Experimental Data and Correlation of Surface Tensions of the Binary and Ternary Systems of Water + Acetonitrile + 2-Propanol at 298.15 K and Atmospheric Pressure

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This paper reports the results of a new experimental study of surface tension for the ternary mixtures of water/acetonitrile/2-propanol. Correlating the excess surface tension of the above-mentioned binary and ternary systems was performed with empirical and thermodynamic based models. The methods of Pando et al. and Ku et al. were used to correlate the ternary surface tension data. The ternary surface tension data were well-correlated using pair additivity and rational functions as the ternary term. The results provide information on the molecular interactions between the unlike molecules that exist at the surface and the bulk.

Introduction

The surface tension of a liquid mixture is not a simple function of the surface tension of the pure components, because in a mixture the composition of the surface is not the same as that of the bulk.[1−4] Alcohols, either alone or in solutions (water, acetonitrile), are very widely used in the chemical, pharmaceutical, chromatography, and cosmetic industries.[5−16] In the present paper we report surface tensions of the ternary system water/acetonitrile/2-propanol and of the corresponding binary mixtures, that is, water/acetonitrile, water/2-propanol, and acetonitrile/2-propanol at 298.15 K and atmospheric pressure. The ternary system water/acetonitrile/2-propanol covers a large range of polarity from the highly polar water and acetonitrile to mildly polar 2-propanol.

A few empirical and thermodynamic-based equations are available to correlate the surface tension; some of them have recently been proposed and are well-founded on a thermodynamic basis. Recently Santos et al. proposed thermodynamic-based equations to correlate the surface tension data with the composition in the binary systems.[17−19] A simple equation was developed from the Butler equation which has been proved to be adequate for highly nonsymmetrical binary systems with large values of excess surface tension.[20] Another surface tension correlation was proposed by Li et al. for liquid mixtures which are based on the Wilson equation for the excess Gibbs energy.[21,22] The other two-parameter equation was developed by Fu et al. which uses the local composition concept due to the Wilson equation.[23] On the other hand, Sonawane and Kumar,[24] Redlich−Kister,[25] and Myers and Scott[26] have developed a correlation of the surface tension of binary mixtures.

In the present work, for the surface tension correlation we used the following models: Redlich−Kister (RK), Santos et al. (SFF), Li et al. (LWW), Fu et al. (FLW), Sonawane and Kumar (SK), and Myers−Scott (MS).

Table 1. Surface Tension, *σ*, of the Pure Components at 298.15 K and Atmospheric Pressure

component	exptl *σ* mN·m^{-1}	literature *σ* mN·m^{-1}
water	72.09	71.98,[a] 72.01,[b] 72.08[c]
acetonitrile	27.76	27.54[b]
2-propanol	20.95	21.19,[b] 20.90[d]

[a] Ref 27. [b] Ref 29. [c] Ref 30. [d] Ref 28.

Experimental Section

Chemicals. Acetonitrile (mass fraction > 0.999) and 2-propanol (mass fraction 0.995) were purchased from Merck and used without further purifications. The water was distilled twice. The purity of reagents was checked by comparing the measured surface tension at 298.15 K with those reported in the literature.[27−30] The resultant values are in good agreement with values found in the literature and are reported in Table 1.

Apparatus and Procedure. The surface tensions of the pure liquids and their mixtures were measured using the platinum−iridium ring method with a KSV (Sigma 70, Finland) tensiometer. The platinum−iridium ring was cleaned with chromosulfuric acid and boiling distilled water. Each measurement was repeated up to 10 times to check for reproducibility. The uncertainty of the surface tension measurement is ± 0.2 mN·m^{-1} of the final value of surface tension, and the corresponding reproducibility is ± 0.01 mN·m^{-1}. The temperature was kept constant by a water bath circulator (Pharmacia Biotech) and with the uncertainty ± 0.1 K. The binary and ternary mixtures were prepared by mass using a Sartorius analytical balance (model BP 121S, accurate to ± 0.1 mg). The uncertainty of the mole fractions was estimated to be within ± 0.0001.

Results and Discussion

The deviations from ideal behavior can be quantified by the excess surface tension, σ^E, defined as

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$$\sigma^{\mathrm{E}} = \sigma - \sum_{i}^{n} x_i \sigma_i^* \qquad (1)$$

where σ is the surface tension of the mixture, σ_i^* is the surface tension of the component i, x_i is the mole fraction of the component i, and n is the number of components.

The relevant equations for all of the models for surface tension calculation, in this section, are the following models.

The binary systems were fitted by a Redlich−Kister (edited by Mosteiro et al.) equation:[25,31]

$$\sigma^{\mathrm{E}} = x_i x_j \sum_{p=0}^{p=m} A_p (x_i - x_j)^p + B_0 (x_i - x_j) \qquad (2)$$

where A_p and B_0 are the adjustable parameters determined by a nonlinear least-squares optimization method.

For the correlation of surface tension of binary systems, a simple equation proposed by Santos et al. (SFF)[17] was used to describe the behavior of the observed systems:

$$\sigma^{\mathrm{E}} = x_i x_j (A + B[1 - (x_i - x_j)]^C) \qquad (3)$$

where A, B, and C are adjustable parameters.

A surface tension equation based on the thermodynamic definition of surface tension and the expression of Gibbs free energy is proposed by Li et al. (LWW):[21]

$$\sigma^{\mathrm{E}} = -RT \sum_i \frac{x_i}{\sum_j x_j \Lambda_{ij}} \sum_j x_j \left(\frac{\partial \Lambda_{ij}}{\partial A}\right)_{T,P,X} \qquad (4)$$

where

$$\begin{aligned} \Lambda_{ij} &= \exp\left(-\frac{U_{ij} - U_{ii}}{RT}\right) \\ \left(\frac{\partial \Lambda_{ij}}{\partial A}\right)_{T,P,X} &= -\frac{\Lambda_{ij}}{RT}\left[\frac{\partial (U_{ij} - U_{ii})}{\partial A}\right]_{T,P,X} \end{aligned} \qquad (5)$$

In the preceding relations, $U_{ij} - U_{ii}$ is the difference in the interaction energy between molecular pair ij and the derivative $[\partial(U_{ij} - U_{ii})/\partial A]_{T,P,x}$ reflects the energy change with the increase in surface area. Li et al. made the assumption $U_{ij} = (U_{ii} + U_{jj})/2$; so, the number of adjustable parameters is reduced from four to two for a binary system, that is, $U_{12} - U_{11}$, $[\partial(U_{12} - U_{11})/\partial A]_{T,P,x}$. Hence the resultant equation is given by:

$$\sigma^{\mathrm{E}} = -\frac{x_1 x_2 RT}{x_2 + x_1 \Lambda_{21}} \left(\frac{\partial \Lambda_{21}}{\partial A}\right) \left[1 - \frac{1}{\Lambda_{21}}\right] \qquad (6)$$

Fu et al. (FLW),[23] based on the modified Hildebrand−Scott[32] equation for binary systems, proposed the following equation:

$$\sigma = \frac{x_1 \sigma_1^*}{x_1 + x_2 f_{12}} + \frac{x_2 \sigma_2^*}{x_2 + x_1 f_{21}} - \frac{x_1 x_2 |\sigma_1^* - \sigma_2^*|}{(x_1 + x_2 f_{12})(x_2 + x_1 f_{21})} \qquad (7)$$

where f_{12} and f_{21} are the binary adjustable parameters.

Table 2. Experimental Surface Tension, σ, and Excess Surface Tension, σ^{E}, for the Water (1)/Acetonitrile (2)/2-Propanol (3) System and Its Binary Constituents at 298.15 K and Atmospheric Pressure

x_1	x_2	σ / $\mathrm{mN \cdot m^{-1}}$	σ^{E} / $\mathrm{mN \cdot m^{-1}}$	x_1	x_2	σ / $\mathrm{mN \cdot m^{-1}}$	σ^{E} / $\mathrm{mN \cdot m^{-1}}$
0.9851	0.0149	62.36	−9.07	0.6999	0.1001	26.15	−31.28
0.9702	0.0298	55.92	−14.85	0.6000	0.0998	24.61	−27.70
0.9484	0.0516	49.39	−20.41	0.4992	0.1001	23.76	−23.40
0.9050	0.0950	40.54	−27.34	0.3938	0.1131	23.15	−18.71
0.8773	0.1227	37.97	−28.68	0.3004	0.1001	22.38	−14.61
0.8977	0.1023	39.63	−27.93	0.1947	0.1404	22.14	−9.73
0.8145	0.1855	33.97	−29.90	0.0990	0.1024	21.39	−5.32
0.7459	0.2541	32.92	−27.91	0.5977	0.1999	26.86	−26.02
0.6041	0.3959	31.68	−22.86	0.3982	0.2034	23.78	−18.92
0.5149	0.4851	31.45	−19.14	0.3010	0.2001	22.73	−14.97
0.4087	0.5913	30.95	−14.93	0.2012	0.1995	21.85	−10.75
0.2032	0.7968	29.46	−7.31	0.2006	0.2004	21.90	−10.67
0.9697	0	39.36	−31.18	0.1008	0.2004	21.30	−6.17
0.9598	0	35.83	−34.20	0.6008	0.2995	29.22	−24.49
0.9450	0	32.36	−36.92	0.5005	0.2993	26.51	−22.07
0.8991	0	26.64	−40.29	0.3995	0.3005	24.72	−18.71
0.8502	0	25.04	−39.39	0.2990	0.3001	23.57	−14.71
0.8000	0	24.37	−37.49	0.1955	0.2914	22.47	−10.46
0.7021	0	23.28	−33.58	0.3996	0.4005	26.97	−17.14
0.5993	0	22.74	−28.86	0.3014	0.3958	24.93	−14.13
0.5018	0	22.28	−24.33	0.2005	0.4000	23.72	−10.21
0.2949	0	21.97	−14.06	0.3988	0.5005	28.76	−15.99
0.0990	0	21.65	−4.36	0.3112	0.4921	26.48	−13.74
0	0.9851	27.55	−0.11	0.2039	0.4976	24.79	−9.97
0	0.9701	27.28	−0.28	0.2997	0.6002	28.61	−11.75
0	0.9579	27.10	−0.37	0.1996	0.6002	26.13	−9.12
0	0.8984	26.23	−0.84	0.1041	0.5974	24.45	−5.89
0	0.8001	24.94	−1.46	0.1984	0.6966	27.74	−8.10
0	0.7000	23.84	−1.88	0.0958	0.6985	25.47	−5.14
0	0.6001	22.88	−2.16	0.1002	0.7999	27.73	−3.79
0	0.5398	22.44	−2.19	0.0520	0.8983	27.09	−2.64
0	0.4885	22.15	−2.13	0.9498	0.0252	39.50	−30.19
0	0.3621	21.55	−1.87				
0	0.2001	21.05	−1.26				

Sonawane and Kumar (SK)[24] have derived an equation for correlation of the surface tension data of liquid mixtures at both ambient and high temperatures:

$$\sigma^{\mathrm{E}} = RT\left(x_i x_j \left(\frac{1}{A_i^*} - \frac{1}{A_j^*}\right)\right)(\delta_p + \delta_m x_j) \qquad (8)$$

Two unknown parameters δ_p and δ_m can be evaluated from the experimental surface tension−composition data. A_i^* and A_j^* are the molar surface areas of pure components i and j that were calculated from the correlation proposed by Suarez et al.:[33]

$$A_i^* = 1.021 \cdot 10^8 \, V_{\mathrm{c}}^{6/15} V_{\mathrm{b}}^{4/15} \qquad (9)$$

where V_{c} is the critical molar volume, V_{b} is the bulk liquid molar volume are in $\mathrm{cm^3 \cdot mol^{-1}}$, and A_i^* is in $\mathrm{cm^2 \cdot mol^{-1}}$.

A more flexible representation of the binary excess data is a rational expression proposed by Myers and Scott (MS):[26]

$$\sigma^{\mathrm{E}} = x_i x_j \left(\frac{\sum_{p=0}^{p=m} B_p (x_i - x_j)^p}{1 + \sum_{l=1}^{l=m} C_l (x_i - x_j)^l}\right) \qquad (10)$$

where B_p and C_1 are adjustable parameters.

In Table 2 the measured surface tension data and the corresponding excess surface tensions are presented for the

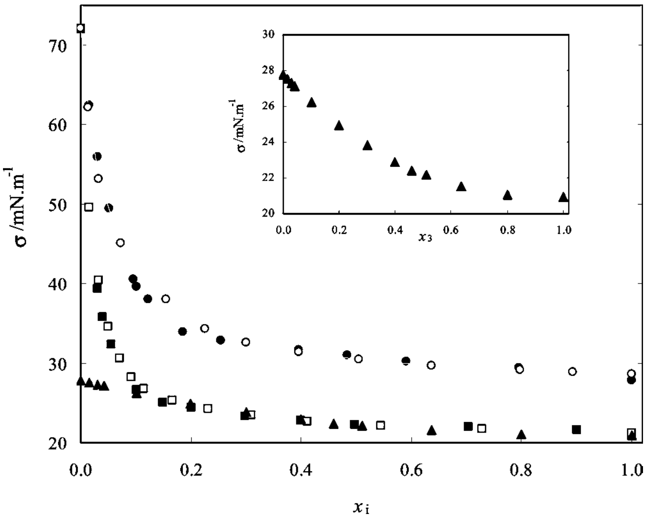

Figure 1. Experimental surface tension, σ, as a function of mole fraction. $x_i = x_3$, ▲, acetonitrile (2)/2-propanol (3); ■, water (1)/2-propanol (3); □, ref 34. $x_i = x_2$, ●, water (1)/acetonitrile (2); ○, ref 30.

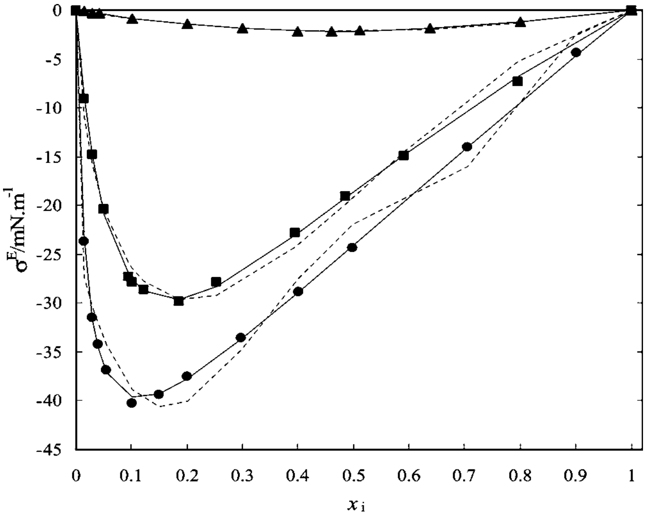

Figure 2. Excess surface tension, σ^E, as a function of mole fraction. The symbols refer to the experimental data. $x_i = x_3$, ●, water (1)/2-propanol (3); ▲, acetonitrile (2)/2-propanol (3). $x_i = x_2$, ■, water (1)/acetonitrile (2). The solid curves represent the best correlation (based on MS model), and the dashed curves represent the worst correlation (based on data in Table 3, model RK-4 for water/acetonitrile and water/2-propanol; model SFF for acetonitrile/2-propanol).

ternary systems and constituent binaries at 298.15 K as a function of the composition.

In Figures 1 to 4, we have plotted the experimental and fitted surface tensions of the binary systems of water/2-propanol, water/acetonitrile, and 2-propanol/acetonetrile as a function of the composition with various models. As can be seen, the agreement between the experimental data and the correlated values are reasonable. In Figures 1 and 3 we have also plotted the values taken from the literature[30,34] which are in excellent agreement with our data. The surface tension deviation, σ^E, of all mixtures shows negative values that increase with the increase in the difference of surface tension values of pure compounds.

The asymmetry in the curves of water/acetonitrile and water/2-propanol indicates that the components with the strongest molecular interactions in each binary mixture settle down in the bulk liquid phase instead of doing it in the surface phase between liquid and vapor phases, moving the curves to the rich region of these compounds.

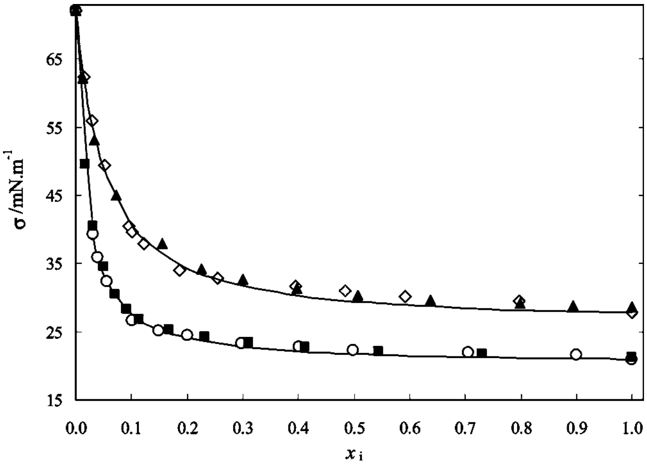

Figure 3. Surface tension, σ, as a function of mole fraction. The symbols refer to the experimental data, and the solid curves represent the correlation with eq 7. $x_i = x_3$, ○, water (1)/2-propanol (3); ■, ref 34; $x_i = x_2$, ◇, water (1)/acetonitrile (2); ▲, ref 30.

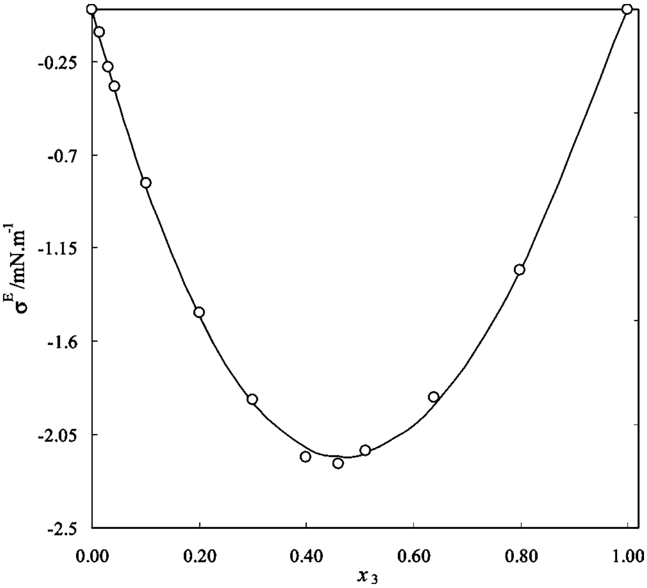

Figure 4. Excess surface tension, σ^E, for the binary system acetonitrile (2)/2-propanol (3) as a function of composition. Symbols correspond to the experimental data of this work, and the curve represents the correlation with eq 8.

In Table 3, the adjusted coefficients of the equations used to correlate the binary data are listed as well as the respective standard deviations of the fittings.

The standard deviation of the fittings, S, is defined as

$$S = \left[\sum_{i=1}^{M} \frac{(\sigma_{\text{exp}}^{E} - \sigma_{\text{calc}}^{E})^2}{M - P} \right]^{1/2} \tag{11}$$

where σ_{exp}^{E} and σ_{calc}^{E} are the experimental and calculated excess surface tensions, M is the number of data points, and P is the number of adjustable parameters used for fitting the experimental data in various equations. As expected, the highest values of the standard deviation are obtained for the water/2-propanol and water/acetonitrile systems which have higher values of σ^E and show markedly asymmetrical variations of this property with the composition. With the exception of the SK model all of the thermodynamic-based equations correlate the surface tension well. The SK model does not give good results when the surface

Table 3. Fitted Coefficients and Standard Deviation, *S*, of the Models Used to Correlate Surface Tension with the Composition for the Binary Systems

system	model	*A*	*B*	*C*	*D*	*S* mN·m^{-1}
water (1)/acetonitrile (2)	SFF	184.93	−261.39	−0.3772		1.10
	RK-4[a]	−72.97	36.26	−120.67	4.77	1.30
	FLW[b]	0.0642	8.084			0.90
	LWW[c]	0.0471	$-8.37 \cdot 10^{-7}$			1.10
	LWW[d]	−910.99	−530.33			1.10
	MS-3[e]	−74.476	1.139	0.2438		0.24
acetonitrile (2)/2-propanol (3)	SFF	526.2	−534.75	−0.0012		0.05
	RK-4[a]	−8.621	1.319	0.434	−0.017	0.02
	SK[f]	0.257	0.0778			0.02
	FLW[b]	0.857	1.204			0.02
	LWW[c]	0.697	$-6.76 \cdot 10^{-6}$			0.05
	LWW[d]	−107.62	−289.17			0.05
	MS-3[e]	−8.632	0.147	0.087		0.02
water (1)/2-propanol (3)	SFF	50.478	−146.92	−0.737		0.89
	RK-4[a]	−89.059	−26.84	−214.47	25.919	2.30
	FLW[b]	0.0203	18.446			0.56
	LWW[c]	0.0165	$-3.39 \cdot 10^{-7}$			0.53
	LWW[d]	−1223.72	−613.10			0.53
	MS-3[e]	−96.21	1.018	0.0520		0.31

[a] The coefficients *A*, *B*, *C*, and *D* correspond to A_0, A_1, A_2, and B_0, respectively. [b] The coefficients *A* and *B* correspond to f_{12} and f_{21}, respectively. [c] The coefficients *A* and *B* correspond to Λ_{21} and $(\partial\Lambda_{21}/\partial A)_{T,P,X}$, respectively. [d] The values *A* and *B* correspond to $U_{12} - U_{11}/R$ (in K) and $10^5 \cdot [\partial U_{12} - U_{11}/\partial A)]_{T,P,X}$ (in K·mol^{-1}·m^{-2}), respectively. [e] The coefficients *A*, *B*, and *C* correspond to B_0, C_1, and C_2, respectively. [f] The coefficients *A* and *B* correspond to δ_p and δ_m, respectively.

tensions of pure components are not comparable. The surface tension of the binary systems was well-correlated using the LWW and FWW models. The RK model with four adjustable parameters does not give good results when σ^E is large (such as water/2-propanol and water/acetonitrile). As can be seen from Figure 2 and Table 3, the MS model correlates the surface tensions of these systems well, even for the system water/2-propanol, which is highly nonsymmetrical with large values of σ^E.

The excess surface tension of the ternary mixtures, σ_T^E, has been correlated using the equation,

$$\sigma_T^E = \sigma_{12}^E + \sigma_{13}^E + \sigma_{23}^E + \sigma_{123}^E \qquad (12)$$

where σ_{ij}^E represents the excess surface tension for the binaries given by eq 10 and σ_{123}^E is a ternary term expressed based on two relations:

(i) Pando et al. edited by Santos et al.[35]

$$\sigma_{123}^E = x_1 x_2 x_3 \frac{D_1 + D_2(x_1 - x_2) + D_3(x_2 - x_3)}{1 + D_4(x_1 - x_2)} \qquad (13)$$

(ii) The model proposed by Ku et al.[28] which is based on the RK equation,

$$\sigma_{123}^E = x_1 x_2 x_3 \sum_{i=0}^{2} \sum_{j=0}^{2-i} C_{ij} x_1^i x_2^j \qquad (14)$$

The adjustable parameters D_i (in eq 13) and C_{ij} (in eq 14) and the standard deviation, *S*, were determined with the optimization algorithm and are given in Table 4. The ternary surface tension data were well-correlated using pair additivity (σ_{ij}^E) and rational functions (σ_{123}^E) as the ternary term. Figure 5 shows a typical plot of the isolines of σ_T^E for the ternary mixture with the Pando et al. model. The values of σ_T^E for the water/acetonitrile/2-propanol system are large and negative. For the equimolar composition (i.e., $x_1 = x_2 = x_3 = 1/3$), σ_T^E values of ternary mixtures are −15.41 mN·m^{-1}. It is observed that by the addition of 2-propanol to a pseudobinary mixture (water/acetonitrile) the values of σ_T^E increase. This may be inferred as

Table 4. Coefficients of Equations 13 and 14 Fitted to the Excess Surface Tension, σ^E, for the Ternary System Water (1)/Acetonitrile (2)/2-Propanol (3)

Pando et al.	D_1	D_2	D_3	D_4	*S* mN·m^{-1}
	121.71	203.15	175.41	−1.03	0.43

Ku et al.	C_{00}	C_{10}	C_{01}	C_{11}	C_{20}	*S* mN·m^{-1}
	110.42	−603.73	24.66	−14.71	1736.3	0.69

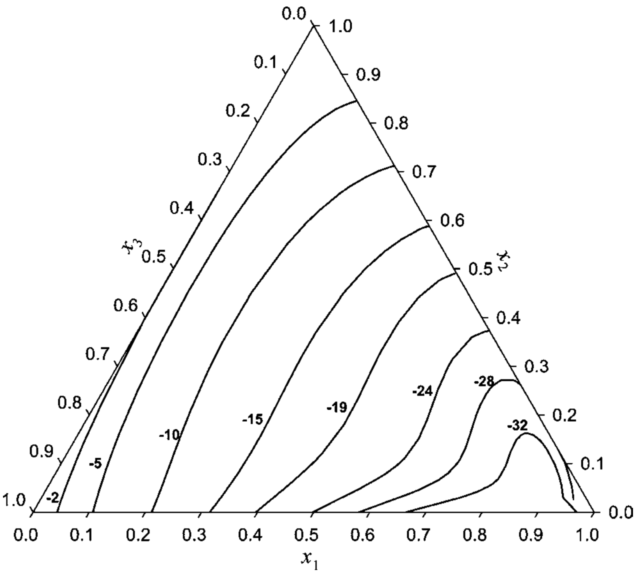

Figure 5. Iso-lines of σ_T^E for the ternary system water (1)/acetonitrile (2)/2-propanol (3) calculated from eqs 12 and 13.

the occurrence of specific interactions between water and acetonitrile molecules in bulk and the tendency of 2-propanol to surface.

Conclusion

This investigation provides surface tension data for the ternary mixture of water/acetonitrile/2-propanol and three constituent binary systems over ranges of composition. The σ^E values are negative over the whole mole fraction values and pass through a minimum at $x_1 \approx 0.85$ to 0.95 (in water (1)/2-propanol (3)) and $x_1 \approx 0.75$ to 0.95 (in water (1)/acetonitrile (2)). This behavior is explained by the difference in the distribution of the molecules between the surface and the bulk region of the liquid. The experimental surface tension values for binary and ternary mixtures were correlated by various models. The best results were obtained for binary systems by the Myers−Scott model and for the ternary system by the Pando et al. model.

Literature Cited

(1) Vilares, A.; Giner, B.; Artigas, H.; Lafuente, C.; Royo, F. Study of the Surface Tensions of Cyclohexane or Methylcyclohexane with Some Cyclic Ethers. *J. Solution Chem.* **2005**, *34*, 205–209.
(2) Ali, A.; Tarig, M. Surface Thermodynamic Behaviour of Benzene + 1,1,2,2-Tetrachloroethane at Different Temperatures: An Experimental and Theoretical Study. *Phys. Chem. Liq.* **2008**, *46*, 47–58.
(3) Rafati, A. A.; Ghasemian, E.; Iloukhani, H. Surface Tension and Surface Properties of Binary Mixtures of 1,4-Dioxane or *N*,*N*-Dimethyl Formamide with *n*-Alkyl Acetates. *J. Chem. Eng. Data* **2009**, *54*, 3224–3228.
(4) Rafati, A. A.; Ghasemian, E. Study of Surface Tension and Surface Properties of Binary Alcohol/*n*-Alkyl Acetate Mixtures. *J. Colloid Interface Sci.* **2008**, *328*, 385–390.
(5) Kromidas, S. *HPLC Made to Measure*; John Wiley-VCH: New York, 2006.
(6) Granberg, R. A.; Rasmuson, A. C. Solubility of Paracetamol in Binary Ternary Mixtures of Water + Acetone + Toluene. *J. Chem. Eng. Data* **2000**, *45*, 478–483.
(7) Mendes-Tatsis, M. A.; Pursell, M.; Tang, S.; San Miguel, G. *The Effect of Ionic Surfactants on the Mass Transfer at the Liquid-Liquid Interface for a Toluene/Water/Acetone System*, International Solvent Extraction Conference, Cape Town, South Africa, March 17−21, 2002.
(8) Brodkorb, M. J.; Slater, M. J. *Multicomponent Kinetics in Liquid-Liquid Systems: an Experimental Study*, Solvent Extraction for the 21st Century, Proceedings of ISEC '99, Barcelona, Spain, July 11−16, 1999, 2001.
(9) Tourneau, M.; Wolf, S.; Stichlmair, J. Influence of Interfacial Convections on Mass Transfer in Liquid-Liquid Systems at Plane Interfaces. *DECHEMA Monogr.* **2000**, *136*, 277–293.
(10) Wolf, S. Interfacial Convective Flows in Mass Transfer in Liquid-Liquid Systems. *Fortschritt-Berichte VDI, Reihe 3: Verfahrenstechnik 584*; VDI Verlag GmbH: Düsseldorf, 1999.
(11) Pertler, M.; Haeberl, M.; Rommel, W.; Blass, E. Mass Transfer Across Liquid-Phase Boundaries. *Chem. Eng. Process.* **1995**, *34*, 269–277.
(12) Jasper, J. J. Surface Tension of Pure Liquid Compounds. *J. Phys. Chem. Ref. Data* **1972**, *1*, 841–1009.
(13) Daubert, T. E.; Danner, R. P. *Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation*; Hemisphere: New York, 1989.
(14) Wielebinski, D.; Findenegg, G. H. Measurement of Interfacial Tension in Simple Two-Phase Ternary Systems Along an Isothermal Linear Path to the Critical Point. *J. Phys. Chem.* **1984**, *88*, 4397–4401.
(15) Nagarajan, N.; Gasem, K. A. M.; Robinson, R. L., Jr. Equilibrium Phase Compositions, Phase Densities, and Interfacial Tensions of CO_2 + Hydrocarbon Systems. 6. CO_2 + *n*-butane + *n*-decane. *J. Chem. Eng. Data* **1990**, *35*, 228–231.
(16) Poling, B. E.; Prausnitz, J. M.; O'Connell, J. P. *The Properties of Gases and Liquids*; McGraw Hill: New York, 2001.
(17) Santos, B. M. S.; Ferreira, A. G. M.; Fonseca, I. M. A. Surface and Interfacial Tensions of the Systems Water + *n*-Butyl acetate + Methanol and Water + *n*-Pentyl Acetate + Methanol at 303.15 K. *Fluid Phase Equilib.* **2003**, *208*, 1–21.
(18) Kijevcanin, M. L.; Ribeiro, I. S. A.; Ferreira, A. G. M.; Fonseca, I. M. A. Densities, Viscosities, and Surface and Interfacial Tensions of the Ternary Mixture Water + Ethyl Butyrate + Methanol at 303.15 K. *J. Chem. Eng. Data* **2003**, *48*, 1266–1270.
(19) Kijevcanin, M. J.; Ribeiro, I. S. A.; Ferreira, A. G. M.; Fonseca, I. M. A. Water + Esters + Methanol: Experimental Data, Correlation and Prediction of Surface and Interfacial Tensions at 303.15 K and Atmospheric Pressure. *Fluid Phase Equilib.* **2004**, *218*, 141–148.
(20) Butler, J. A. V. The Thermodynamics of the Surfaces of Solutions. *Proc. R. Soc. London A* **1932**, *135*, 348–375.
(21) Li, C.; Wang, W.; Wang, Z. A Surface Tension Model for Liquid Mixtures Based on the Wilson Equation. *Fluid Phase Equilib.* **2000**, *175*, 185–196.
(22) Wilson, G. M. Vapor-Liquid Equilibrium. XI. A New Expression for the Excess Free Energy of Mixing. *J. Am. Chem. Soc.* **1964**, *86*, 127–131.
(23) Fu, J.; Li, B.; Wang, Z. Estimation of Fluid-Fluid Interfacial Tensions of Multicomponent Mixtures. *Chem. Eng. Sci.* **1986**, *41*, 2673–2679.
(24) Sonawane, P. D.; Kumar, A. A New Equation for the Correlation of Surface Tension-Composition Data of Solvent-Solvent and Solvent-Fused Salt Mixtures. *Fluid Phase Equilib.* **1999**, *157*, 17–28.
(25) Redlich, O. J.; Kister, A. T. Algebraic Representation of Thermodynamic Properties and the Classification of Solutions. *Ind. Eng. Chem.* **1948**, *40*, 345–348.
(26) Myers, D. B.; Scott, R. L. Thermodynamic Functions for Nonelectrolyte Solutions. *Ind. Eng. Chem.* **1963**, *55*, 43–46.
(27) IAPWS. IAPWS Release on Surface Tension of Ordinary Water Substance September. http://www.iapws.org/1994.
(28) Ku, H.; Wang, C.; Tu, C. Densities, Viscosities, Refractive Indexes, and Surface Tensions for Binary and Ternary Mixtures of Tetrahydofuran, 2-Propanol, and 2,2,4-Trimethylpentane. *J. Chem. Eng. Data* **2008**, *53*, 566–573.
(29) Wohlfarth, C.; Wohlfarth, B. Surface Tension of Pure Liquids and Binary Liquid Mixtures. *Landoldt-Börnstein New Series Group IV Physical Chemistry*, Vol. 16; Springer: Heidelberg, 1997.
(30) Maximino, R. B. Surface tension and density of binary mixtures of monoalcohols, water and acetonitrile: equation of correlation of the surface tension. *Phys. Chem. Liq.* **2009**, *47*, 475–486.
(31) Mosteiro, L.; Mariano, A. B.; Casas, L. M.; Pineiro, M. M.; Legido, J. L. Analysis of Surface Tension, Density, and Speed of Sound for the Ternary Mixture Dimethyl Carbonate + *p*-Xylene + *n*-Octane. *J. Chem. Eng. Data* **2009**, *54*, 1056–1062.
(32) Hildebrand, J. M.; Scott, R. *Solubility of Nonelectrolytes*, 3rd ed.; Dover: New York, 1964.
(33) Poling, B. E.; Prausnitz, J. M.; O'Connell, J. P. *The Properties of Gases and Liquids*, 5th ed.; McGraw-Hill: New York, 2004.
(34) Vazquez, G.; Alvarez, E.; Navaza, J. M. Surface Tension of Alcohol Water + Water from 20 to 50 °C. *J. Chem. Eng. Data* **1995**, *40*, 611–614.
(35) Pando, C.; Renuncio, J. A. R.; Calzon, J. A. G.; Christensen, J. J.; Izatt, R. M. Correlation and Prediction of Ternary Excess Enthalpy Data. *J. Solution Chem.* **1987**, *16*, 503–527.

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