glucose+Water	Txy	334-386	20-101.3	82	[16],[42]
Glucose+Water	ϕ	298-333	-	138	[8],[43],[44],[45],[46]
Glucose+MeOH	Tx	295-323	-	3	[17]
Glucose+Water+MeOH	Tx	310-353	-	83	[23],[47]
Glucose+EtOH	Tx	295-323	-	3	[17]
Glucose+Water+EtOH	Tx	273-333	-	90	[7]*,[13],[14],[21],[48],[49]*
Glucose+MeOH+EtOH	Tx	313,333	-	21	[23]

^a Tx: solid solubility data; Txy: constant-pressure VLE data; Pxy: constant-temperature VLE data; ϕ : osmotic coefficient data (converted to activity coefficient for regression).

^b Pressures in parentheses refer to partial vapor pressures.

Table 5: Data for fructose-containing systems.

System	Type ^a	T/K	P/kPa ^b	Points	Sources
Fructose+Water	Tx	269-343	-	17	[12],[38],[50]
Fructose+Water	Pxy	308	(5.1-5.6)	21	[8]
Fructose+Water	Txy	334-403	20-101.3	84	[16],[42]
Fructose+Water	ϕ	273-308	-	25	[8],[51]
Fructose+MeOH	Tx	295-313	-	3	[17]
Fructose+Water+MeOH	Tx	293-333	-	67	[1],[15],[47]
Fructose+EtOH	Tx	295-313	-	3	[17]
Fructose+Water+EtOH	Tx	273-333	-	120	[1],[13],[15],[24]
Fructose+MeOH+EtOH	Tx	298-333	-	32	[15]

^a Tx: solid solubility data; Txy: constant-pressure VLE data; Pxy: constant-temperature VLE data; ϕ : osmotic coefficient data (converted to activity coefficient for regression).

^b Pressures in parentheses refer to partial vapor pressures.

Table 6: Data for sucrose-containing systems.

System	Type ^a	T/K	P/kPa ^b	Points	Sources
Sucrose+Water	Tx	263-343	-	8	[12],[39]
Sucrose+Water	Pxy	298	(2.7-3.2)	16	[52]
Sucrose+Water	Txy	373-415	101.3	23	[42],[53]
Sucrose+Water	ϕ	273-308	-	106	[8],[44],[51],[52],[54],[55],[56]*
Sucrose+Water+MeOH	Tx	298-352	-	103	[9],[22],[47]*
Sucrose+Water+EtOH	Tx	273-333	-	78	[9],[13],[22],[48]
Sucrose+MeOH+EtOH	Tx	298-333	-	52	[9],[22]

^a Tx: solid solubility data; Txy: constant-pressure VLE data; Pxy: constant-temperature VLE data; ϕ : osmotic coefficient data (converted to activity coefficient for regression).

^b Pressures in parentheses refer to partial vapor pressures.

Table 7 summarizes the experimental data for systems containing more than one sugar. These sources were not included in the regressions but were used for model validation.

Table 7: Data for systems containing multiple sugars in water (aq) and water-EtOH (aq+et) mixtures.

Sugars (solvent)	Type ^a	T/K	P/kPa	Points	Source
Glucose+Sucrose (aq)	Txy	374-382	101.3	9	[42]
Fructose+Sucrose (aq)	Txy	374-387	101.3	9	[42]
Glucose+Fructose (aq)	Txy	374-393	101.3	10	[42]
Glucose+Fructose+Sucrose (aq)	Txy	374-392	101.3	10	[42]
Glucose+Sucrose (aq)	Tx	303,343	-	16	[36],[12]
Fructose+Sucrose (aq)	Tx	303,343	-	15	[36],[12]
Glucose+Fructose (aq+et)	Tx	303	-	70	[57]

^a Txy: constant-pressure VLE data; Tx: solid solubility data.

MODEL RESULTS

All available data for single sugars, excluding certain sets as discussed above, were used to regress the necessary parameters for each sugar and each model in turn – temperature-dependent K_{sp} , temperature-dependent τ_{ij} for each model, and δ^A , δ^D , and r for the aNRTL model – simultaneously, using the regression tool built into Aspen Properties V11.²⁷ The parameters were all regressed together to get the most accurate result for the sugar-specific solubility (K_{sp}) and association (δ^A , δ^D , r) parameters. Aspen Properties reports two statistics for its regressions. The residual root mean squared error ($RMSE$) is defined as:²⁷

$$RMSE = \sqrt{\frac{WSS}{K - n}} \quad (16)$$

where K is the total number of data points, n is the number of parameters, and the weighted sum of squares (WSS) is defined as:

$$WSS = \sum_{l=1}^g w_l \left[\sum_{i=1}^k \sum_{j=1}^m \left(\frac{Z_{ij} - ZM_{ij}}{\sigma_{ij}} \right)^2 \right]_l \quad (17)$$

ZM_{ij} is the measured data, Z_{ij} is the calculated value, σ_{ij} is the standard deviation assigned to the data point, w_l is the weighting factor assigned to the data group, l is the data group number, g is the total number of data groups, i is the data point number, k is the total number of data points within data group l , j is the measured variable (T , P , x , etc.) number, and m the total number of variables associated with data point i .

While RMSE uses the number of parameters to penalize overfitting of the data, there are additional statistical tests that are more sensitive to superfluous parameters such as the Mallows,⁵⁸ Akaike, and Bayesian information criteria,⁵⁹ which balance the likelihood function against the number of parameters. When tested, they were found to give similar results qualitatively. Consequently, only the Bayesian information criterion (BIC) is reported in this paper since it appeared to be the most sensitive to overfitting of the data. The BIC is defined as:

$$BIC = K \ln \left(\frac{SSE}{K} \right) + n \ln K \quad (18)$$

where SSE is the sum of the squared errors. Since Aspen Properties only reports the WSS , it was more practical to replace SSE in Equation (18) with WSS as defined in Equation (17). This can be

justified for a qualitative comparison of two models derived from the same data set, since the weighting factors w_l and σ_{ij} is identical for both cases. The weighting of the error makes it more likely for WSS to be less than K , resulting in a negative value of the modified BIC . When looking at two models derived from the same set of data, the preferred model is the one with the lower (more negative) value of modified BIC . The exact values of the statistical parameters, along with a discussion of the process for assigning standard deviations to experimental data, is included in the Supporting Information. **Table 8** shows the association parameters regressed for each sugar, along with the values of RMSE and modified BIC for the NRTRL and aNRTRL models. The values of v_i^A and v_i^D for each sugar were chosen based on the number of available hydrogen bond acceptor and donor sites on the hydroxy groups of each sugar. The structure of the most common form of each sugar can be seen in **Figure 2**.

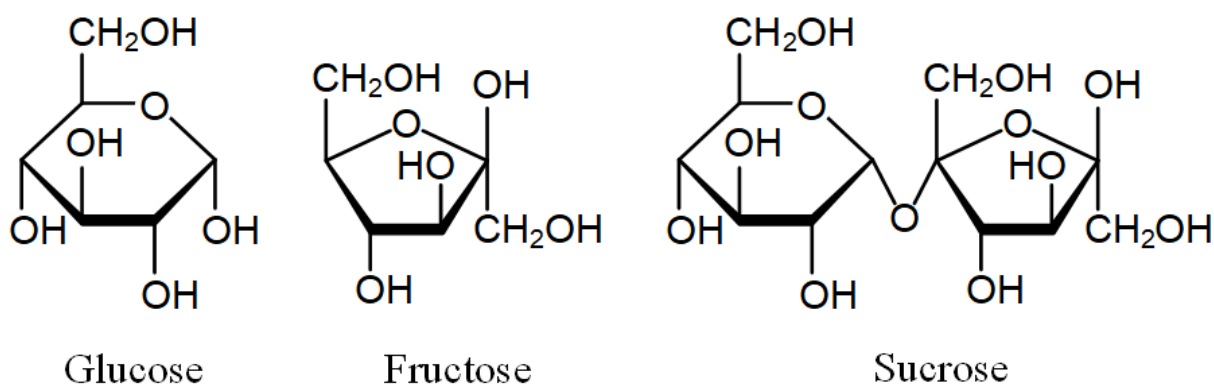


Figure 2: Molecular structure of the three representative sugars.

In each case, the aNRTRL model is a significant improvement over the base NRTRL model. This improvement is most pronounced for sucrose, which has the highest number of associating hydroxy groups and the highest association strength, and least significant for fructose, which has the lowest estimated association strength. One possible explanation for the low association strength of fructose is the size of the molecule. As a furanose ring, its hydroxy groups are closer

together than those of glucose or sucrose, and the two methylene groups result in a higher degree of flexibility than is found in glucose. This configuration could result in a high degree of intramolecular association, resulting in the low observed association strength with external sites. The parameter r_i was included in the regression, in every case reflecting a reduction from that estimated using Bondi’s group contribution method²⁹ (8.46 for glucose, 7.69 for fructose, and 14.31 for sucrose). Fixing r_i results consistently in a drastic increase in *RMSE* and modified *BIC* compared to the baseline NRTL and aNRTL with variable r_i models. While the r_i in the combinatorial term of aNRTL has a definite physical significance, that term has only a small effect on the activity calculations, while the r_i of the association term is more open to interpretation. This should be carefully considered as the aNRTL model is extended further, but that is beyond the scope of the present work. Still, it can be hypothesized that a reduction in r_i for large, complex molecules with many association sites may better reflect the actual size of these molecules in solution, which could be expected to decrease when the effects of relatively strong association are spread over the large number of association sites. This hypothesis is supported by the trend of fructose having the lowest association strength and the least reduction in r_i .

Table 8: Regressed association parameters for the three sugars and *RMSE* and modified *BIC* for the NRTL and aNRTL models.

Sugar	ν_i^A	ν_i^D	δ_i^A	δ_i^D	r_i	<i>RMSE</i>		Modified <i>BIC</i>	
						(NRTL)	(aNRTL)	(NRTL)	(aNRTL)
Glucose	10	5	1.31 ± 0.09	0.07 ± 0.02	4.90 ± 0.29	0.94	0.85	-7	-94
Fructose	10	5	0.07 ± 0.02	0.00 ± 0.00	4.65 ± 0.25	0.98	0.88	32	-36
Sucrose	16	8	2.00 ± 0.06	0.80 ± 0.20	9.54 ± 0.31	0.70	0.51	-186	-381

Table 9 and **Table 10** present the NRTL model and aNRTL residual binary interaction parameters for each of the three sugars in each of the three solvents, as well as the K_{sp} solubility parameter for the solid sugars associated with each model. The τ parameters show a consistent trend between the two models, with the τ_{ij} increasing from negative to positive from water to MeOH to EtOH while τ_{ji} remains strongly positive. The introduction of the association term through the aNRTL model shifts most τ parameters in the positive direction, as the attractive forces of association are captured by the association term. The negative shift in τ_{ij} from NRTL to aNRTL for fructose is a result of including the combinatorial (Flory-Huggins) term while the effects of association are almost negligible. The solubility parameters are similar for both models and are consistent with the thermodynamic properties of each sugar, reflecting the fundamental nature of solid solubility.

Table 9: Regressed NRTL and K_{sp} parameters.

Comp. i	Comp. j	a_{ij}	b_{ij}/K	a_{ji}	b_{ji}/K	$a_{ij} = a_{ji}$	$\tau_{ij}(298K)$	$\tau_{ji}(298K)$
Glucose	Water	0.53 ± 0.32	-966 ± 147	-5.53 ± 0.72	2850 ± 260	0.3	-2.71 ± 0.59	4.03 ± 1.13
Glucose	MeOH	-0.55 ± 0.07		3.00 ± 0.13		0.3	-0.55 ± 0.07	3.00 ± 0.13
Glucose	EtOH	2.65 ± 0.89		2.36 ± 0.14		0.3	2.65 ± 0.89	2.36 ± 0.14
Fructose	Water	-7.53 ± 0.46	1868 ± 182	13.79 ± 0.84	-3937 ± 214	0.3	-1.27 ± 0.76	0.58 ± 1.10
Fructose	MeOH	-0.66 ± 0.04		3.17 ± 0.10		0.3	-0.66 ± 0.04	3.17 ± 0.10
Fructose	EtOH		334 ± 27		782 ± 27	0.3	1.12 ± 0.09	2.62 ± 0.09
Sucrose	Water	-0.70 ± 0.33	-691 ± 58	-3.32 ± 1.22	2096 ± 314	0.3	-3.02 ± 0.44	3.72 ± 1.61
Sucrose	MeOH	-1.60 ± 0.11		5.78 ± 0.51		0.3	-1.60 ± 0.11	5.78 ± 0.51
Sucrose	EtOH	-0.42 ± 0.14		4.70 ± 0.12		0.3	-0.42 ± 0.14	4.70 ± 0.12
K-salt		a_i	b_i/K	$K_{sp,i}(298K)$				
Glucose(s)		7.93 ± 0.32	-3421 ± 122	-3.55 ± 0.52				
Fructose(s)		5.51 ± 0.41	-2155 ± 140	-1.72 ± 0.62				
Sucrose(s)		2.99 ± 0.59	-2320 ± 218	-4.79 ± 0.94				

Table 10: Regressed aNRTL residual term and K_{sp} parameters.

Comp. i	Comp. j	a_{ij}	b_{ij}/K	a_{ji}	b_{ji}/K	$a_{ij} = a_{ji}$	$\tau_{ij}(298K)$	$\tau_{ji}(298K)$
Glucose	Water	1.03 ± 0.32	-377 ± 147	-3.59 ± 0.72	3201 ± 260	0.3	-0.24 ± 0.59	7.15 ± 1.13
Glucose	MeOH	0.40 ± 0.13		4.36 ± 0.13		0.3	0.40 ± 0.13	4.36 ± 0.13
Glucose	EtOH	4.44 ± 4.69		4.39 ± 0.37		0.3	4.44 ± 4.69	4.39 ± 0.37
Fructose	Water	-7.83 ± 0.49	1526 ± 224	12.95 ± 0.85	-3559 ± 214	0.3	-2.71 ± 0.90	1.01 ± 1.11
Fructose	MeOH	-1.10 ± 0.06		2.47 ± 0.16		0.3	-1.10 ± 0.06	2.47 ± 0.16
Fructose	EtOH		276 ± 34		628 ± 38	0.3	0.93 ± 0.11	2.11 ± 0.13
Sucrose	Water	-0.79 ± 0.86	-197 ± 340	-9.16 ± 0.86	4717 ± 258	0.3	0.13 ± 1.43	6.67 ± 1.22
Sucrose	MeOH	0.06 ± 0.23		6.16 ± 0.24		0.3	0.06 ± 0.23	6.16 ± 0.24
Sucrose	EtOH	3.73 ± 5.11		5.09 ± 0.42		0.3	3.73 ± 5.11	5.09 ± 0.42
K-salt		a	b/K	$K_{sp}(298K)$				
Glucose(s)		6.33 ± 0.45	-2705 ± 187	-2.75 ± 0.77				
Fructose(s)		3.03 ± 0.60	-1176 ± 210	-0.92 ± 0.92				
Sucrose(s)		6.04 ± 0.75	-2885 ± 274	-3.64 ± 1.19				

The following subsections cover the results for each of the sugars in turn, then compare model predictions to experimental data for multi-sugar systems.

Glucose

Figure 3 includes a comparison of model predictions to experimental VLE data for the glucose-water system. Both models effectively capture the range of experimental data, with the aNRTL model performing slightly better at higher temperatures and glucose mass fractions.

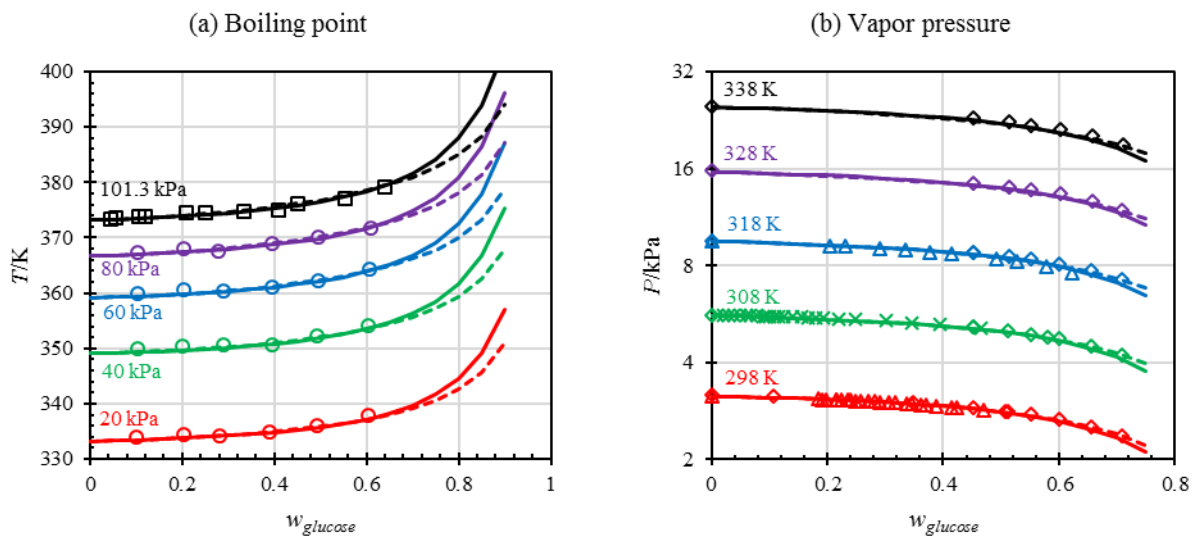


Figure 3: (a) Boiling point elevation and (b) vapor pressure of water with different mass fractions of glucose, including both the (—) NRTL and (- -) aNRTL model and data from (□) Abderafi and Bounahmidi,⁴² (○) Maximo et al.,¹⁶ (◇) Taylor and Rowlinson,⁴¹ (△) Cooke et al.,¹⁸ and (×) Ebrahimi and Sadeghi.⁸

Figure 4 compares model results and experimental data for solubility of glucose in select water-EtOH mixed-solvents. The solubility of glucose in pure water is exactly captured by both models. Even after the exclusion of some data sets, the data for water-EtOH mixed-solvents are not completely consistent. Particularly due to the very low solubility of most sugars in EtOH, it is not surprising that individual data sources and the models themselves have a high degree of relative error when the solvent has high EtOH concentrations. Considering these inconsistencies, both models perform well at matching the solubility of glucose in water-EtOH mixed-solvents within the range of the data. The aNRTL model is an improvement over the NRTL model when it comes to matching the trends present in the data sets across the entire range of ethanol concentrations. The aNRTL model predicts a consistent reduction in solubility as temperature decreases

(reciprocal temperature increases), while the NRTL model shows much less of an effect, especially for systems with higher water-to-EtOH ratios.

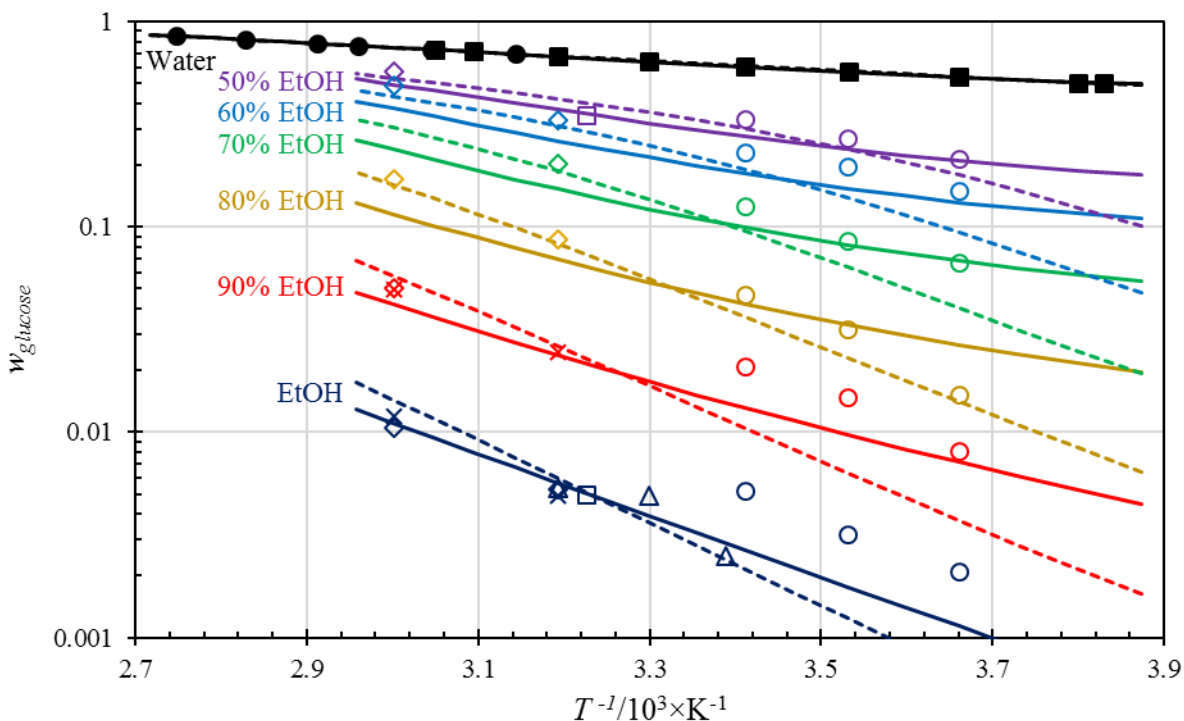


Figure 4: Mass solubility of glucose in various mass fraction water-EtOH solutions, including both the (—) NRTL and (- -) aNRTL model, and data from (■) Young,³⁷ (●) Jackson and Silsbee,³⁵ (○) Gong et al.,¹³ (△) Montanes et al.,¹⁷ (◇) Peres and Macedo,²¹ (□) Bouchard et al.,⁴⁸ and (×) Leontarakis et al.¹⁴

Figure 5 compares model results and experimental data for glucose solubility in the water-MeOH and MeOH-EtOH mixed-solvents. Both models represent the data reasonably well, once again considering the spread of the available data, with the aNRTL model being a slight improvement in capturing all but the outlying data of Montanes et al.¹⁷

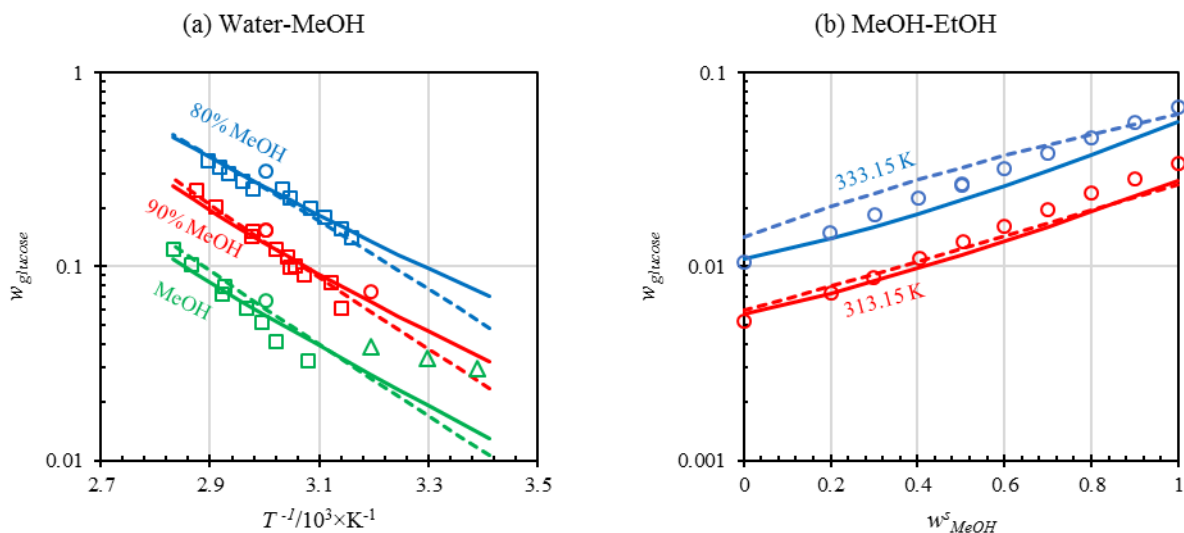


Figure 5: Solubility of glucose in different mass fractions of (a) water-MeOH and (b) MeOH-EtOH solutions, including the (—) NRTL and (- -) aNRTL model and data from (○) Peres and Macedo,²³ (△) Montanes et al.,¹⁷ and (□) van Putten et al.⁴⁷ w^s is mass fraction in the solute-free solvent.

Fructose

Figure 6 includes a comparison of model predictions to experimental VLE data for the fructose-water system. Both models effectively capture the range of experimental data, although the aNRTL model gives slightly better results at higher temperatures and fructose mass fractions.

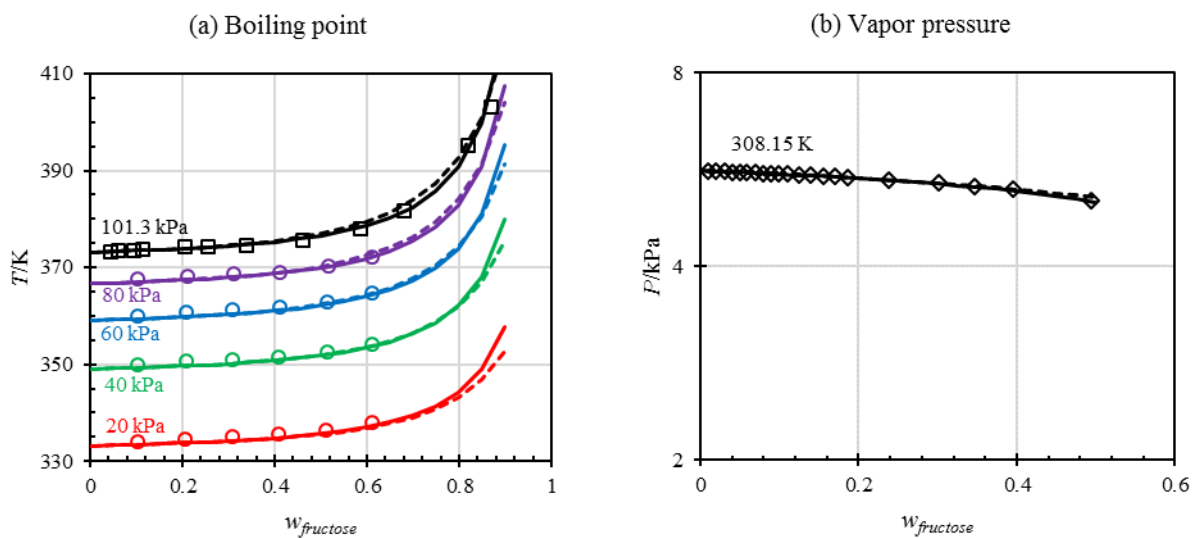


Figure 6: (a) Boiling point elevation and (b) vapor pressure of water with different mass fractions of fructose, including both the (—) NRTL and (- -) aNRTL model, and data from (\square) Abderafi and Bounahmidi,⁴² (\circ) Maximo et al.,¹⁶ (\diamond) Ebrahimi and Sadeghi.⁸

Figure 7 compares model results and experimental data for the solubility of fructose in water-EtOH mixed-solvents. Fructose is significantly more soluble in alcohols than glucose or sucrose and is reported to have much higher solubility at higher temperatures. This increased solubility in alcohols supports the low calculated association strength, since the alcohols also contain non-associating regions that set them apart from water, which is made up entirely of hydrogen bond donor and acceptor sites. Both models capture the solubility of fructose in pure water. Since fructose has very weak association strength, there is little difference between the models when predicting the solubility of fructose in EtOH-water mixed-solvents, although the aNRTL model shows a slight improvement in pure EtOH and at higher water concentrations.

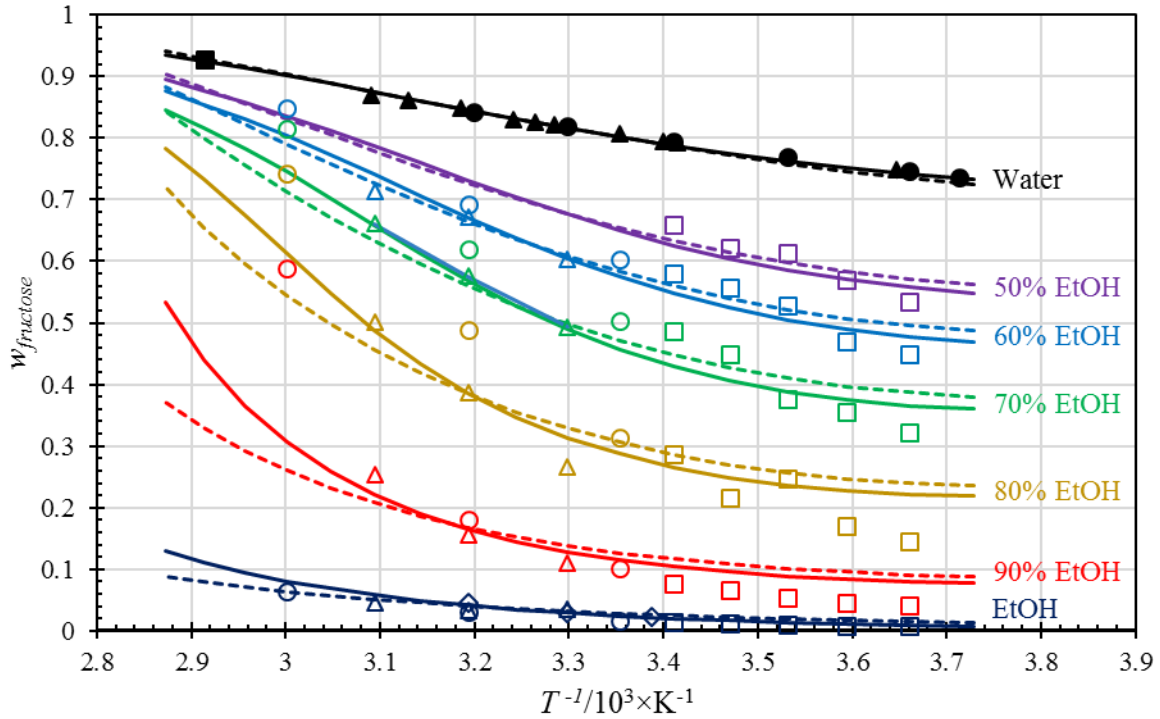


Figure 7: Solubility of fructose in various mass fraction water-EtOH solutions, including both the (—) NRTL and (- -) aNRTL model, and data from (●) Young et al.,³⁸ (▲) Vasatko and Smelik,⁵⁰ (■) Abed et al.,¹² (○) Macedo and Peres,¹⁵ (△) Flood et al.,²⁴ (◇) Montanes et al.,¹⁷ and (□) Gong et al.¹³

Figure 8 compares model predictions to experimental data for fructose solubility in water-MeOH and MeOH-EtOH mixed-solvents. Neither model seems to have an advantage when describing both systems, with the NRTL model performing better under certain conditions and the aNRTL performing better under others.

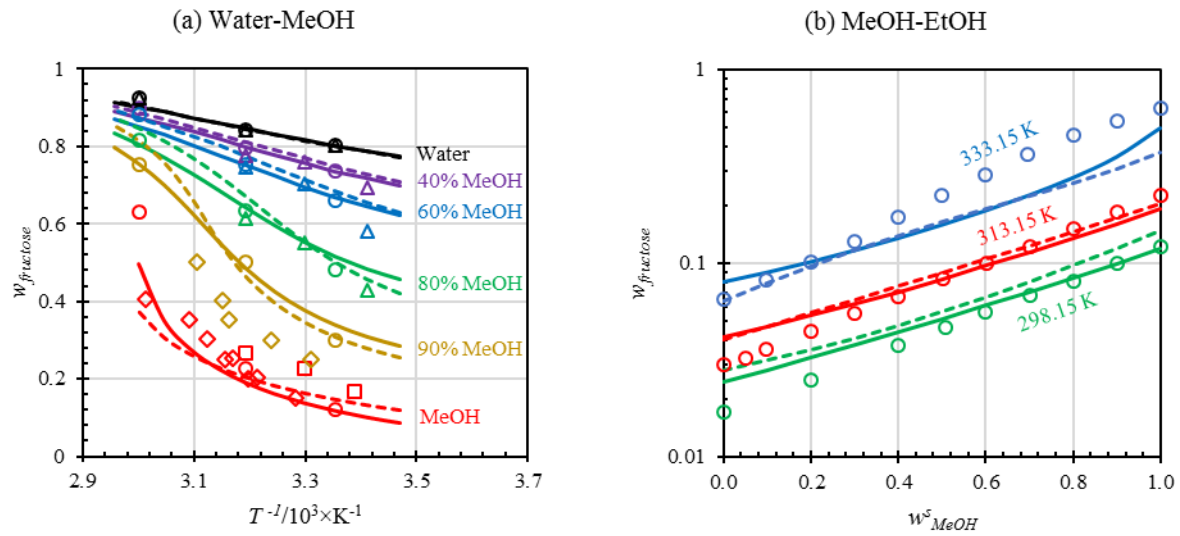


Figure 8: Solubility of fructose in various mass fraction (a) water-MeOH and (b) MeOH-EtOH solutions, including the (—) NRTL and (- -) aNRTL model and data from (○) Macedo and Peres,¹⁵ (□) Montanes et al.,¹⁷ (△) Alavi et al.,¹ and (◇) van Putten et al.⁴⁷ w^s is mass fraction in the solute-free solution.

Sucrose

Figure 9 compares model predictions to experimental data for sucrose-water binary VLE. Both models accurately capture the available data, with the aNRTL model performing better for boiling point elevation of solutions with high sucrose mass fractions.

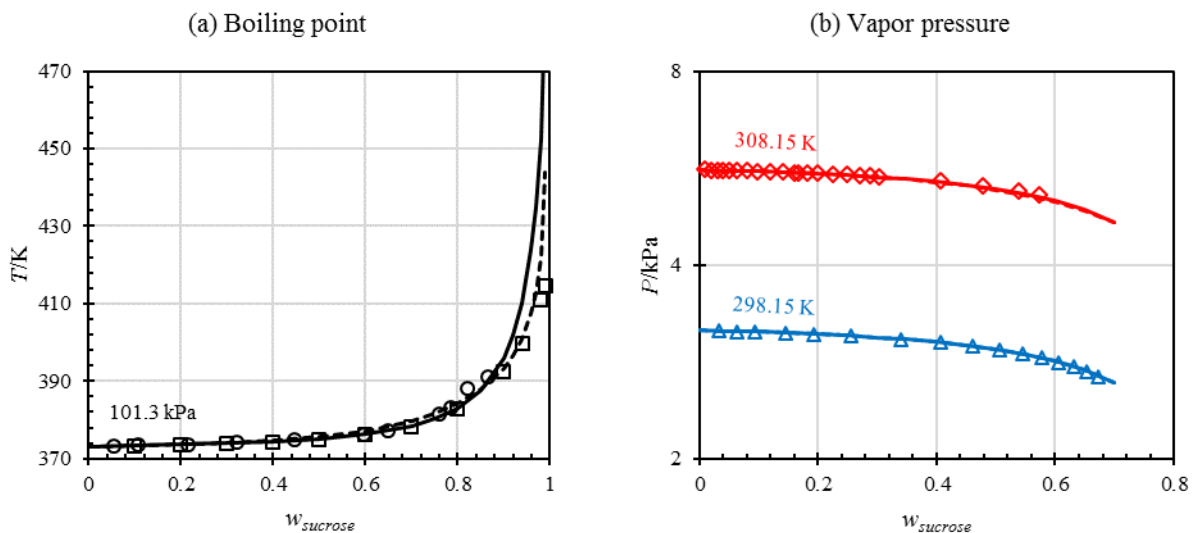


Figure 9: (a) Boiling point elevation and (b) vapor pressure of sucrose-water solutions, including both the (—) NRTL and (- -) aNRTL model, and data from (○) Abderafi and Bounahmidi,⁴² (□) Leschke,⁵³ (◇) Ebrahimi and Sadeghi,⁸ and (△) Robinson et al.⁵²

Figure 10 compares model results and experimental data for the solubility of sucrose in water-EtOH mixed-solvents. Both models exactly match the solubility of sucrose in water and perform well within the variation of the available data for water-EtOH mixed-solvents. Even more so than with with glucose, the aNRTL model more closely matches the curvature of the experimental data in all cases except for pure EtOH, where the very low solubility invites a large degree of uncertainty.

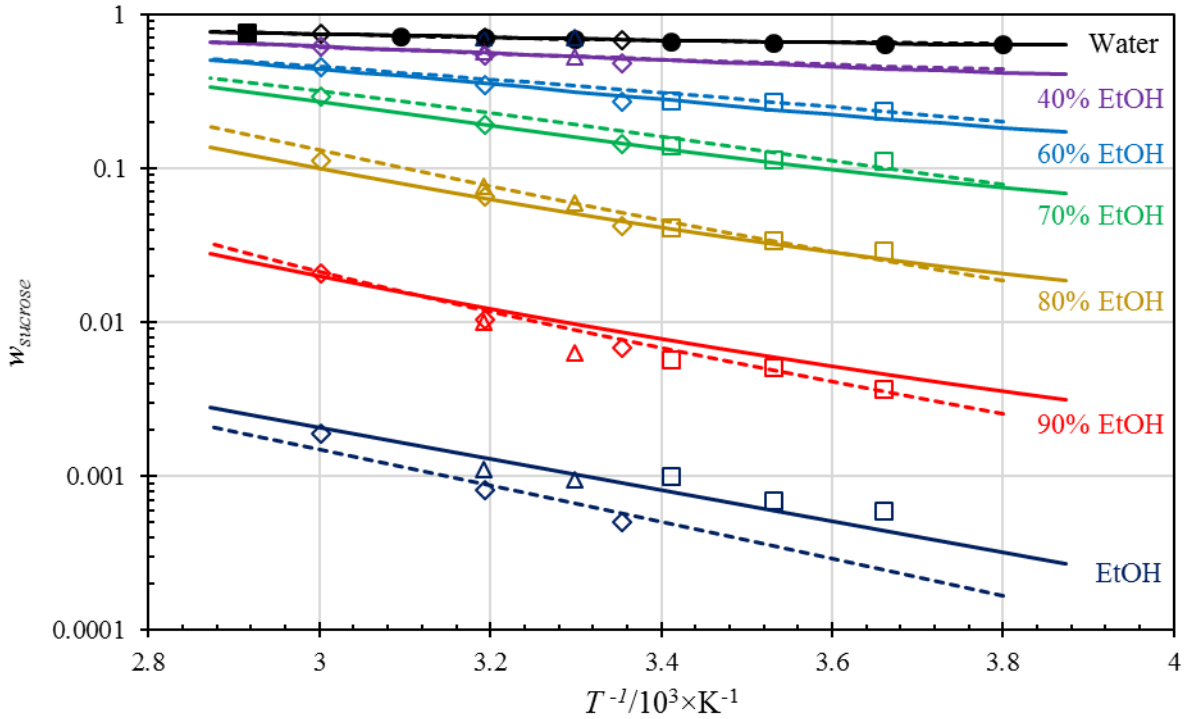


Figure 10: Solubility of sucrose in various mass fraction water-EtOH solutions, including both the (—) NRTL and (- -) aNRTL model, and data from (●) Young and Jones,³⁹ (■) Abed et al.,¹² (△) Galvao et al.,⁹ (◇) Peres and Macedo,²² and (□) Gong et al.¹³

Figure 11 compares model predictions to experimental data for sucrose solubility in water-MeOH and MeOH-EtOH mixed-solvents. Both models perform well at capturing the data, with the aNRTL model doing slightly better at matching sucrose solubility in water-MeOH systems and significantly better at matching sucrose solubility in MeOH-EtOH.

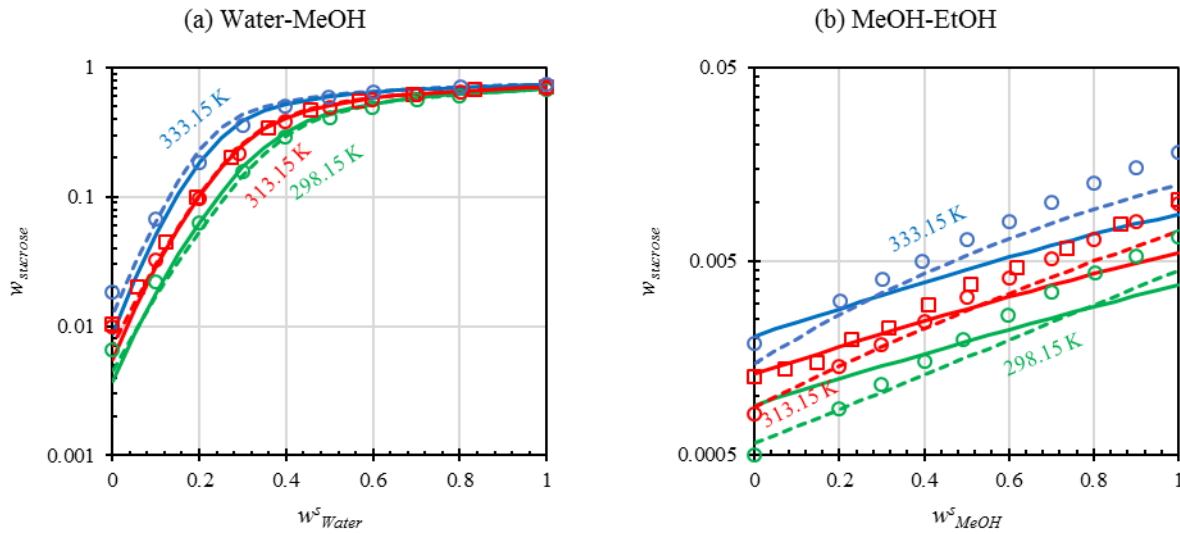


Figure 11: Solubility of sucrose in (a) water-MeOH and (b) MeOH-EtOH solutions, including the (—) NRTL and (- -) aNRTL model and data from (○) Macedo and Peres,¹⁵ and (□) Galvao et al.⁹ w^s is mass fraction in the solute-free solution.

Multi-sugar systems

The utility of these models for overall process modeling hinges on their ability to predict the phase behavior of mixtures containing multiple solutes. To test this ability, the parameters regressed from pure sugar data have been applied to mixtures containing two or more sugars and compared to the available experimental data.

Abderafi and Bounahmidi⁴² measured the boiling points of aqueous solutions of glucose, fructose, sucrose, mixtures of two sugars, and the mixture containing all three. While their data for binary sugar-water systems follow the behavior of similar measurements by other authors and can be well-described by the models, their data for multiple sugars have unusual curvature at low sugar mass fractions. This is particularly obvious in the case of mixtures of glucose and fructose, which each have a similar effect on boiling point elevation. It is unexpected that combining the two

might result in a significantly higher boiling point rise at low mass fractions than either of the substituent species, then level off and then follow the expected trends at high mass fractions. In solutions of sugar mixtures that contained sucrose, the sucrose was present in 20:1 mass ratio to the other sugar(s). This causes the predicted boiling point to be close to the boiling point of pure sucrose, while the reported boiling point rise frequently exceeded that caused by any of the sugars on their own. It is possible that the sugars, especially sucrose, degraded to some extent at the experimental conditions. In spite of these irregularities, both models capture the overall trends of the data as seen in **Figure 12**.

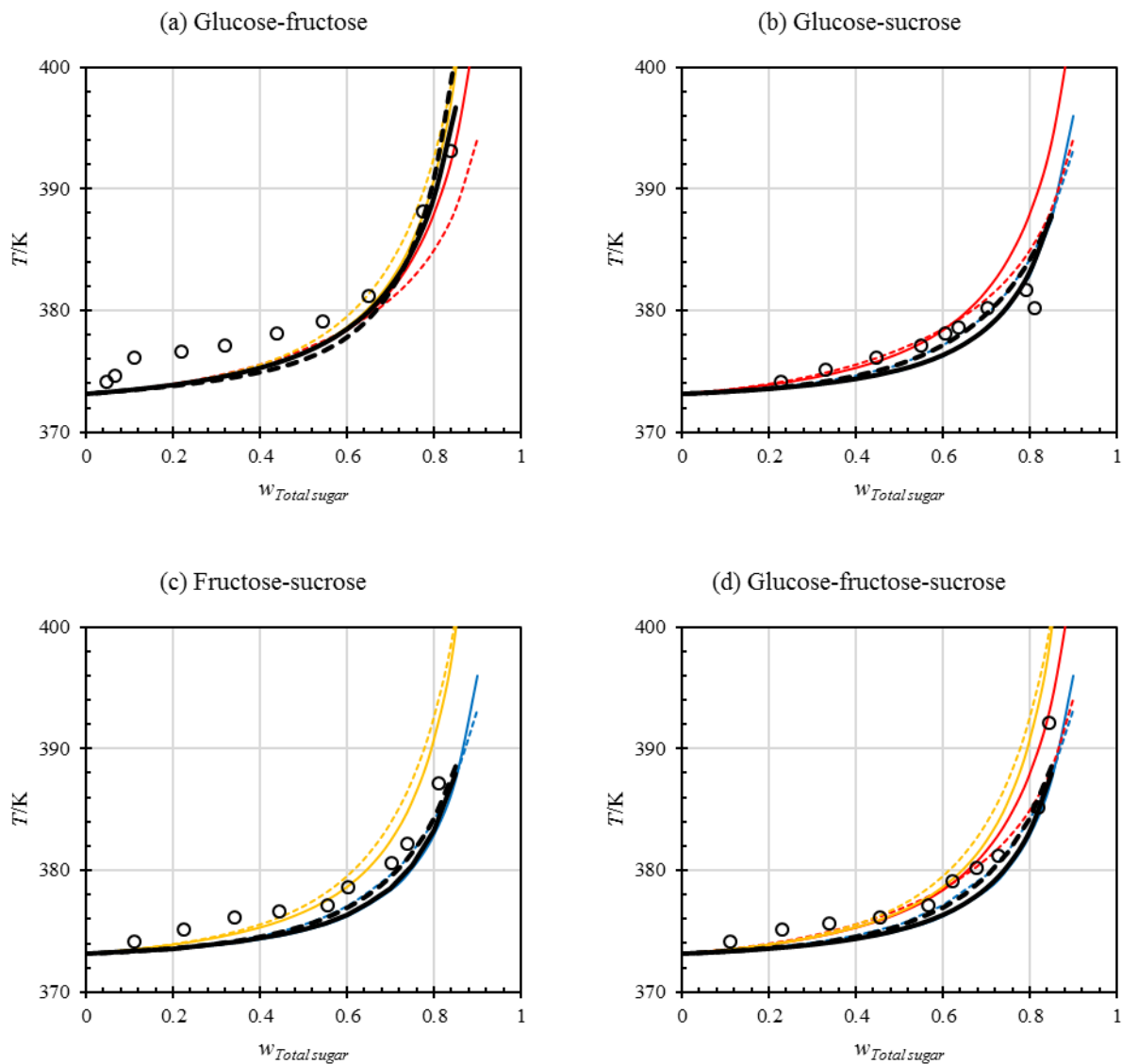


Figure 12. Boiling point elevation of (a) glucose+fructose(1:1)-, (b) glucose+sucrose(1:20)-, (c) fructose+sucrose(1:20)-, and (d) glucose+fructose+sucrose(1:1:20)-water solutions (mass ratios), including the (—) NRTL and (- -) aNRTL model and data from (○) Abderafi and Bounahmidi.⁴² Colored lines indicate the boiling point rise accurately predicted by each model for the pure sugars as a reference: red lines refer to glucose, orange to fructose, blue to sucrose, and black to total sugar.

Kelly³⁶ and Abed et al.¹² reported the solubility of mixtures of glucose or fructose and sucrose in water at 303.15 and 343.15 K, respectively. The models both accurately predict the solubility of each sugar in the mixture, as seen in **Figure 13**. Both models capture the invariant point for the glucose-sucrose system, the inverted “peak” in total sugar solubility observed where both sugars are found in the solid phase. To the left and right of this point, the sugar in the solid phase corresponds to the left and right single-sugar system, respectively. For example, to the left of the invariant point in **Figure 13(b)**, fructose is in the solid phase, while to the right of the invariant point sucrose is in the solid phase. As observed by the experimentalists, the location of the invariant point corresponds to the relative solubility of the two sugars, with the similarly soluble glucose and fructose having an invariant point where the dissolved mass of the sugars is roughly equal, while the invariant point of the fructose-sucrose system is in a location with higher fructose mass fraction.

The NRTL model closely captures the invariant point for the fructose-sucrose system, while the aNRTL model predicts the invariant point shifted to the right with a very indistinct local maximum. As the aNRTL model performs so well overall, and accurately predicts the invariant point for glucose-sucrose and fructose-glucose mixtures, it seems that this particular combination is an outlier of model performance. The most likely cause is that the great difference in association strength causes a slight offset in the predicted solubility of each sugar, which is amplified when adding them together to calculate the total solubility.

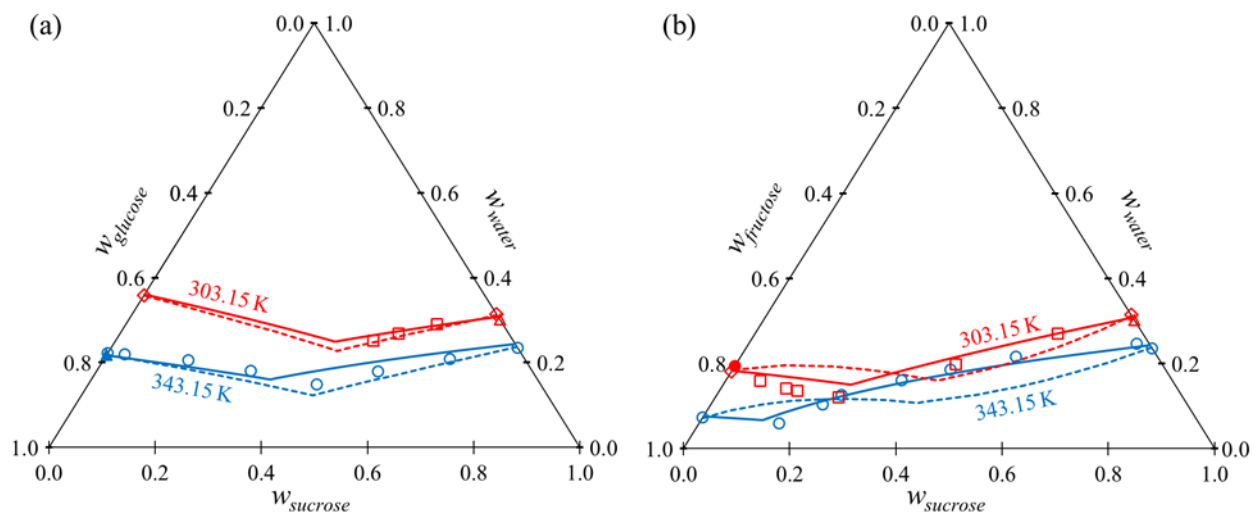


Figure 13: Mutual solubility of (a) glucose+sucrose and (b) fructose+sucrose, including the (—) NRTL and (- -) aNRTL models and data from (○) Abed et al.¹², (□) Kelly³⁶, (◇) Young et al.³⁷⁻³⁹, (△) Galvao et al.⁹, (▲) Jackson and Silsbee,³⁵ and (●) Alavi et al.¹

Flood and Puagsa⁵⁷ measured the solubility of glucose-fructose dissolved in three EtOH-water solutions at 303.15 K. **Figure 14** compares the model results to experimental data for these systems and systems with higher concentrations of water. The models are offset from the data at 40% and 60% EtOH solutions, perhaps due to the presence of metastable glucose·monohydrate³⁴ in the solid phase. There is no corroborating data for pure glucose in these solvent mixtures at 303.15 K, but the models are consistent with the other available data around this temperature. When the model and Flood and Puagsa's⁵⁷ data agree with the pure glucose solubility, as for 80% EtOH solution the predictions are within the spread of the data. Both models predict the invariant point for mixtures of the two sugars consistent with the maximum measured solubility.

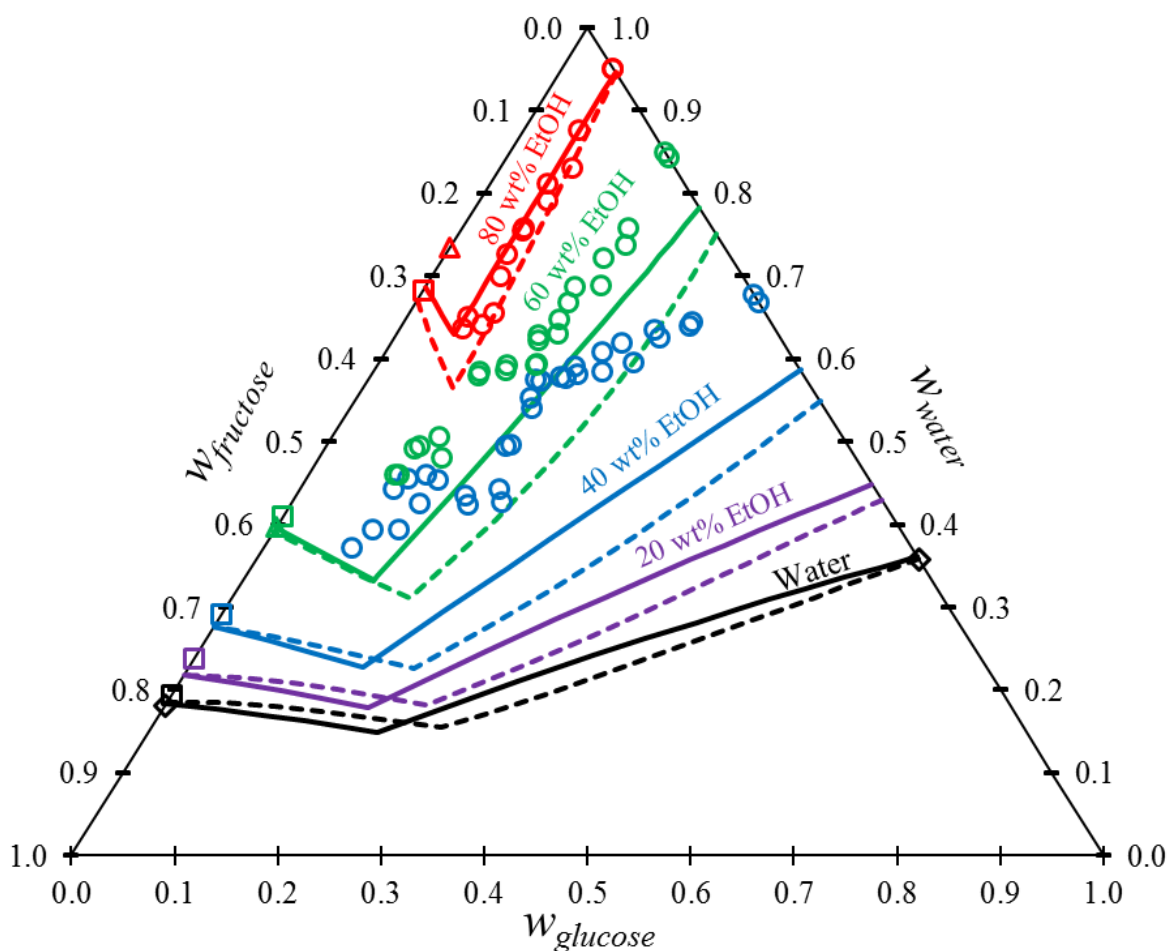


Figure 14: Mutual solubility of glucose-fructose in EtOH-water solutions at 303.15 K, including the (—) NRTL and (- -) aNRTL models and data from (○) Flood and Puagsa⁵⁷, (□) Alavi et al.¹, (△) Flood et al.²⁴, and (◇) Young et al.³⁷⁻³⁸

CONCLUSIONS

Both models presented here provide an accurate description of the experimental data in all but a few outlying cases. The NRTL model works well because, due to the high concentration of hydroxyl groups on each of the sugars, water, and alcohols, the species are quite similar from an interaction standpoint. Accordingly, the NRTL model may be used to adequately describe the phase equilibrium of sugar-containing systems when aNRTL parameters are not available for the

other components and it is not practical to regress them. The inclusion of the association term provides an improvement over the base NRTL model that is most effective for sucrose, effective for glucose, and least effective for fructose. The aNRTL model is thus able to better predict the solubility of glucose and sucrose, consistently matching the curvature of the data. Both models demonstrate the ability to accurately predict the phase behavior of systems containing multiple sugars from only sugar-solvent binary parameters. This bodes well for the continued use of NRTL, and especially aNRTL, to describe other sugars, such as xylose, and the anhydrous derivatives of xylose and glucose, xylosan and levoglucosan, which are important products of biomass pyrolysis. The well-defined association parameters and consistency of the interaction parameters, in their progression from water to MeOH to EtOH, are promising signs that these models can be readily extended to include additional solvents and similarly structured sugars. Additional measurements of the boiling point rise of multi-sugar systems would be needed to validate the single set of available data. To further extend the predictive ability of aNRTL requires additional data for the phase equilibrium of sugars in non-associating solvents. With the recently developed association-NRTL-Segment Activity Coefficient (aNRTL-SAC) model,³¹ the phase behavior of each sugar in a few solvents can be used to regress sugar-specific parameters that will apply in any solvent or solvent mixture without any additional regression.

ASSOCIATED CONTENT

Supporting Information.

The following files are available free of charge.

Assignment of standard deviations and error analysis for parameter regression (.pdf)

Microsoft Excel workbook containing data used in parameter regression (.xlsx)

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Notes

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Supporting Information

for

Modeling Phase Equilibrium of Common Sugars Glucose, Fructose, and Sucrose in Mixed Solvents

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4 pages, 1 table, 1 reference list

Assignment of standard deviations for data regression

Especially when dealing with older data, it is common for authors not to report the error in their measurements. When a standard deviation is given, there is little consistency between authors in how they account for error, if they describe their methods at all. To avoid bias toward the data that happens to report the lowest error, the authors of this work assigned standard values of error to the experimental measurements. These standards were relaxed or tightened to account for data sets that deviate from comparable sets or data points that had particularly small values. For example, the boiling point measurements of Abderafi and Bounahmidi¹ were given a higher standard deviation as their data sets tended to deviate from other sets of boiling point data (Maximo et al.², Leschke³). As another example, due to the low solubility of glucose and sucrose in methanol and ethanol, some data sets were given 20-30% standard deviation when the concentration of sugar dropped below 10% of the standard assigned value of 0.005 fraction.

Vapor-liquid equilibrium (VLE) data that was collected at a constant temperature or pressure was given a standard deviation of 0 for the respective state variable. The sugars were assumed to be nonvolatile, so the concentrations of sugar in the vapor phase for VLE measurements were set to 0 with a standard deviation of 0. For activity of water data, the activity coefficient of the sugar was left blank and given a standard deviation of 100%.

Every data set used for data regression is included in the Microsoft Excel workbook in the Supplemental Information in the same format as it was entered into Aspen Properties.⁴ The source of each data set is identified by "Author List (Year)" at the top of each data table, with the reader referred to the references list in the manuscript for citation details. If needed, a source journal abbreviation is included to differentiate between referenced documents published by the same author(s) in the same year. For each data set, the first column represents the usage of the numbers in that row: STD-DEV (assignment of standard deviation), DATA (data used in regression), and Ignore (applied to very few points that

were rejected for abnormal behavior). The rows marked STD-DEV apply to all of the rows beneath them, with any new STD-DEV superseding the last. For any system with C components, $C-1$ component concentrations are assigned standard deviations, with the last component concentration automatically calculated and assigned a standard deviation of 0. All in all, the 1202 data points used in data regression contained approximately 2950 values.

Error analysis

The Aspen Properties regression program calculates the weighted sum of squares (WSS) and the residual root mean squared error ($RMSE$) as a measure of goodness of fit for regressed property model parameters (see manuscript for definitions). With a large data set, these measures become desensitized to the addition of potentially spurious parameters. Information criteria, which balance the likelihood function against the number of parameters, provide a way to avoid this problem. Three information criteria were calculated in addition to the WSS and $RMSE$ reported by Aspen Properties. These were the Mallows information criterion (MIC),⁵

$$MIC = (K - q) \left(\frac{SSE}{SSE_q} \right) + 2n - K \quad (S-1)$$

the Akaike information criterion (AIC),⁶

$$AIC = K \ln \left(\frac{SSE}{K} \right) + 2n \quad (S-2)$$

and the Bayesian information criterion (BIC).⁶

$$BIC = K \ln \left(\frac{SSE}{K} \right) + n \ln K \quad (S-3)$$

where K is the number of data points, n is the number of parameters, q is the number of parameters of the full (reference) model, SSE is the sum of squared error, and SSE_q is the sum of squared error for the reference model with q parameters. As mentioned in the manuscript, SSE was replaced by WSS (automatically calculated and reported by Aspen Properties) for comparison of the models. This means that the information criteria reported here are modified versions, and because of this, the values of the modified AIC and BIC are often negative.

Table S-1 presents the results of the statistical analysis of the models. The aNRTL with variable r was chosen as the full, $n = q$, model for comparison of the MIC . All four measures – $RMSE$ and the three modified information criteria – agree that the aNRTL (with variable r) model provides the best fit of the three options investigated. Fixing r reduces the number of adjustable parameters, but significantly increases the sum of squares and, thus, the values of the information criteria.

Table S-1: Comparison between measures of goodness of fit for the three model alternatives (*MIC*, *AIC*, and *BIC* modified to use *WSS* in place of *SSE*).

GLUCOSE							
Model	<i>n</i>	<i>WSS</i>	<i>RMSE</i>	<i>K</i>	<i>MIC</i>	<i>AIC</i>	<i>BIC</i>
NRTL	10	438.2	0.9438	503	121.7	-49.3	-7.1
aNRTL	13	355.1	0.8522	503	13.0	-149.1	-94.2
aNRTL (<i>r</i> fixed)	12	800.5	1.2781	503	625.5	257.7	308.3
FRUCTOSE							
Model	<i>n</i>	<i>WSS</i>	<i>RMSE</i>	<i>K</i>	<i>MIC</i>	<i>AIC</i>	<i>BIC</i>
NRTL	10	343.8	0.9785	370	100.1	-7.2	31.9
aNRTL	13	272.7	0.8752	370	13.0	-86.9	-36.1
aNRTL (<i>r</i> fixed)	12	467.7	1.1446	370	266.3	110.7	157.6
SUCROSE							
Model	<i>n</i>	<i>WSS</i>	<i>RMSE</i>	<i>K</i>	<i>MIC</i>	<i>AIC</i>	<i>BIC</i>
NRTL	10	156.9	0.7025	329	294.3	-223.5	-185.6
aNRTL	13	82.20	0.5108	329	13.0	-430.3	-381.0
aNRTL (<i>r</i> fixed)	12	178.95	0.7525	329	383.0	-176.3	-130.8

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				DATA	40	33.087	26.84416	40.0688				
				DATA	40	43.069	27.39747	29.5335				
				DATA	40	51.806	28.68266	19.5113				
				DATA	40	61.612	30.57182	7.81618				
				DATA	40	67.332	32.668	0				
				DATA	60	1.056	0	98.944				
				DATA	60	5.064	9.515435	85.4206				
				DATA	60	17.077	16.49919	66.4238				
				DATA	60	31.907	19.38063	48.7124				
				DATA	60	48.984	20.73086	30.2851				
				DATA	60	56.887	21.50735	21.6056				
				DATA	60	63.247	22.00476	14.7482				
				DATA	60	71.13	23.09282	5.77718				
				DATA	60	75.071	24.929	0				
				Leontarakis & al. (2005)								
				X: Mole Fraction								
				Usage	TEMPERAT	X	X	X				
					C	GLUCOSE	WATER	ETHANOL				
				STD-DEV	0.5	30%	0.005	0				
				DATA	40	0.001264	0	0.998736				
				DATA	60	0.003066	0	0.996934				
				DATA	40	0.006032	0.21989	0.774078				
				DATA	60	0.01232	0.218499	0.769181				
				Alves, Almeida e Silva, & Giuletta (2007)								
				X: Mass Percent			EXCLUDED FROM REGRESSION					
				Usage	TEMPERAT	X	X	X				
					C	GLUCOSE	ETHANOL	WATER				
				STD-DEV	0.1	0.5	0.5	0				
				DATA	10	40.4	0	59.6				
				DATA	20	47.8	0	52.2				
				DATA	30	53.4	0	46.6				
				DATA	40	60.3	0	39.7				
				DATA	50	67.2	0	32.8				

Solubility		Glucose-Methanol-Ethanol Solubility					Glucose-Methanol-Water Solubility			
Peres, & Fornari (2007)		Peres & Macedo (1997, I&ECR)					Peres & Macedo (1997, I&ECR)			
X		X: Mass Percent					X: Mass Percent			
GLUCOSE	METHANOL	Usage	TEMPERAT	X	X	X	Usage	TEMPERAT	X	X
0.005	0		C	GLUCOSE	ETHANOL	METHANOL		C	GLUCOSE	WATER
0.029649	0.970351	STD-DEV	0.1	0.5	0.5	0	STD-DEV	0.1	0.5	0.5
0.033748	0.966252	DATA	40	3.406	0	96.594	DATA	40	3.405	0
0.038725	0.961275	DATA	40	2.847	9.710442	87.4426	DATA	40	7.477	9.216216
		DATA	40	2.385	19.50836	78.1066	DATA	40	15.811	16.85295
		DATA	40	1.96	29.44141	68.5986	DATA	40	27.722	21.66244
		DATA	40	1.62	39.33134	59.0487	DATA	40	37.851	23.97646
		DATA	40	1.337	48.8372	49.8258	DATA	40	47.452	25.85467
		DATA	40	1.098	58.83284	40.0692	DATA	40	53.797	27.00658
		DATA	40	0.88	69.56737	29.5526	DATA	40	62.622	29.80073
		DATA	40	0.726	79.1462	20.1278	DATA	40	62.665	29.78474
		DATA	40	0.523	99.477	0	DATA	40	67.332	32.668
		DATA	60	6.643	0	93.357	DATA	60	6.643	0
		DATA	60	5.526	9.464405	85.0096	DATA	60	15.358	8.492132
		DATA	60	4.635	19.03676	76.3282	DATA	60	15.523	8.532177
		DATA	60	3.864	28.84753	67.2885	DATA	60	31.181	13.78376
		DATA	60	3.219	38.71046	58.0705	DATA	60	45.586	16.13974
		DATA	60	2.64	48.43757	48.9224	DATA	60	56.08	17.6128
		DATA	60	2.672	48.54039	48.7876	DATA	60	62.122	18.64469
		DATA	60	2.244	58.56171	39.1943	DATA	60	66.57	19.90355
		DATA	60	1.85	68.62844	29.5216	DATA	60	71.768	22.23552
		DATA	60	1.502	78.8772	19.6208	DATA	60	75.071	24.929
		DATA	60	1.056	98.944	0				
							van Putten, Winkelman, Keihan, van der Wa			
							X: Mole Fraction			
		Usage	TEMPERAT	X	X	X	Usage	TEMPERAT	X	X
			K	GLUCOSE	METHANO			K	GLUCOSE	METHANO
		STD-DEV	0.1	0.005	0.005		STD-DEV	0.1	0.005	0.005
		DATA	341.75	0.015076	0.984924		DATA	341.75	0.015076	0.984924

								DATA	348.85	0.019913	0.980087
								DATA	353.05	0.024188	0.975812
								DATA	330.95	0.007584	0.992416
								DATA	333.85	0.009598	0.990402
								DATA	337.15	0.011443	0.988557
								DATA	342.05	0.013614	0.986386
								DATA	324.85	0.005926	0.994074
								DATA	343.95	0.023684	0.892751
								DATA	347.25	0.029365	0.887556
								DATA	339.35	0.020508	0.897722
								DATA	344.65	0.024801	0.893787
								DATA	347.45	0.02898	0.889956
								DATA	323.35	0.008809	0.909623
								DATA	329.55	0.010899	0.908254
								DATA	334.85	0.014634	0.904824
								DATA	339.85	0.018955	0.900856
								DATA	328.35	0.017893	0.815555
								DATA	335.65	0.028564	0.806694
								DATA	320.45	0.014494	0.813881
								DATA	325.45	0.01599	0.812646
								DATA	327.15	0.017982	0.811001
								DATA	328.85	0.020455	0.808958
								DATA	330.95	0.022437	0.807321
								DATA	318.35	0.010614	0.824891
								DATA	336.05	0.026568	0.811589
								DATA	343.55	0.039994	0.800395
								DATA	347.65	0.051913	0.790458
								DATA	332.65	0.040096	0.730603
								DATA	338.05	0.050183	0.722926
								DATA	341.95	0.058809	0.71636
								DATA	345.45	0.069703	0.708069
								DATA	319.05	0.021405	0.729596
								DATA	322.25	0.025148	0.726805
								DATA	324.95	0.029113	0.723849
								DATA	327.75	0.033812	0.720345

0	DATA	37	0.0072	0.9928	0.999952	X: Mole Fraction	EXCLUDED FROM R
0	DATA	37	0.0107	0.9893	0.999887	Usage	TEMPERAT X X
0	DATA	37	0.0142	0.9858	0.999795		C GLUCOSE WATER
0	DATA	37	0.0177	0.9823	0.999677	STD-DEV	0.1 0.005 0
0	DATA	37	0.0212	0.9788	0.999509	DATA	20 0.08029 0.91971
0	DATA	37	0.0246	0.9754	0.999308	DATA	25 0.09447 0.90553
0	DATA	37	0.028	0.972	0.999015	DATA	30 0.11386 0.88614
0.083566	DATA	37	0.0314	0.9686	0.998674		
0.083079	DATA	37	0.0348	0.9652	0.998285		
0.081771	DATA	37	0.0431	0.9569	0.997035	Saldana, Alvarez, & Haldar (2012)	
0.081412	DATA	37	0.0513	0.9487	0.995463	X: Mass Fraction	EXCLUDED FROM R
0.081063	DATA	37	0.0593	0.9407	0.993632	Usage	TEMPERAT PRESSURE X
0.081568	DATA	37	0.0672	0.9328	0.991501		K bar GLUCOSE
0.080848	DATA	37	0.075	0.925	0.989153	STD-DEV	0.1 0.1 0.005
0.080542	DATA	37	0.0826	0.9174	0.986707	DATA	303 15 0.33687
0.080189	DATA	37	0.0902	0.9098	0.984023	DATA	323 15 0.397227
0.166552	DATA	37	0.0975	0.9025	0.981209	DATA	343 15 0.434389
0.164742	DATA	37	0.1048	0.8952	0.978294	DATA	373 15 0.5905
0.171625	DATA	37	0.112	0.888	0.975184	DATA	393 15 0.662618
0.171365	DATA	37	0.119	0.881	0.971882	DATA	413 15 0.755262
0.171018	DATA	37	0.126	0.874	0.96839	DATA	433 15 0.809124
0.170587	DATA	37	0.1328	0.8672	0.96486	DATA	303 80 0.291283
0.170242	DATA	37	0.1395	0.8605	0.961162	DATA	323 80 0.342105
0.164495	DATA	37	0.1461	0.8539	0.957301	DATA	343 80 0.387255
0.161843	DATA	37	0.1527	0.8473	0.953107	DATA	373 80 0.545661
0.159611	DATA	60	0.0826	0.9174	0.987152	DATA	393 80 0.617298
0.157629	DATA	60	0.0902	0.9098	0.984608	DATA	413 80 0.698159
0.229301	DATA	60	0.0975	0.9025	0.981951	DATA	433 80 0.742467
0.226891	DATA	60	0.1048	0.8952	0.979096	DATA	303 120 0.297753
0.224831	DATA	60	0.112	0.888	0.976168	DATA	323 120 0.339498
0.222228	DATA	60	0.119	0.881	0.973196	DATA	343 120 0.388379
0.248999	DATA	60	0.126	0.874	0.970066	DATA	373 120 0.538106
0.248047	DATA	60	0.1328	0.8672	0.966783	DATA	393 120 0.608457
0.247038	DATA	60	0.1395	0.8605	0.963347	DATA	413 120 0.684244
0.245842	DATA	60	0.1461	0.8539	0.959926	DATA	433 120 0.722684

0.244797	DATA	60	0.1527	0.8473		0.956375				
0.242001										
0.241065	Stokes & Robinson (1966)									
0.240055	X: Mole Fraction		T: 25 C							
0.238876	Usage	X	X	GAMMA	GAMMA					
0.237413		GLUCOSE	WATER	GLUCOSE	WATER					
0.238321	STD-DEV	0.005	0%	100%	0.005					
0.291243	DATA	0.0182	0.9818		0.999626					
0.290655	DATA	0.0348	0.9652		0.997565					
0.288697	DATA	0.0513	0.9487		0.994333					
0.286435	DATA	0.0672	0.9328		0.990002					
0.283985	DATA	0.0826	0.9174		0.984754					
0.299239	DATA	0.0975	0.9025		0.978666					
0.310832	DATA	0.112	0.888		0.972114					
0.309351	DATA	0.119	0.881		0.968735					
0.30797										
0.306054	Miyajima, Sawada, & Nakagaki (1983)									
0.304214	X: Mole Fraction		T: 25 C							
0.363344	Usage	X	X	GAMMA	GAMMA					
0.361495		GLUCOSE	WATER	GLUCOSE	WATER					
0.359416	STD-DEV	0.005	0	100%	0.005					
0.339379	DATA	0.0018	0.9982		0.999996					
0.324419	DATA	0.0036	0.9964		0.999986					
0.378212	DATA	0.0054	0.9946		0.999964					
0.375875	DATA	0.0072	0.9928		0.999938					
0.373619	DATA	0.0089	0.9911		0.999896					
0.370587	DATA	0.0107	0.9893		0.999833					
	DATA	0.0125	0.9875		0.999769					
	DATA	0.0142	0.9858		0.99968					
	DATA	0.016	0.984		0.999577					
	DATA	0.0177	0.9823		0.99946					
	DATA	0.0212	0.9788		0.999185					
	DATA	0.0246	0.9754		0.998829					
	DATA	0.028	0.972		0.998439					
	DATA	0.0314	0.9686		0.997961					

	DATA	0.0348	0.9652		0.997422				
	DATA	0.0431	0.9569		0.995824				
	DATA	0.0513	0.9487		0.993957				
	DATA	0.0593	0.9407		0.991754				
	DATA	0.0672	0.9328		0.98936				
	DATA	0.075	0.925		0.98675				
	DATA	0.0826	0.9174		0.983956				
	DATA	0.0902	0.9098		0.981005				
	DATA	0.0975	0.9025		0.977926				
	Hu & Wang (1997)								
	X: Mole Fraction		T: 298.15 K						
	Usage	X	X	GAMMA	GAMMA				
		GLUCOSE	WATER	GLUCOSE	WATER				
	STD-DEV	0.005	0	100%	0.005				
	DATA	0.010757	0.989243		0.999829				
	DATA	0.010762	0.989238		0.999834				
	DATA	0.010799	0.989201		0.999832				
	DATA	0.014538	0.985462		0.999651				
	DATA	0.0149	0.9851		0.999611				
	DATA	0.017745	0.982255		0.999453				
	DATA	0.017783	0.982217		0.999448				
	DATA	0.018454	0.981546		0.999383				
	DATA	0.027004	0.972996		0.998569				
	DATA	0.035557	0.964443		0.997182				
	DATA	0.04204	0.95796		0.995893				
	DATA	0.054449	0.945551		0.992994				
	DATA	0.059529	0.940471		0.991514				
	DATA	0.067158	0.932842		0.989201				
	DATA	0.074867	0.925133		0.986507				
	DATA	0.081086	0.918914		0.984333				
	DATA	0.088457	0.911543		0.98144				
	DATA	0.097436	0.902564		0.977611				
	DATA	0.113948	0.886052		0.970314				

Ebrahimi & Sadeghi (2016)				
X: Mole Fraction		T: 308.15 K		
Usage	X	X	GAMMA	GAMMA
	GLUCOSE	WATER	GLUCOSE	WATER
STD-DEV	0.005	0	100%	0.005
DATA	0.001002	0.998998		1.000002
DATA	0.002024	0.997976		1.000024
DATA	0.003026	0.996974		1.000026
DATA	0.004012	0.995988		1.000012
DATA	0.00522	0.99478		0.99992
DATA	0.006335	0.993665		0.999935
DATA	0.007298	0.992702		0.999898
DATA	0.008529	0.991471		0.999928
DATA	0.009603	0.990397		0.999902
DATA	0.010178	0.989822		0.999877
DATA	0.011062	0.988938		0.99986
DATA	0.012128	0.987872		0.999826
DATA	0.013063	0.986937		0.99976
DATA	0.014142	0.985858		0.999739
DATA	0.016103	0.983897		0.999698
DATA	0.018032	0.981968		0.999625
DATA	0.019593	0.980407		0.999482
DATA	0.021419	0.978581		0.999407
DATA	0.023272	0.976728		0.999357
DATA	0.027485	0.972515		0.998956
DATA	0.032094	0.967906		0.998444
DATA	0.041219	0.958781		0.997204
DATA	0.050384	0.949616		0.995456
DATA	0.06132	0.93868		0.992884
DATA	0.080306	0.919694		0.98685

Glucose-Water Boiling Point							Glucose-Water Vapor Pressure		
Abderafi & Bounahmidi (1994)							Taylor & Rowlinson (1955)		
X/Y: Mass Fraction							X/Y: Mole Fraction		
Usage	TEMPERATURE	PRESSURE	X	X	Y	Y	Usage	TEMPERATURE	PRESSURE
	C	N/sqm	GLUCOSE	WATER	GLUCOSE	WATER		C	mmHg
STD-DEV	0.1	0	0.01	0	0	0	STD-DEV	0	1
DATA	100.2	101320	0.045	0.955	0	1	DATA	25	23.756
DATA	100.4	101320	0.055	0.945	0	1	DATA	25	23.476
DATA	100.6	101320	0.105	0.895	0	1	DATA	25	22.563
DATA	100.7	101320	0.12	0.88	0	1	DATA	25	21.727
DATA	101.3	101320	0.21	0.79	0	1	DATA	25	21.151
DATA	101.4	101320	0.25	0.75	0	1	DATA	25	21.117
DATA	101.6	101320	0.335	0.665	0	1	DATA	25	20.668
DATA	101.8	101320	0.41	0.59	0	1	DATA	25	19.943
DATA	103	101320	0.45	0.55	0	1	DATA	25	19.002
DATA	104	101320	0.555	0.445	0	1	DATA	25	17.751
DATA	106	101320	0.64	0.36	0	1	DATA	35	42.175
Ignore	107.7	101320	0.815	0.185	0	1	DATA	35	38.666
Ignore	113	101320	0.875	0.125	0	1	DATA	35	38.59
							DATA	35	37.504
							DATA	35	36.781
Maximo, Meirelles, & Batista (2010)							DATA	35	36.097
X/Y: Mass Percent							DATA	35	35.484
Usage	TEMPERATURE	PRESSURE	X	X	Y	Y	DATA	35	33.619
	K	kPa	GLUCOSE	WATER	GLUCOSE	WATER	DATA	35	31.585
STD-DEV	0.1	0	0.5	0	0	0	DATA	45	71.88
DATA	333.9	20	10.2	89.8	0	100	DATA	45	65.86
DATA	334.4	20	20.3	79.7	0	100	DATA	45	65.8
DATA	334.3	20	28	72	0	100	DATA	45	63.95
DATA	335	20	39.1	60.9	0	100	DATA	45	62.74
DATA	336.1	20	49.2	50.8	0	100	DATA	45	60.59
DATA	337.9	20	60.4	39.6	0	100	DATA	45	57.8
DATA	340.2	26.7	10.2	89.8	0	100	DATA	45	54.11
DATA	340.7	26.7	20.3	79.7	0	100			

REGRESSION	DATA	340.8	26.7	28.7	71.3	0	100	DATA	55	118.04
	DATA	341.1	26.7	39.1	60.9	0	100	DATA	55	108.15
	DATA	342.4	26.7	49.2	50.8	0	100	DATA	55	105.18
	DATA	344.3	26.7	60.4	39.6	0	100	DATA	55	102.97
	DATA	345.6	33.3	10.3	89.7	0	100	DATA	55	100.12
	DATA	346.2	33.3	20.2	79.8	0	100	DATA	55	95.24
	DATA	346.1	33.3	28.9	71.1	0	100	DATA	55	89.19
	DATA	346.7	33.3	39.3	60.7	0	100	DATA	65	187.54
	DATA	347.7	33.3	49.2	50.8	0	100	DATA	65	172.06
REGRESSION	DATA	349.6	33.3	60.5	39.5	0	100	DATA	65	167.69
X	DATA	349.9	40	10.3	89.7	0	100	DATA	65	163.98
WATER	DATA	350.4	40	20.2	79.8	0	100	DATA	65	159.45
0	DATA	350.7	40	29	71	0	100	DATA	65	151.57
0.66313	DATA	350.7	40	39.5	60.5	0	100	DATA	65	142.34
0.602773	DATA	352.3	40	49.3	50.7	0	100			
0.565611	DATA	354.1	40	60.5	39.5	0	100	Cooke, Jonsdottir, & Westh (2002)		
0.4095	DATA	353.7	46.7	10.3	89.7	0	100	X/Y: Mole Fraction		
0.337382	DATA	354.4	46.7	20.2	79.8	0	100	Usage	TEMPERAT	PRESSURE
0.244738	DATA	354	46.7	28.9	71.1	0	100		K	kPa
0.190876	DATA	354.9	46.7	39.4	60.6	0	100	STD-DEV	0	0.5
0.708717	DATA	355.7	46.7	49.3	50.7	0	100	DATA	298.06	3.152
0.657895	DATA	357.6	46.7	60.5	39.5	0	100	DATA	298.06	3.075
0.612745	DATA	357	53.3	10.3	89.7	0	100	DATA	298.06	3.07
0.454339	DATA	357.7	53.3	20.2	79.8	0	100	DATA	298.06	3.067
0.382702	DATA	357.4	53.3	28.8	71.2	0	100	DATA	298.06	3.059
0.301841	DATA	358.1	53.3	39.3	60.7	0	100	DATA	298.06	3.054
0.257533	DATA	359.2	53.3	49.4	50.6	0	100	DATA	298.06	3.061
0.702247	DATA	361	53.3	60.6	39.4	0	100	DATA	298.06	3.048
0.660502	DATA	360	60	10.3	89.7	0	100	DATA	298.06	3.048
0.611621	DATA	360.7	60	20.3	79.7	0	100	DATA	298.06	3.038
0.461894	DATA	360.4	60	29	71	0	100	DATA	298.06	3.038
0.391543	DATA	361.1	60	39.4	60.6	0	100	DATA	298.06	3.027
0.315756	DATA	362.2	60	49.5	50.5	0	100	DATA	298.06	3.018
0.277316	DATA	364.3	60	60.6	39.4	0	100	DATA	298.06	3.01
	DATA	362.7	66.7	10.4	89.6	0	100	DATA	298.06	3

Pressure			
X	X	Y	Y
GLUCOSE	WATER	GLUCOSE	WATER
0.005	0	0	0
0	1	0	1
0.0118	0.9882	0	1
0.0508	0.9492	0	1
0.0761	0.9239	0	1
0.0934	0.9066	0	1
0.095	0.905	0	1
0.1091	0.8909	0	1
0.1304	0.8696	0	1
0.1598	0.8402	0	1
0.195	0.805	0	1
0	1	0	1
0.0761	0.9239	0	1
0.0761	0.9239	0	1
0.0951	0.9049	0	1
0.1093	0.8907	0	1
0.1212	0.8788	0	1
0.1305	0.8695	0	1
0.1601	0.8399	0	1
0.1954	0.8046	0	1
0	1	0	1
0.0763	0.9237	0	1
0.0763	0.9237	0	1
0.0953	0.9047	0	1
0.1095	0.8905	0	1
0.1308	0.8692	0	1
0.1603	0.8397	0	1
0.1959	0.8041	0	1

0	1	0	1
0.0763	0.9237	0	1
0.0955	0.9045	0	1
0.1096	0.8904	0	1
0.131	0.869	0	1
0.1606	0.8394	0	1
0.1962	0.8038	0	1
0	1	0	1
0.0763	0.9237	0	1
0.0953	0.9047	0	1
0.1098	0.8902	0	1
0.1313	0.8687	0	1
0.1611	0.8389	0	1
0.1969	0.8031	0	1
)			
X	X	Y	Y
GLUCOSE	WATER	GLUCOSE	WATER
0.005	0	0	0%
0	1	0	1
0.022108	0.977892	0	1
0.023007	0.976993	0	1
0.023995	0.976005	0	1
0.026569	0.973431	0	1
0.026742	0.973258	0	1
0.028142	0.971858	0	1
0.02978	0.97022	0	1
0.030608	0.969392	0	1
0.03201	0.96799	0	1
0.03361	0.96639	0	1
0.03572	0.96428	0	1
0.03761	0.96239	0	1
0.03937	0.96063	0	1
0.0424	0.9576	0	1

0.04439	0.95561	0	1
0.0484	0.9516	0	1
0.05007	0.94993	0	1
0.05337	0.94663	0	1
0.05574	0.94426	0	1
0.05958	0.94042	0	1
0.06605	0.93395	0	1
0.06854	0.93146	0	1
0.0815	0.9185	0	1
0.0948	0.9052	0	1
0.0998	0.9002	0	1
0.1195	0.8805	0	1
0.1286	0.8714	0	1
0.1382	0.8618	0	1
0	1	0	1
0.025011	0.974989	0	1
0.029211	0.970789	0	1
0.03917	0.96083	0	1
0.04791	0.95209	0	1
0.05699	0.94301	0	1
0.06607	0.93393	0	1
0.08855	0.91145	0	1
0.10023	0.89977	0	1
0.12058	0.87942	0	1
0.141	0.859	0	1
0.1614	0.8386	0	1
0.1819	0.8181	0	1
0.2024	0.7976	0	1
0.2285	0.7715	0	1
X	Y	Y	
WATER	GLUCOSE	WATER	
0%	0	0	

Fructose-Ethanol Solubility

Montanes, Olano, Ibanez, & Fornari (2007)

X: Mole Fraction

Usage	TEMPERAT C	X FRUCTOSE	X ETHANOL
STD-DEV	0.1	0.001	0
DATA	22	0.005677	0.994323
DATA	30	0.007418	0.992582
DATA	40	0.012139	0.987861

Fructose-Ethanol-Water Solubility

Flood, Addai-Mensah, Johns, & White (1996)

X: Mass Fraction

Usage	TEMPERAT C	X FRUCTOSE	X ETHANOL	X WATER
STD-DEV	0.1	0.005	0.005	0
DATA	30	0.754	0.074	0.172
DATA	30	0.603	0.237	0.16
DATA	30	0.493	0.354	0.153
DATA	30	0.37	0.492	0.138
DATA	30	0.359	0.508	0.133
DATA	30	0.266	0.586	0.148
DATA	30	0.23	0.65	0.12
DATA	30	0.158	0.713	0.129
DATA	30	0.206	0.683	0.111
DATA	30	0.162	0.731	0.107
DATA	30	0.11	0.798	0.092
DATA	30	0.076	0.852	0.072
DATA	30	0.054	0.896	0.05
DATA	30	0.046	0.927	0.027
DATA	30	0.035	0.962	0.003
DATA	40	0.774	0.068	0.158
DATA	40	0.672	0.196	0.132
DATA	40	0.576	0.296	0.128
DATA	40	0.451	0.425	0.124
DATA	40	0.386	0.49	0.124
DATA	40	0.26	0.627	0.113
DATA	40	0.3	0.595	0.105
DATA	40	0.278	0.621	0.101
DATA	40	0.256	0.644	0.1
DATA	40	0.203	0.703	0.094
DATA	40	0.156	0.757	0.087
DATA	40	0.105	0.825	0.07
DATA	40	0.098	0.854	0.048
DATA	40	0.076	0.898	0.026
DATA	40	0.033	0.964	0.003
DATA	50	0.812	0.056	0.132
DATA	50	0.714	0.171	0.115
DATA	50	0.661	0.237	0.102
DATA	50	0.501	0.398	0.101
DATA	50	0.348	0.552	0.1
DATA	50	0.254	0.669	0.077
DATA	50	0.171	0.764	0.065
DATA	50	0.119	0.834	0.047
DATA	50	0.082	0.892	0.026
DATA	50	0.045	0.952	0.003

Macedo & Peres (2001)**X: Mass Percent**

Usage	TEMPERAT C	X FRUCTOSE	X WATER	X ETHANOL
STD-DEV	0.1	0.5	0.5	0
DATA	25	1.702	0	98.298
DATA	25	10.207	9.00085	80.7921
DATA	25	31.332	13.71369	54.9543
DATA	25	50.278	14.90815	34.8139
DATA	25	60.243	15.85946	23.8975
DATA	25	66.641	16.66315	16.6958
DATA	25	70.991	17.35231	11.6567
DATA	25	76.96	18.48753	4.55247
DATA	25	80.104	19.896	0
DATA	40	3.008	0	96.992
DATA	40	7.602	4.643	87.755
DATA	40	18.147	8.21722	73.6358
DATA	40	48.874	10.27581	40.8502
DATA	40	61.902	11.38559	26.7124
DATA	40	69.224	12.28301	18.493
DATA	40	74.436	12.76564	12.7984
DATA	40	77.87	13.25698	8.87302
DATA	40	81.964	14.32563	3.71037
DATA	40	84.365	15.635	0
DATA	60	6.501	0	93.499
DATA	60	20.204	3.92118	75.8748
DATA	60	58.828	4.05915	37.1128
DATA	60	74.307	5.10006	20.5929
DATA	60	81.596	5.52967	12.8743
DATA	60	84.825	6.09322	9.08178
DATA	60	86.719	6.61248	6.66852
DATA	60	88.978	6.70082	4.32118
DATA	60	91.247	7.15435	1.59865
DATA	60	92.449	7.551	0

Gong, Wang, & Qu. Thermo. Chem. Eng. Data. (2011)**X: Mass Fraction**

Usage	TEMPERAT K	X FRUCTOSE	X ETHANOL	X WATER
STD-DEV	0.1	0.005	0.005	0
DATA	273.2	0.007	0.993	0
DATA	273.2	0.0405	0.86355	0.09595
DATA	273.2	0.1462	0.68304	0.17076
DATA	273.2	0.3216	0.47488	0.20352
DATA	273.2	0.4487	0.33078	0.22052
DATA	273.2	0.5344	0.2328	0.2328

DATA	278.2	0.0079	0.9921	0
DATA	278.2	0.0455	0.85905	0.09545
DATA	278.2	0.1701	0.66392	0.16598
DATA	278.2	0.3557	0.45101	0.19329
DATA	278.2	0.4691	0.31854	0.21236
DATA	278.2	0.569	0.2155	0.2155
DATA	283.2	0.0109	0.9891	0
DATA	283.2	0.053	0.8523	0.0947
DATA	283.2	0.2166	0.62672	0.15668
DATA	283.2	0.3755	0.43715	0.18735
DATA	283.2	0.5277	0.28338	0.18892
DATA	283.2	0.6127	0.19365	0.19365
DATA	288.2	0.0121	0.9879	0
DATA	288.2	0.0655	0.84105	0.09345
DATA	288.2	0.2483	0.60136	0.15034
DATA	288.2	0.4498	0.38514	0.16506
DATA	288.2	0.5576	0.26544	0.17696
DATA	288.2	0.6222	0.1889	0.1889
DATA	293.2	0.0143	0.9857	0
DATA	293.2	0.0769	0.83079	0.09231
DATA	293.2	0.2874	0.57008	0.14252
DATA	293.2	0.487	0.3591	0.1539
DATA	293.2	0.5808	0.25152	0.16768
DATA	293.2	0.66	0.17	0.17

Alavi, Pazuki, & Raisi. J. Food Sci. (2014)

X: Mole Percent

Usage	TEMPERAT C	X FRUCTOSE	X WATER	X ETHANOL
STD-DEV	0.1	0.5	0.5	0
DATA	20	7.5	36.0745	56.4255
DATA	30	8.3	35.7625	55.9375
DATA	40	15.15	33.091	51.759
DATA	20	17.8	51.8104	30.3896
DATA	30	18.55	51.3377	30.1123
DATA	40	25.26	47.1084	27.6316
DATA	20	23.3	60.8397	15.8603
DATA	30	24.37	59.9909	15.6391
DATA	40	28.8	56.477	14.723
DATA	20	25.5	67.8655	6.6345
DATA	30	26.8	66.6813	6.5187
DATA	40	31.77	62.1539	6.0761
DATA	20	27.44	69.5387	3.0213
DATA	30	28.1	68.9061	2.9939
DATA	40	32.5	64.6894	2.8106
DATA	20	28.19	71.81	0
DATA	30	29.33	70.67	0

DATA

40

33.49

66.51

0

Fructose-Methanol Solubility

Montanes, Olano, Ibanez, & Fornari (2007)

X: Mass Fraction

Usage	TEMPERAT C	X FRUCTOSE	X METHANOL
STD-DEV	0.1	0.005	0
DATA	22	0.167314	0.832686
DATA	30	0.226138	0.773862
DATA	40	0.264937	0.735063

Fructose-Methanol-Ethanol Solubil

Macedo & Peres (2001)

X: Mass Percent

Usage	TEMPERAT C	X FRUCTOSE	X ETHANOL
STD-DEV	0.1	0.5	0.5
DATA	25	12.107	0
DATA	25	10.021	9.0114
DATA	25	8.113	18.41783
DATA	25	6.79	27.95554
DATA	25	5.602	37.88003
DATA	25	4.652	46.9217
DATA	25	3.746	57.68887
DATA	25	2.492	77.9869
DATA	25	1.702	98.298
DATA	40	22.534	0
DATA	40	18.297	8.11638
DATA	40	15.037	17.00704
DATA	40	12.248	26.22732
DATA	40	10.002	35.938
DATA	40	8.286	45.691
DATA	40	6.734	55.98758
DATA	40	5.505	66.10209
DATA	40	4.454	76.54763
DATA	40	3.602	86.87291
DATA	40	3.235	91.91707
DATA	40	3.008	96.992
DATA	60	62.978	0
DATA	60	54.121	4.54615
DATA	60	45.674	10.83695
DATA	60	36.467	19.35025
DATA	60	28.554	28.682
DATA	60	22.457	38.93977
DATA	60	17.401	49.62631
DATA	60	12.997	61.01955
DATA	60	10.204	71.76317
DATA	60	8.179	82.75919
DATA	60	6.501	93.499

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Fructose-Methanol-Water Solubility

Fructose-Water A

Macedo & Peres (2001)

X: Mass Percent

Lerici, Piva, Dalla Rosa

X: Mole Fraction

X	Usage	TEMPERAT C	X	X	X
METHANOL			FRUCTOSE	WATER	METHANOL
0	STD-DEV	0.1	0.5	0.5	0
87.893	DATA	25	12.107	0	87.893
80.9676	DATA	25	30.011	6.9891	62.9999
73.4692	DATA	25	48.221	10.3558	41.4232
65.2545	DATA	25	59.378	12.19269	28.4293
56.518	DATA	25	65.922	13.61109	20.4669
48.4263	DATA	25	70.826	14.61121	14.5628
38.5651	DATA	25	73.692	15.73981	10.5682
19.5211	DATA	25	77.356	17.80724	4.83676
0	DATA	25	80.104	19.896	0
77.466	DATA	40	22.534	0	77.466
73.5866	DATA	40	36.389	3.16719	60.4438
67.956	DATA	40	50.025	4.9945	44.9805
61.5247	DATA	40	63.255	7.32328	29.4217
54.06	DATA	40	71.147	8.68648	20.1665
46.023	DATA	40	75.33	9.8606	14.8094
37.2784	DATA	40	77.967	11.04206	10.9909
28.3929	DATA	40	79.659	11.94668	8.39432
18.9984	DATA	40	82.602	13.99878	3.39922
9.52509	DATA	40	84.365	15.635	0
4.84793	DATA	60	62.978	0	37.022
0	DATA	60	70.492	1.47894	28.0291
37.022	DATA	60	75.447	2.55032	22.0027
41.3329	DATA	60	81.582	3.66942	14.7486
43.489	DATA	60	85.793	4.2692	9.9378
44.1827	DATA	60	88.154	4.74646	7.09954
42.764	DATA	60	89.109	5.44114	5.44986
38.6032	DATA	60	89.866	6.04047	4.09353
32.9727	DATA	60	91.387	6.82124	1.79176
25.9835	DATA	60	92.449	7.551	0

Alavi, Pazuki, & Raisi (2014)

X: Mole Percent

Ebrahimi & Sadeghi (2

X: Mole Fraction

Usage	X
	FRUCTOSE
STD-DEV	0.005
DATA	0.010988
DATA	0.01734
DATA	0.041094
DATA	0.062497
STD-DEV	20%
DATA	0.001006
DATA	0.002023
DATA	0.003078
DATA	0.004119
DATA	0.005238
DATA	0.006205
DATA	0.007483
DATA	0.008559
DATA	0.009755
DATA	0.01094
DATA	0.012322
DATA	0.013983
DATA	0.015986
DATA	0.018085
DATA	0.020105
DATA	0.02229
DATA	0.030405
DATA	0.041467
DATA	0.050467
DATA	0.061295
DATA	0.089014

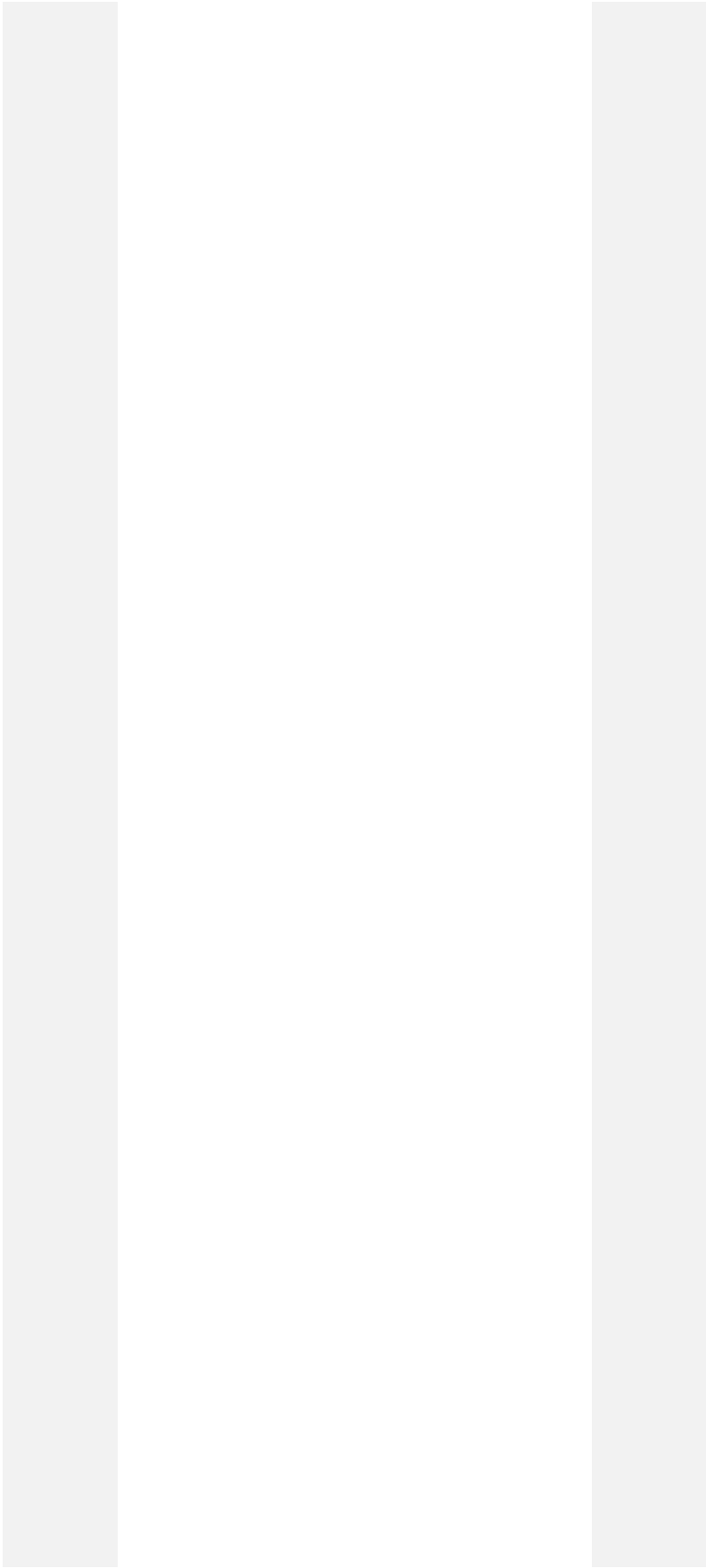
Usage	TEMPERAT C	X	X	X
		FRUCTOSE	WATER	METHANOL
STD-DEV	0.1	0.5	0.5	0
DATA	20	10.4	27.5772	62.0228
DATA	30	15.9	25.8844	58.2156
DATA	40	19.7	24.7148	55.5852
DATA	20	15.8	45.6765	38.5235
DATA	30	24.4	41.0112	34.5888

DATA	40	28.7	38.6786	32.6214
DATA	20	21.4	57.1701	21.4299
DATA	30	27.86	52.4714	19.6686
DATA	40	29.46	51.3076	19.2324
DATA	20	23.5	67.0719	9.4281
DATA	30	28.2	62.9512	8.8488
DATA	40	32.28	59.374	8.346
DATA	20	24.96	70.6276	4.4124
DATA	30	29.6	66.2604	4.1396
DATA	40	33.68	62.4204	3.8996
DATA	20	27.6	72.4	0
DATA	30	30.16	69.84	0
DATA	40	34.4	65.6	0

van Putten, Winkelman, Keihan, van der Waal, Jong, & Heeres (2014)

X: Mole Fraction

Usage	TEMPERAT K	X FRUCTOSE	X METHANO	X WATER
STD-DEV	0.1	0.005	0.005	0
DATA	304.55	0.030739	0.969261	0
DATA	312.85	0.043053	0.956947	0
DATA	316.75	0.056334	0.943666	0
DATA	311.25	0.043173	0.956827	0
DATA	315.55	0.056645	0.943355	0
DATA	320.05	0.071706	0.928294	0
DATA	323.35	0.088511	0.911489	0
DATA	331.75	0.107878	0.892122	0
DATA	300.15	0.030348	0.891063	0.078589
DATA	306.55	0.041703	0.880629	0.077669
DATA	311.35	0.054698	0.868686	0.076616
DATA	316.75	0.08475	0.840015	0.075235
DATA	313.35	0.069116	0.854363	0.07652
DATA	317.75	0.08501	0.839776	0.075214
DATA	324.75	0.103381	0.822916	0.073704
DATA	302.15	0.052385	0.788436	0.159179
DATA	308.65	0.066166	0.77697	0.156864
DATA	316.05	0.082599	0.763297	0.154104
DATA	317.35	0.099708	0.75085	0.149442
DATA	321.95	0.142722	0.714976	0.142302



DATA
DATA
DATA
DATA

-Water Boiling Point

Bounahmidi (1994)

Fraction

TEMPERAT	PRESSURE	X	X	Y	Y
C	N/sqm	FRUCTOSE	WATER	FRUCTOSE	WATER
0.5	500	0.01	0	0	0
100.1	101320	0.045	0.955	0	1
100.3	101320	0.06	0.94	0	1
100.4	101320	0.095	0.905	0	1
100.6	101320	0.115	0.885	0	1
101.1	101320	0.205	0.795	0	1
101.2	101320	0.255	0.745	0	1
101.3	101320	0.34	0.66	0	1
102.5	101320	0.46	0.54	0	1
104.9	101320	0.585	0.415	0	1
108.4	101320	0.68	0.32	0	1
1	500	0.01	0	0	0
122	101320	0.82	0.18	0	1
130	101320	0.87	0.13	0	1

Leirelles, & Batista (2010)

Percent

TEMPERAT	PRESSURE	X	X	Y	Y
K	kPa	FRUCTOSE	WATER	FRUCTOSE	WATER
0.5	0.1	0.5	0	0	0
334.1	20	10.3	89.7	0	100
334.5	20	20.6	79.4	0	100
335.2	20	30.9	69.1	0	100
335.5	20	40.9	59.1	0	100
336.5	20	51.2	48.8	0	100
337.9	20	61	39	0	100
340.8	26.7	10.3	89.7	0	100
341.2	26.7	20.7	79.3	0	100
341.5	26.7	30.8	69.2	0	100
342.1	26.7	40.9	59.1	0	100
343	26.7	51.3	48.7	0	100
344.6	26.7	61	39	0	100
345.8	33.3	10.3	89.7	0	100
346.2	33.3	20.7	79.3	0	100
346.7	33.3	30.6	69.4	0	100
347.1	33.3	40.9	59.1	0	100
348.2	33.3	51.4	48.6	0	100
349.8	33.3	61.1	38.9	0	100
350	40	10.3	89.7	0	100
350.6	40	20.8	79.2	0	100
351.1	40	30.7	69.3	0	100

Fructose-Water Vapor Pre

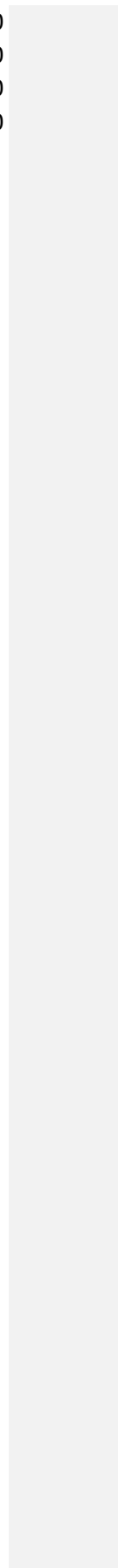
Ebrahimi & Sadeghi (2016)

X/Y: Mole Fraction T: 308.15 K

Usage	PRESSURE	X
	kPa	FRUCTOSE
STD-DEV	0.1	0.005
DATA	5.6264	0.001006
DATA	5.6207	0.002023
DATA	5.6145	0.003078
DATA	5.6089	0.004119
DATA	5.6026	0.005238
DATA	5.597	0.006205
DATA	5.5897	0.007483
DATA	5.5835	0.008559
DATA	5.5767	0.009755
DATA	5.5705	0.01094
DATA	5.5626	0.012322
DATA	5.553	0.013983
DATA	5.5417	0.015986
DATA	5.5293	0.018085
DATA	5.518	0.020105
DATA	5.5056	0.02229
DATA	5.4582	0.030405
DATA	5.3916	0.041467
DATA	5.3357	0.050467
DATA	5.2663	0.061295
DATA	5.0727	0.089014

351.4	40	40.9	59.1	0	100
352.5	40	51.5	48.5	0	100
354.2	40	61.1	38.9	0	100
353.9	46.7	10.3	89.7	0	100
354.4	46.7	20.9	79.1	0	100
355	46.7	30.8	69.2	0	100
355.4	46.7	40.9	59.1	0	100
356.4	46.7	51.6	48.4	0	100
358	46.7	61.2	38.8	0	100
357.2	53.3	10.3	89.7	0	100
357.8	53.3	20.9	79.1	0	100
358.3	53.3	30.8	69.2	0	100
358.5	53.3	41.1	58.9	0	100
359.7	53.3	51.6	48.4	0	100
361.4	53.3	61.2	38.8	0	100
360.1	60	10.3	89.7	0	100
360.7	60	20.9	79.1	0	100
361.2	60	30.8	69.2	0	100
361.7	60	41.2	58.8	0	100
362.8	60	51.5	48.5	0	100
364.7	60	61.2	38.8	0	100
362.7	66.7	10.4	89.6	0	100
363.4	66.7	20.9	79.1	0	100
364	66.7	31	69	0	100
364.4	66.7	41.2	58.8	0	100
365.5	66.7	51.5	48.5	0	100
367.2	66.7	61.1	38.9	0	100
365.3	73.3	10.4	89.6	0	100
366	73.3	20.9	79.1	0	100
366.4	73.3	31.2	68.8	0	100
367	73.3	41.2	58.8	0	100
368	73.3	51.6	48.4	0	100
369.9	73.3	61.1	38.9	0	100
367.7	80	10.4	89.6	0	100
368.2	80	21	79	0	100
368.7	80	31.2	68.8	0	100
369	80	41	59	0	100
370.4	80	51.8	48.2	0	100
372.2	80	61	39	0	100
369.8	86.7	10.4	89.6	0	100
370.5	86.7	21	79	0	100
370.8	86.7	31.2	68.8	0	100
371.3	86.7	40.9	59.1	0	100
372.8	86.7	51.9	48.1	0	100
374.3	86.7	60.8	39.2	0	100
372.1	93.6	10.4	89.6	0	100
372.8	93.6	21.1	78.9	0	100

373.2	93.6	31.2	68.8	0	100
374.2	93.6	41.3	58.7	0	100
375.1	93.6	52	48	0	100
376.7	93.6	61.2	38.8	0	100



ssure

X	Y	Y
WATER	FRUCTOSE	WATER
0	0	0
0.998994	0	1
0.997977	0	1
0.996922	0	1
0.995881	0	1
0.994762	0	1
0.993795	0	1
0.992517	0	1
0.991441	0	1
0.990245	0	1
0.98906	0	1
0.987678	0	1
0.986017	0	1
0.984014	0	1
0.981915	0	1
0.979895	0	1
0.97771	0	1
0.969595	0	1
0.958533	0	1
0.949533	0	1
0.938705	0	1
0.910986	0	1

Methanol-Water Solubility			
acedo (1997, CarbRes)			
Percent			
TEMPERAT	X	X	X
C	SUCROSE	WATER	METHANOL
0.1	0.5	0.5	0
25	0.6627	0	99.3373
25	2.2217	9.684941	88.0934
25	6.3312	18.71409	74.9547
25	15.741	25.23051	59.0285
25	28.9476	28.24901	42.8034
25	41.1992	29.38688	29.4139
25	49.8836	30.03777	20.0786
25	56.849	30.21951	12.9315
25	61.0928	31.11409	7.79311
25	67.4623	32.5377	0
40	0.9962	0	99.0038
40	3.2821	9.766574	86.9513
40	9.7585	18.03837	72.2031
40	21.6473	22.89309	55.4596
40	37.9694	24.646	37.3846
40	49.7914	25.14547	25.0631
40	56.1027	26.26463	17.6327
40	61.4483	26.98233	11.5694
40	64.933	28.05535	7.01165
40	70.1888	29.8112	0
60	1.8309	0	98.1691
60	6.7843	9.318774	83.8969
60	18.498	16.21482	65.2872
60	36.0736	19.11527	44.8111
60	50.0608	19.86931	30.0699
60	58.7036	20.54991	20.7465
60	64.4322	21.32325	14.2445

Sucrose-Water Activity Coefficient				
Scatchard, Hamer, & Wood (1938)				
X: Mole Fraction		T: 298.15 K		
Usage	X	X	GAMMA	GAMMA
	SUCROSE	WATER	SUCROSE	WATER
STD-DEV	0.005	0	100%	0.005
DATA	0.001798	0.998202		0.999985
DATA	0.00359	0.99641		0.999939
DATA	0.005375	0.994625		0.999859
DATA	0.007154	0.992846		0.999744
DATA	0.008927	0.991073		0.999593
DATA	0.010693	0.989307		0.999404
DATA	0.012453	0.987547		0.999177
DATA	0.014207	0.985793		0.998911
DATA	0.015955	0.984045		0.998604
DATA	0.017696	0.982304		0.998258
DATA	0.021161	0.978839		0.997445
DATA	0.024601	0.975399		0.996464
DATA	0.028016	0.971984		0.995324
DATA	0.031409	0.968591		0.994034
DATA	0.034777	0.965223		0.992603
DATA	0.043097	0.956903		0.988455
DATA	0.051274	0.948726		0.983499
DATA	0.059313	0.940687		0.97777
DATA	0.067216	0.932784		0.971338
DATA	0.074988	0.925012		0.964291
DATA	0.082632	0.917368		0.956799
DATA	0.09015	0.90985		0.948975
DATA	0.097546	0.902454		0.941517
Robinson, Smith, & Smith (1942)				
X: Mole Fraction		T: 298.15 K		
Usage	X	X	GAMMA	GAMMA

Sucrose-Water Solubility	
Young & Jones (1949)	
X: Mass Percent	
Usage	TEMPERAT
	C
STD-DEV	0.5
DATA	-10
DATA	0
DATA	10
DATA	20
DATA	30
DATA	40
DATA	50
Abed, Gabas, Delia, &	
X: Mass Fraction	
Usage	TEMPERAT
	C
STD-DEV	0.5
DATA	70

Solubility		Sucrose-Water Boiling Point						Sucrose-Water Vapor Pressure		
		Leschke (1987)						Robinson, Smith, & Smith (1942)		
		X: Mass Percent			P: 101.325 kPa			X: Mole Fraction		T: 298.15 K
X	X	Usage	TEMPERAT	X	X	Y	Y	Usage	PRESSURE	X
SUCROSE	WATER		C	SUCROSE	WATER	SUCROSE	WATER		mmHg	SUCROSE
0.5	0	STD-DEV	0.1	1	0	0	0	STD-DEV	0.05	0.001
63.7	36.3	DATA	100.2	10	90	0	100	DATA	23.713	0.001798
64.4	35.6	DATA	100.3	20	80	0	100	DATA	23.669	0.00359
65.4	34.6	DATA	100.6	30	70	0	100	DATA	23.625	0.005375
66.8	33.2	DATA	101.1	40	60	0	100	DATA	23.534	0.008927
68.6	31.4	DATA	101.8	50	50	0	100	DATA	23.441	0.012453
70.4	29.6	DATA	103	60	40	0	100	DATA	23.294	0.017696
72.3	27.7	DATA	105.1	70	30	0	100	DATA	23.035	0.026311
		DATA	109.5	80	20	0	100	DATA	22.757	0.034777
		DATA	119.4	90	10	0	100	DATA	22.462	0.043097
		STD-DEV	10	1	99	0	100	DATA	22.154	0.051274
		DATA	126.7	94	6	0	100	DATA	21.835	0.059313
		DATA	137.9	98	2	0	100	DATA	21.506	0.067216
		DATA	141.4	99	1	0	100	DATA	21.175	0.074988
								DATA	20.84	0.082632
								DATA	20.5	0.09015
								DATA	20.154	0.097546
		Abderafi & Bounahmidi (1994)								
		X: Mass Fraction			P: 101.325 kPa					
		Usage	TEMPERAT	X	X	Y	Y			
			C	SUCROSE	WATER	SUCROSE	WATER			
		STD-DEV	0.1	0.01	0	0	0%			
		DATA	100.1	0.055	0.945	0	1			
		DATA	100.3	0.106	0.894	0	1			
		DATA	100.4	0.215	0.785	0	1			
		DATA	101.2	0.32	0.68	0	1			
		DATA	101.8	0.445	0.555	0	1			
		DATA	103	0.596	0.404	0	1			
		DATA	104	0.65	0.35	0	1			
		DATA	108.2	0.76	0.24	0	1			

60	70.7825	23.3965	5.821		SUCROSE	WATER	SUCROSE	WATER			
60	74.378	25.622	0		STD-DEV	0.005	0	100%	0.005		
					DATA	0.001798	0.998202		0.999985		
, Winkelman, Keihan, van der Waal, Jong, & Heeres (20					DATA	0.00359	0.99641		0.999939		
action	EXCLUDED FROM REGRESSION				DATA	0.005375	0.994625		0.999859		
TEMPERAT	X	X	X		DATA	0.008927	0.991073		0.99959		
K	SUCROSE	WATER	METHANOL		DATA	0.012453	0.987547		0.99917		
0.1	0.005	0.005	0		DATA	0.017696	0.982304		0.998225		
335.95	0.002579	0.997421	0		DATA	0.026311	0.973689		0.995826		
335.35	0.001897	0.998103	0		DATA	0.034777	0.965223		0.992445		
334.45	0.001897	0.998103	0		DATA	0.043097	0.956903		0.988115		
349.15	0.002914	0.997086	0		DATA	0.051274	0.948726		0.98294		
348.35	0.002914	0.997086	0		DATA	0.059313	0.940687		0.977054		
350.95	0.003952	0.996048	0		DATA	0.067216	0.932784		0.970546		
351.95	0.003952	0.996048	0		DATA	0.074988	0.925012		0.963625		
341.25	0.004855	0.908329	0.086816		DATA	0.082632	0.917368		0.956254		
346.55	0.007286	0.90611	0.086604		DATA	0.09015	0.90985		0.948409		
330.85	0.002725	0.915297	0.081978		DATA	0.097546	0.902454		0.940041		
331.35	0.002725	0.915297	0.081978								
340.25	0.003725	0.914379	0.081896		Robinson & Stokes (1961)						
338.85	0.003725	0.914379	0.081896		X: Mole Fraction		T: 298.15 K				
351.45	0.005795	0.912479	0.081726		Usage	X	X	GAMMA	GAMMA		
349.85	0.005795	0.912479	0.081726			SUCROSE	WATER	SUCROSE	WATER		
327.05	0.004671	0.826534	0.168794		STD-DEV	0.005	0	100%	0.005		
333.25	0.007014	0.824589	0.168397		DATA	0.006746	0.993254		0.999781		
334.65	0.009784	0.822289	0.167927		DATA	0.009043	0.990957		0.999595		
345.85	0.012594	0.819956	0.167451		DATA	0.012969	0.987031		0.999132		
321.75	0.00367	0.830947	0.165384		DATA	0.013107	0.986893		0.999112		
329.05	0.004652	0.830128	0.165221		DATA	0.015208	0.984792		0.99878		
328.75	0.004652	0.830128	0.165221		DATA	0.016034	0.983966		0.998634		
343.15	0.007939	0.827386	0.164675		DATA	0.017391	0.982609		0.998373		
343.05	0.007939	0.827386	0.164675		DATA	0.020906	0.979094		0.99758		
347.55	0.009543	0.826048	0.164409		DATA	0.026004	0.973996		0.996116		
346.85	0.009543	0.826048	0.164409		DATA	0.027434	0.972566		0.995637		
341.05	0.014759	0.742888	0.242354		DATA	0.030276	0.969724		0.994596		

327.15	0.009272	0.747025	0.243703	DATA	0.031219	0.968781		0.994224				
325.85	0.007223	0.753126	0.239651	DATA	0.032454	0.967546		0.993717				
322.85	0.007223	0.753126	0.239651	DATA	0.032953	0.967047		0.993506				
329.85	0.009224	0.751608	0.239168	DATA	0.033305	0.966695		0.993354				
329.55	0.009224	0.751608	0.239168	DATA	0.040696	0.959304		0.989756				
335.05	0.011248	0.750073	0.238679	DATA	0.047542	0.952458		0.985724				
334.95	0.011248	0.750073	0.238679	DATA	0.048962	0.951038		0.984808				
340.05	0.014492	0.747612	0.237896	DATA	0.050608	0.949392		0.983712				
340.15	0.014492	0.747612	0.237896	DATA	0.05532	0.94468		0.980384				
344.55	0.017499	0.747833	0.234668	DATA	0.057604	0.942396		0.978674				
344.45	0.017499	0.747833	0.234668	DATA	0.068364	0.931636		0.969857				
348.35	0.020539	0.745519	0.233942	DATA	0.071582	0.928418		0.967006				
348.35	0.020539	0.745519	0.233942	DATA	0.073366	0.926634		0.965387				
344.65	0.027164	0.686461	0.286375	DATA	0.0775	0.9225		0.961544				
349.35	0.034078	0.681582	0.28434	DATA	0.082448	0.917552		0.956787				
324.55	0.012961	0.679535	0.307504	DATA	0.084234	0.915766		0.955031				
324.95	0.012961	0.679535	0.307504	DATA	0.094535	0.905465		0.944559				
339.15	0.019496	0.675036	0.305468									
339.05	0.019496	0.675036	0.305468									
335.35	0.022388	0.673045	0.304567									
335.35	0.022388	0.673045	0.304567									
336.75	0.033188	0.596197	0.370615									
343.35	0.040716	0.591555	0.367729									
352.25	0.049605	0.586074	0.364322									
329.15	0.025802	0.600752	0.373446									
bazza, Sarturi, Goulart, & Conte (2016)				Stokes & Robinson (1966)								
action				X: Mole Fraction	T: 298.15 K							
TEMPERAT	X	X	X	Usage	X	X	GAMMA	GAMMA				
K	SUCROSE	METHANO	WATER		SUCROSE	WATER	SUCROSE	WATER				
0.1	0.005	0.005	0	STD-DEV	0.005	0	100%	0.005				
303.2	0.008134	0.991866	0	DATA	0.0177	0.9823		0.998309				
303.2	0.014626	0.92743	0.057944	DATA	0.0348	0.9652		0.992689				
303.2	0.032468	0.848285	0.119247	DATA	0.0513	0.9487		0.983271				
303.2	0.074915	0.745376	0.179709	DATA	0.0672	0.9328		0.970855				
				DATA	0.0826	0.9174		0.9566				
				DATA	0.0975	0.9025		0.941415				
				Chuang & Toledo (1976) EXCLUDED FROM REGRESSION								
				X: Mole Fraction	T: 298.15 K							
				Usage	X	X	GAMMA	GAMMA				
					SUCROSE	WATER	SUCROSE	WATER				
				STD-DEV	0.005	0	100%	0.005				

303.2	0.159546	0.611299	0.229155	DATA	0.003271	0.996729		0.996259				
303.2	0.27223	0.465833	0.261937	DATA	0.00941	0.99059		0.991328				
303.2	0.414636	0.317538	0.267826	DATA	0.034974	0.965026		0.978212				
303.2	0.518577	0.208226	0.273197	DATA	0.093788	0.906212		0.925832				
303.2	0.617732	0.11765	0.264618									
303.2	0.664085	0.055477	0.280438	Lerici, Piva, Dalla Rosa (1983)								
303.2	0.698458	0	0.301542	X: Mole Fraction			T: 298.15 K					
313.2	0.010324	0.989676	0	Usage	X	X	GAMMA	GAMMA				
313.2	0.020116	0.922203	0.057681		SUCROSE	WATER	SUCROSE	WATER				
313.2	0.044455	0.83784	0.117705	STD-DEV	0.005	0	100%	0.005				
313.2	0.099994	0.725235	0.174771	DATA	0.002762	0.997238		0.998759				
313.2	0.201882	0.580507	0.217611	DATA	0.005814	0.994186		0.997801				
313.2	0.343116	0.42046	0.236424	DATA	0.009202	0.990798		0.997176				
313.2	0.468493	0.288432	0.243075	DATA	0.012986	0.987014		0.995934				
313.2	0.556299	0.19191	0.251791	DATA	0.022058	0.977942		0.992901				
313.2	0.622578	0.116159	0.261263	DATA	0.033897	0.966103		0.988507				
313.2	0.673142	0.053931	0.272927									
313.2	0.707301	0	0.292699	Ebrahimi & Sadeghi (2016)								
				X: Mole Fraction			T: 308.15 K					
				Usage	X	X	GAMMA	GAMMA				
					SUCROSE	WATER	SUCROSE	WATER				
				STD-DEV	0.005	0	100%	0.005				
				DATA	0.000533	0.999467		1.000033				
				DATA	0.001046	0.998954		1.000046				
				DATA	0.001626	0.998374		1.000026				
				DATA	0.002173	0.997827		0.999973				
				DATA	0.002756	0.997244		0.999956				
				DATA	0.003569	0.996431		0.999968				
				DATA	0.004546	0.995454		0.999845				
				DATA	0.005655	0.994345		0.999854				
				DATA	0.007044	0.992956		0.999743				
				DATA	0.00852	0.99148		0.999617				
				DATA	0.009929	0.990071		0.999525				
				DATA	0.010379	0.989621		0.999474				
				DATA	0.011539	0.988461		0.999432				

				DATA	0.012919	0.987081		0.99931		
				DATA	0.015068	0.984932		0.999054		
				DATA	0.017192	0.982808		0.998872		
				DATA	0.019215	0.980785		0.998486		
				DATA	0.020912	0.979088		0.998378		
				DATA	0.022448	0.977552		0.998003		
				DATA	0.034705	0.965295		0.993996		
				DATA	0.046047	0.953953		0.989252		
				DATA	0.057905	0.942095		0.983021		
				DATA	0.066068	0.933932		0.978336		