Application of Abraham solvation parameters for surface tension prediction of mono-solvents and solvent mixtures at various temperatures

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ABSTRACT

A combined form of the Jouyban–Acree model and the Abraham solvation parameters was used to predict the surface tension of binary and ternary solvent mixtures at various temperatures. The new equations have been tested by comparisons with the experimental results for 364 binary and 79 ternary mixtures reported in the literature. After the training procedures, the models were used for the prediction of the surface tension of mixed solvent systems. The mean relative deviations (MRDs) between predicted and experimental surface tensions are used as an accuracy criterion. The overall MRD for binary mixtures was 6.5% and the corresponding value for ternary mixtures was 11.2%. These versions of the models require the experimental surface tension of the mono-solvents as input data. An attempt has been made here to correlate the surface tension of the mono-solvents at various temperatures using Abraham parameters. The model calculates the surface tension with the MRD of 11.0%. A combined version of the models was presented to predict the surface tension of binary and ternary mixtures without using any experimental input data in which the MRDs of 14.6 and 11.7% were obtained. Results show that the addition of solvation parameters may lead to an improvement in the calculated surface tension and show good agreement between theory and experiment.

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1. Introduction

Surface tension is a very complicated property of a liquid which reflects the intermolecular interaction and forces in liquids. When a new surface is being formed, surface active chemicals diffuse to the surface and align. During this process, interfacial tension is changing rapidly and continuously. Surface tension depends upon many variables such as temperature, composition of the solution, measurement time and viscosity of the liquid [1,2]. Surface tension of a liquid mixture (σ_m) is not a simple function of the surface tension of pure components. Experimental data on surface tension of liquid mixtures are very scarce in the literature therefore reliable methods for surface tension prediction are useful in many industrial applications and will save laborious experimental measurement time. Considerable effort has been made to develop theoretical or semi-theoretical models to predict surface tension. Details of these models, as well as comparisons of their abilities to accurately predict the surface tension of solvent mixtures, are available in the literature [3].

The linear solvation (or Abraham) parameters were used to correlate the surface tension of 299 organic compounds at 20 °C by Freitas et al. [4]. Their model also uses an arbitrary variable, i.e. number of carbon atoms for alkanes (N_C), and is expressed as:

$$\sigma_i = 14.9 + 4.35A_i^{Exp} - 1.3B_i^{Exp} + 11.3S_i^{Exp} + 10.9E_i + 3.0V_i + 0.8N_C \quad (1)$$

where A_i^{Exp}, B_i^{Exp}, S_i^{Exp}, E_i and V_i are the Abraham parameters of the organic compounds taken from the literature [5–7]. The numerical values of A_i^{Exp}, B_i^{Exp} and S_i^{Exp} were derived from experimental solubility data of the compounds dissolved in a number of organic solvents with known Abraham solvent parameters [8], E_i was calculated from refractive index data [9] and V_i was computed using a group contribution method of McGowan and Abraham [10]. Eq. (1) possesses no variable representing temperature effects on the surface tension, therefore it could be used to calculate the surface tension data at a given temperature, i.e. 20 °C.

There have been previous attempts to model the surface tension of solvent mixtures. The Redlich–Kister extension correlates the excess surface tension of the mixture (σ^E) to solvent composition:

$$\sigma^E = \sigma_m - (x_1\sigma_1 + x_2\sigma_2) \quad (2)$$

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and the Redlich–Kister extension is:

$$\sigma^E = (x_1(1-x_1))\left[S_0 + S_1(1-2x_1) + S_2(1-2x_1)^2\right] \tag{3}$$

where S_0–S_2 are the model constants calculated by regressing $\left[\frac{\sigma^E}{x_1(1-x_1)}\right]$ versus $(1-2x_1)$ and $(1-2x_1)^2$ using a least square analysis [11].

A polynomial function of solvent composition was also used to correlate the surface tension data as:

$$\log \sigma_m = C_0 + \sum_{i=1}^{m} C_i x_1^i \tag{4}$$

where C_0 and C_i are the model constants.

As an alternative, a non-linear equation was proposed to correlate the surface tension data as:

$$\sigma_m = \sigma_1 - \left[1 + \frac{bx_1}{1-ax_1}\right]x_2(\sigma_1-\sigma_2) \tag{5}$$

where a and b are the model constants. This method has been investigated as Eq. (6) [12].

$$\frac{\sigma_1-\sigma_m}{\sigma_1-\sigma_2} = \left(1 + \frac{bx_1}{1-ax_2}\right)x_2 \tag{6}$$

The Jouyban–Acree model was presented to predict the physico-chemical property of solvent mixtures including the surface tension at various temperatures of the solvent composition:

$$\log \sigma_{m,T} = x_1 \log \sigma_{1,T} + x_2 \log \sigma_{2,T} + \frac{x_1x_2}{T}\left[\sum_{i=0}^{2}J_i(x_1-x_2)^i\right] \tag{7}$$

in which J_i is the model constant. Eq. (7) provides reasonably accurate results with the overall MRD<4% for surface tension correlation of 26 binary and ternary solvent mixture at various temperatures. A previous work by our group indicates that the prediction capability of Jouyban–Acree model was better than models proposed by Lee and co-workers and Hoke and Patton [13]. In order to provide a more comprehensive and predictive model, it is possible to include the physico-chemical properties of the solvents which influence the surface tension of the mixture. Abraham and co-workers proposed a linear solvation energy relationship (LSER) equation to calculate various physico-chemical properties (PP) [14]:

$$\log PP = c + eE + sS + aA + bB + vV \tag{8}$$

in which c, e, s, a, b and v are the model constants, E is the excess molar refraction, S is the dipolarity/polarizability of the analyte, A denotes the analyte's hydrogen-bond acidity, B stands for the analyte's hydrogen-bond basicity and V is the McGowan volume of the analytes (for the numerical values of these parameters see Table 1). The numerical values of c, e, s, a, b and v terms are not available for some solvents and there is no available software to compute these parameters, however, the numerical values of E, S, A, B and V could be calculated using Pharma-Algorithm software. In treating the solute–solvent interactions, both parameters are required, but in the case of the physico-chemical properties of two solvents in the absence of any solute, the solute parameters of Abraham could also be employed to represent the interactions between two solvents in the mixtures. Abraham solvation parameters are known for 4000 organic compounds and the rest can be computed through Pharma Algorithm® Software [15]. Table 1 lists the Abraham parameters of the solvents investigated in this work. As noticed above, Abraham parameters have been used to correlate the surface tension [4] and also the interfacial tension data of organic compounds [16–18].

This work continues our study on the influence of Abraham solvation parameters on the prediction of the physicochemical properties of the solutions [19,20]. Any change in the surface tension of the solvent is due to intermolecular interactions in the solution which could be represented using Abraham parameters. By considering this hypothesis and the effect of temperature on the variations of surface tension, the following equation could be proposed to represent the surface tension of the mono-solvents at various temperatures:

$$\log \sigma_{i,T} = \alpha_0 + \alpha_1 E_i + \alpha_2 S_i + \alpha_3 A_i + \alpha_4 B_i + \alpha_5 V_i \\ + \frac{(\alpha_6 + \alpha_7 E_i + \alpha_8 S_i + \alpha_9 A_i + \alpha_{10}B_i + \alpha_{11}V_i)}{T} \tag{9}$$

in which α terms are the model constants. The J_i terms in Eq. (7) are due to the various solvent–solvent interactions in the mixture represented by Abraham parameters and thus Eq. (7) could be re-written as:

$$\log \sigma_{m,T} = x_1 \log \sigma_{1,T} + x_2 \log \sigma_{2,T} + \frac{x_1x_2}{T}\Big[W_0 + W_1(E_1-E_2)^2 \\ + W_2(S_1-S_2)^2 + W_3(A_1-A_2)^2 + W_4(B_1-B_2)^2 \\ + W_5(V_1-V_2)^2\Big] + \frac{x_1x_2(x_1-x_2)}{T}\Big[W'_0 + W'_1(E_1-E_2)^2 \\ + W'_2(S_1-S_2)^2 + W'_3(A_1-A_2)^2 + W'_4(B_1-B_2)^2 \\ + W'_5(V_1-V_2)^2\Big] + \frac{x_1x_2(x_1-x_2)}{T}\Big[W''_0 + W''_1(E_1-E_2)^2 \\ + W''_2(S_1-S_2)^2 + W''_3(A_1-A_2)^2 + W''_4(B_1-B_2)^2 \\ + W''_5(V_1-V_2)^2\Big] \tag{10}$$

where W terms are the model constants which represent the two and three body interaction energies of the solvents. From a mathematical point of view, they are adjustable curve-fit parameters determined from regressing $(\log \sigma_{m,T} - x_1 \log \sigma_{1,T} - x_2 \log \sigma_{2,T})$ against $\frac{x_1x_2}{T}$, $\frac{x_1x_2(E_1-E_2)^2}{T}$, $\frac{x_1x_2(S_1-S_2)^2}{T}$, $\frac{x_1x_2(A_1-A_2)^2}{T}$, $\frac{x_1x_2(B_1-B_2)^2}{T}$, $\frac{x_1x_2(V_1-V_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)}{T}$, $\frac{x_1x_2(x_1-x_2)(E_1-E_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)(S_1-S_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)(A_1-A_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)(B_1-B_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)(V_1-V_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2(E_1-E_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2(S_1-S_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2(A_1-A_2)^2}{T}$, $\frac{x_1x_2(x_1-x_2)^2(B_1-B_2)^2}{T}$ and $\frac{x_1x_2(x_1-x_2)^2(V_1-V_2)^2}{T}$ using a no intercept least square analysis. The Abraham solvation parameters account for all the probable interactions between solvents 1 and 2 in the system. The model can be used to predict the surface tension of different binary mixtures at various temperatures by employing the corresponding experimental σ_1 and σ_2 values of the mono-solvents at T. This means that in order to predict the surface tension of a binary solvent mixture at a given temperature, two experimental data is required. The number of required data points will be increased to ten when surface tensions at five temperatures are predicted. On the other hand, trained version of Eq. (9), i.e. Eq. (12), is able to predict the surface tension data employing the numerical values of Abraham parameters. The number of experimental data points required in the computation process of $\sigma_{m,T}$, can be reduced by combining Eqs. (9) and (10). The suggested procedure allows the prediction of the surface tension of binary and ternary mixtures as a function of temperature and solvent composition. One might be interested in the comparison of the proposed model for the surface tension of solvent mixtures however, to the best of our knowledge there is no globally trained model to calculate the surface tension data of solvents at various temperatures to be compared with the proposed model.

2. Experimental data and computational methods

Details of the collected data sets from the literatures [11,21–63] are given in Tables 2 and 3. These data sets include both aqueous and non-aqueous binary and ternary mixtures at various temperatures. In all computations, solvents 1, 2 and 3 are defined as $\sigma_1\langle\sigma_2\langle\sigma_3$. The fitness

Table 1
Abraham solute parameters for the solvents investigated in this work computed by Pharma-Algorithm, temperature range and the mean relative deviations (MRD).

No.	Solvent	E	S	A	B	V	T range	MRD
1	1-2-Butanediol	0.41	0.71	0.54	0.62	0.79	298	0.3
2	1-Amino-2-propanol	0.43	0.71	0.46	0.97	0.69	298–323	8.5
3	1-Butanol	0.20	0.46	0.31	0.31	0.73	288–308	6.6
4	1-Chlorobutane	0.12	0.32	0.00	0.04	0.79	298	0.4
5	1-Decanol	0.19	0.48	0.31	0.33	1.58	298	3.7
6	1-Heptanol	0.20	0.47	0.31	0.32	1.15	298	0.1
7	1-Hexanol	0.20	0.46	0.31	0.32	1.01	288–308	3.3
8	1-Nonanol	0.20	0.48	0.31	0.33	1.44	298	1.9
9	1-Octanol	0.20	0.47	0.31	0.32	1.29	288–308	0.9
10	1-Pentanol	0.20	0.46	0.31	0.32	0.87	298	3.4
11	1-Propanol	0.21	0.45	0.31	0.31	0.59	293–323	7.5
12	1,3-Butanediol	0.42	0.71	0.63	0.62	0.79	298–303	16.2
13	1,3-Dioxalone	0.29	0.57	0.00	0.43	0.54	298	16.3
14	1,3-Propanediol	0.41	0.72	0.63	0.59	0.65	298–323	42.2
15	1,4-Butanediol	0.41	0.73	0.63	0.59	0.79	298–303	30.8
16	1,4-Dioxane	0.29	0.58	0.00	0.44	0.68	288–308	15.6
17	2-(Ethylamino)ethanol	0.37	0.58	0.38	0.84	0.83	293–323	4.4
18	2-(Methylamino)ethanol	0.37	0.58	0.38	0.84	0.69	293–323	15.2
19	2-3-Butanediol	0.42	0.69	0.54	0.65	0.79	298	3.8
20	2-Amino-2-methyl-1-propanol	0.40	0.66	0.46	0.98	0.83	298–323	3.8
21	2-Butanol	0.21	0.44	0.31	0.33	0.73	298	11.3
22	2-Chlorobutane	0.13	0.31	0.00	0.06	0.79	298	6.9
23	2-Methyl-1-butanol	0.21	0.44	0.31	0.34	0.87	293–323	9.6
24	2-Methyl-1-chloropropane	0.26	0.37	0.00	0.11	0.75	298	15.9
25	2-Methyl-1-propanol	0.21	0.44	0.31	0.34	0.73	298	17.0
26	2-Methyl-2-butanol	0.19	0.39	0.31	0.35	0.87	293–323	7.6
27	2-Methyl-2-chloropropane	0.11	0.26	0.00	0.07	0.79	298	21.3
28	2-Methyl-2-propanol	0.19	0.39	0.31	0.35	0.73	298	25.1
29	2-Propanol	0.22	0.43	0.31	0.34	0.59	293–323	20.4
30	3-Amino-1-propanol	0.41	0.77	0.52	0.85	0.69	298–323	24.8
31	3-Methyl-1-butanol	0.21	0.44	0.31	0.34	0.87	293–323	6.7
32	Acetic acid	0.17	0.61	0.57	0.36	0.46	293–323	7.3
33	Acetone	0.22	0.67	0.00	0.34	0.55	293–323	17.0
34	Acetonitrile	0.19	0.72	0.00	0.20	0.40	298–318	12.0
35	Benzene	0.56	0.69	0.00	0.12	0.72	293–303	10.3
36	Butyl acetate	0.06	0.59	0.00	0.37	1.03	298	0.5
37	Carbon tetrachloride	0.42	0.55	0.00	0.00	0.74	288–318	6.6
38	Carbondisulfide	1.07	1.00	0.00	0.00	0.49	293–318	33.8
39	Cyclohexane	0.21	0.28	0.00	0.02	0.85	288–328	0.9
40	Decane	−0.01	0.21	0.00	0.05	1.52	293–333	5.5
41	Dichloromethane	0.22	0.38	0.09	0.00	0.49	293–308	11.9
42	Diethanolamine	0.58	0.82	0.64	1.19	0.89	298–323	18.2
43	Diethylsulfoxide	0.52	1.38	0.00	0.72	0.89	298–328	7.6
44	Diisopropylsulfoxide	0.54	1.35	0.00	0.78	1.18	298–328	24.0
45	Dimethylsulfoxide	0.52	1.37	0.00	0.71	0.61	298–328	13.2
46	Dipropylsulfoxide	0.52	1.39	0.00	0.73	1.18	298–328	20.0
47	Docosane	−0.03	0.26	0.00	0.09	3.21	313–343	3.6
48	Eicosane	−0.03	0.25	0.00	0.09	2.93	313–343	4.3
49	Ethanol	0.21	0.45	0.31	0.31	0.45	288–323	13.6
50	Ethyl acetate	0.07	0.58	0.00	0.36	0.75	298	2.6
51	Ethylene glycol	0.41	0.71	0.54	0.58	0.51	283–323	38.0
52	Formic acid	0.20	0.67	0.57	0.34	0.32	293–323	32.0
53	Heptane	0.00	0.20	0.00	0.05	1.09	288–343	10.7
54	Hexadecane	−0.02	0.23	0.00	0.07	2.36	293–333	10.1
55	Hexyl acetate	0.06	0.60	0.00	0.38	1.31	298	2.0
56	m-Xylene	0.61	0.58	0.00	0.12	1.00	298	13.9
57	Methanol	0.21	0.44	0.31	0.30	0.31	293–323	9.7
58	Methyl acetate	0.07	0.57	0.00	0.36	3.97	298	24.1
59	Methyl iodide	0.62	0.46	0.00	0.05	0.51	288–308	0.7
60	Monoethanolamine	0.42	0.72	0.46	0.94	0.55	298–323	34.9
61	n-Decane	−0.01	0.21	0.00	0.05	1.52	293–333	5.6
62	n-Hexadecane	−0.02	0.23	0.00	0.07	2.36	313–343	6.4
63	N-methyldiethanolamine	0.64	0.80	0.48	1.25	1.03	288–313	2.6
64	n-Nonane	−0.01	0.20	0.00	0.05	1.38	288–308	0.6
65	N,N-dimethylformamide	0.35	1.11	0.00	0.63	0.65	288–328	12.6
66	Nitrobenzene	0.83	1.26	0.00	0.21	0.89	293–303	5.8
67	o-Xylene	0.61	0.58	0.00	0.12	1.00	298	9.1
68	p-Xylene	0.61	0.58	0.00	0.12	1.00	298	15.3
69	Pentyl acetate	0.06	0.59	0.00	0.37	1.17	298	0.1
70	Propionic acid	0.17	0.62	0.57	0.57	0.61	293–323	0.9
71	Propyl acetate	0.07	0.58	0.00	0.37	0.89	298	2.5
72	Propyl propanoate	0.06	0.59	0.00	0.37	1.03	298	3.7
73	Propylene glycol	0.41	0.70	0.54	0.61	0.65	298–323	15.8
74	Tetracosane	−0.03	0.26	0.00	0.09	3.21	323–343	2.3

Table 1 (continued)

No.	Solvent	E	S	A	B	V	T range	MRD
75	Tetrahydrofuran	0.25	0.42	0.00	0.22	0.62	298	4.8
76	Toluene	0.58	0.63	0.00	0.12	0.86	288–328	15.3
77	Triethanolamine	0.87	1.04	0.73	1.60	1.23	288–323	11.0
78	Water	0.58	2.55	3.81	4.84	−0.87	283–328	1.1
								11.0

of the experimental data was studied by calculating the correlation co-efficient and the accuracy criteria. The accuracy of the surface tensions was investigated by computing the mean relative deviation (MRD) using:

$$MRD = \frac{100}{N} \sum \left(\frac{\left| \sigma^{Calc} - \sigma^{Exp} \right|}{\sigma^{Exp}} \right) \qquad (11)$$

in which N is the number of compositions of the mixtures. The individual relative deviations (IRDs) are also computed to present the errors of mono-solvents.

3. Results and discussion

3.1. Modeling surface tensions of mono-solvents at various temperatures

Surface tension data of the mono-solvents at various temperatures (collected in this work) were used to train Eq. (9) and the obtained model after excluding the non-significant constants (p > 0.10) is:

$$\log \sigma_{i,T} = 1.245E_i + 0.344A_i + 0.542V_i + \frac{1}{T}(384.020 - 305.012E_i + 22.350S_i - 101.827A_i + 16.608B_i - 152.522V_i). \qquad (12)$$

The model correlates the experimental data (within the range of 15.32 to 74.27 mN m^{-1}) with an F value of 46818, R = 0.999, the maximum IRD of 42.2% for 1,3-propandiol, the minimum IRD of 0.1% for 1-heptanol, and the MRD of 11.0 ± 9.7% (N = 78). Table 1 lists the details of the mono-solvents investigated in this work along with the MRD values for back-calculated data using Eq. (12). It is expected that the model predicts the surface tension of liquids at temperature range of 283 to 343 K with ~11% prediction error. Fig. 1 shows the relative frequency of IRD values for surface tension prediction of mono-solvents using Eq. (12), it is found that in more than 60% of the cases, the IRD value was less than 10%.

The surface tension data sets of Freitas et al. [4,17] were used as prediction data sets for Eq. (12) and the obtained MRD for the surface tensions of 107 mono-solvents at 273–299 K [17] was 11.4 ± 10.0% and for surface tensions of 299 mono-solvents at 293 K [4] was 10.9 ± 10.3%, in which there was no significant mean difference between training data set and prediction data sets. The corresponding MRD for back-calculated data of the surface tensions at 299 K by Eq. (1) was 6.5 ± 5.5% which is significantly less than 10.9% of the proposed model in this work (paired t-test, p < 0.0005). It should be kept in mind that our proposed model possesses a temperature dependence variable and could be used to predict the surface tension at various temperatures. In addition, it employs the computational descriptors which facilitate the prediction procedure and no further experimental effort is required. For further comparison of Eqs. (1) and (12), the surface tensions of Table 1 were predicted using Eq. (1), and the obtained MRDs were 14.2 ± 10.2% which was significantly greater than that of Eq. (12). We do not recommend the users to employ Eq. (1) for predicting the surface tensions of mono-solvents at various temperatures since there is no representing variable within Eq. (1).

3.2. Modeling surface tensions of binary solvents

All available surface tension data of binary solvent mixtures at various temperatures were fitted to Eq. (10) and the obtained model was:

$$\begin{aligned} \log \sigma_{m,T} = {} & x_1 \log \sigma_{1,T} + x_2 \log \sigma_{2,T} + \frac{x_1 x_2}{T} \left[-11.545 - 23.180(S_1 - S_2)^2 - 3.764(A_1 - A_2)^2 + 6.997(V_1 - V_2)^2 \right] \\ & + \frac{x_1 x_2 (x_1 - x_2)}{T} \left[102.261(E_1 - E_2)^2 + 29.458(S_1 - S_2)^2 + 26.850(V_1 - V_2)^2 \right] \\ & + \frac{x_1 x_2 (x_1 - x_2)^2}{T} \left[52.624 - 310.920(E_1 - E_2)^2 - 13.801(A_1 - A_2)^2 - 69.606(V_1 - V_2)^2 \right] \end{aligned} \qquad (13)$$

The model was statistically significant with the F value of 1072 (p < 0.0005) and covered the $\sigma_{m,T}$ range of 15.32 to 74.27 mN m^{-1}. When the surface tension data are back-calculated, the resulted MRDs were in the range of around 0.6% (for cyclohexane + benzene at 293 K) and 31.7% (for propyl acetate + water at 298 K) with the overall MRD (± SD) of 6.5 (± 6.5) % (number of data sets (NDS) = 364, N = 4508). Details of the MRD values for the investigated systems are listed in Table 2. It is found that the aqueous mixtures behave slightly different from non-aqueous mixtures and the overall MRD for aqueous data sets was 10.4 (± 6.8) % (NDS = 172) while the corresponding value for non-aqueous data sets was 3.0 (± 3.5) % (NDS = 192). More complex interactions between water and organic solvents in the aqueous binary mixtures could be a possible reason for this observation.

Table 2
Details of binary solvents studied, along with temperature (T), references, number of compositions of the mixtures (N), and mean relative deviation (MRD) of the computations.

No.	Solvent 1	Solvent 2	T	Ref.	N	Eq. (13)	Eq. (14)
			Overall:			6.5	15.2
1	1-2-Butanediol	Water	298.0	[21]	18	14.9	16.1
2	1-Amino-2-propanol	Water	298.0	[22]	12	5.1	3.8
3	1-Amino-2-propanol	Water	303.0	[22]	12	4.6	3.8
4	1-Amino-2-propanol	Water	308.0	[22]	12	4.2	4.2
5	1-Amino-2-propanol	Water	313.0	[22]	12	3.8	4.4
6	1-Amino-2-propanol	Water	318.0	[22]	12	3.6	5.4
7	1-Amino-2-propanol	Water	323.0	[22]	12	3.6	6.5
8	1-Butanol	1,3-Dioxalone	298.0	[23]	16	3.0	7.7
9	1-Chlorobutane	1-Butanol	298.0	[24]	13	0.9	3.9
10	1-Decanol	1,4-Dioxane	298.0	[25]	14	2.1	0.8
11	1-Heptanol	1,4-Dioxane	298.0	[25]	14	2.5	1.1
12	1-Heptanol	Ethylene glycol	298.0	[26]	21	30.5	32.2
13	1-Heptanol	Tetrahydrofuran	298.0	[27]	19	1.4	2.0
14	1-Hexanol	1,4-Dioxane	298.0	[25]	15	2.5	1.1
15	1-Hexanol	Ethylene glycol	298.0	[26]	19	22.5	25.1
16	1-Hexanol	Tetrahydrofuran	298.0	[27]	16	1.1	2.7
17	1-Octanol	1,4-Dioxane	298.0	[25]	18	2.4	0.9
18	1-Pentanol	1,3-Dioxalone	298.0	[23]	16	3.4	8.0
19	1-Pentanol	Ethylene glycol	298.0	[26]	21	23.2	26.6
20	1-Propanol	1,3-Dioxalone	298.0	[23]	13	1.8	5.7
21	1-Propanol	1,4-Dioxane	298.0	[28]	16	0.9	4.5
22	1-Propanol	Water	293.0	[29]	14	18.3	25.4
23	1-Propanol	Water	298.0	[29]	14	19.2	26.2
24	1-Propanol	Water	303.0	[29]	14	19.9	26.9
25	1-Propanol	Water	308.0	[29]	14	20.7	27.7
26	1-Propanol	Water	313.0	[29]	14	21.5	28.3
27	1-Propanol	Water	318.0	[29]	14	22.4	29.2
28	1-Propanol	Water	323.0	[29]	14	23.1	29.9
29	1,3-Butanediol	Water	298.0	[21]	18	4.4	4.4
30	1,3-Butanediol	Water	303.0	[30]	18	5.9	8.1
31	1,3-Propanediol	Water	298.0	[31]	7	14.2	11.9
32	1,3-Propanediol	Water	303.0	[30]	18	4.7	3.0
33	1,3-Propanediol	Water	303.0	[31]	7	14.3	11.9
34	1,3-Propanediol	Water	308.0	[31]	7	14.3	11.9
35	1,3-Propanediol	Water	313.0	[31]	7	14.2	11.9
36	1,3-Propanediol	Water	318.0	[31]	7	14.2	11.9
37	1,3-Propanediol	Water	323.0	[31]	7	14.0	11.8
38	1,4-Butanediol	Water	298.0	[21]	18	6.4	7.6
39	1,4-Butanediol	Water	303.0	[30]	18	5.0	4.2
40	1,4-Dioxane	Nitrobenzene	293.0	[32]	10	3.2	3.3
41	1,4-Dioxane	Nitrobenzene	303.0	[32]	11	4.0	4.2
42	1,4-Dioxane	Water	298.0	[33]	15	4.4	21.1
43	2-(Ethylamino)ethanol	Water	293.0	[34]	14	6.4	7.4
44	2-(Ethylamino)ethanol	Water	298.0	[34]	14	6.6	8.0
45	2-(Ethylamino)ethanol	Water	303.0	[34]	14	6.8	8.6
46	2-(Ethylamino)ethanol	Water	308.0	[34]	14	7.2	9.2
47	2-(Ethylamino)ethanol	Water	313.0	[34]	14	7.6	9.8
48	2-(Ethylamino)ethanol	Water	318.0	[34]	14	8.1	10.5
49	2-(Ethylamino)ethanol	Water	323.0	[34]	14	8.5	11.0
50	2-(Methylamino)ethanol	Water	293.0	[34]	14	6.7	4.0
51	2-(Methylamino)ethanol	Water	298.0	[34]	14	6.1	3.7
52	2-(Methylamino)ethanol	Water	303.0	[34]	14	5.6	3.3
53	2-(Methylamino)ethanol	Water	308.0	[34]	14	5.1	3.0
54	2-(Methylamino)ethanol	Water	313.0	[34]	14	4.6	2.8
55	2-(Methylamino)ethanol	Water	318.0	[34]	14	4.1	2.6
56	2-(Methylamino)ethanol	Water	323.0	[34]	14	3.6	2.6
57	2-3-Butanediol	Water	298.0	[21]	18	7.9	7.5
58	2-Amino-2-methyl-1-propanol	Water	298.0	[35]	14	10.6	11.1
59	2-Amino-2-methyl-1-propanol	Water	303.0	[35]	14	11.2	11.6
60	2-Amino-2-methyl-1-propanol	Water	308.0	[35]	14	11.7	12.2
61	2-Amino-2-methyl-1-propanol	Water	313.0	[35]	14	12.1	12.6
62	2-Amino-2-methyl-1-propanol	Water	318.0	[35]	14	12.9	13.3
63	2-Amino-2-methyl-1-propanol	Water	323.0	[35]	14	13.3	13.8
64	2-Butanol	1-Chlorobutane	298.0	[24]	13	0.9	0.9
65	2-Butanol	1-Decanol	298.0	[36]	11	3.1	4.4
66	2-Butanol	1,3-Dioxalone	298.0	[23]	14	3.5	2.1
67	2-Chlorobutane	1-Butanol	298.0	[24]	13	0.9	4.1
68	2-Chlorobutane	2-Butanol	298.0	[24]	13	1.1	4.6
69	2-Chlorobutane	2-Methyl-1-propanol	298.0	[24]	13	0.8	3.6
70	2-Methyl-1-chloropropane	1-Butanol	298.0	[24]	13	0.9	4.6
71	2-Methyl-1-chloropropane	2-Butanol	298.0	[24]	13	1.0	4.9
72	2-Methyl-1-chloropropane	2-Methyl-1-propanol	298.0	[24]	13	1.0	3.8
73	2-Methyl-1-propanol	1-Chlorobutane	298.0	[24]	13	0.9	3.2

Table 2 (continued)

No.	Solvent 1	Solvent 2	T	Ref.	N	Eq. (13)	Eq. (14)
74	2-Methyl-1-propanol	1-Decanol	298.0	[36]	10	3.2	4.6
75	2-Methyl-2-chloropropane	1-Butanol	298.0	[24]	13	2.0	5.5
76	2-Methyl-2-chloropropane	2-Butanol	298.0	[24]	13	0.9	4.1
77	2-Methyl-2-chloropropane	2-Methyl-1-propanol	298.0	[24]	13	1.3	3.9
78	2-Methyl-2-chloropropane	2-Methyl-2-propanol	298.0	[24]	13	1.0	4.4
79	2-Methyl-2-propanol	1-Chlorobutane	298.0	[24]	13	1.0	4.5
80	2-Methyl-2-propanol	1-Decanol	298.0	[36]	10	4.3	5.6
81	2-Methyl-2-propanol	2-Chlorobutane	298.0	[24]	13	0.9	4.4
82	2-Methyl-2-propanol	2-Methyl-1-chloropropane	298.0	[24]	13	1.0	4.7
83	2-Propanol	1,3-Dioxalone	298.0	[23]	14	3.2	7.8
84	2-Propanol	Water	293.0	[29]	14	10.8	17.6
85	2-Propanol	Water	298.0	[29]	14	11.7	18.5
86	2-Propanol	Water	303.0	[29]	14	12.6	19.3
87	2-Propanol	Water	308.0	[29]	14	13.4	20.1
88	2-Propanol	Water	313.0	[29]	14	14.1	20.7
89	2-Propanol	Water	318.0	[29]	14	15.0	21.6
90	2-Propanol	Water	323.0	[29]	14	15.8	22.3
91	3-Amino-1-propanol	Water	298.0	[22]	12	9.0	6.2
92	3-Amino-1-propanol	Water	303.0	[22]	12	8.3	5.6
93	3-Amino-1-propanol	Water	308.0	[22]	12	7.8	5.2
94	3-Amino-1-propanol	Water	313.0	[22]	12	7.2	4.8
95	3-Amino-1-propanol	Water	318.0	[22]	12	6.4	4.3
96	3-Amino-1-propanol	Water	323.0	[22]	12	5.8	4.0
97	Acetic acid	Water	293.0	[37]	14	4.7	9.1
98	Acetic acid	Water	298.0	[37]	14	5.3	9.7
99	Acetic acid	Water	303.0	[37]	14	5.8	10.2
100	Acetic acid	Water	308.0	[37]	14	6.3	10.7
101	Acetic acid	Water	313.0	[37]	14	6.8	11.1
102	Acetic acid	Water	318.0	[37]	14	7.5	11.7
103	Acetic acid	Water	323.0	[37]	14	7.9	12.1
104	Acetone	Water	293.0	[38]	16	12.5	53.8
105	Acetone	Water	298.0	[38]	9	11.0	43.0
106	Acetone	Water	311.0	[38]	16	14.3	33.4
107	Acetone	Water	323.0	[38]	18	15.4	39.2
108	Acetonitrile	Water	298.0	[39]	13	5.4	45.8
109	Benzene	1,4-Dioxane	293.0	[32]	8	1.1	2.2
110	Benzene	1,4-Dioxane	303.0	[32]	8	1.2	2.3
111	Benzene	Nitrobenzene	293.0	[32]	11	0.9	0.9
112	Benzene	Nitrobenzene	293.0	[40]	11	0.9	0.9
113	Benzene	Nitrobenzene	303.0	[32]	11	0.7	0.6
114	Benzene	Nitrobenzene	303.0	[40]	11	0.7	0.6
115	Butyl acetate	1,4-Dioxane	298.0	[41]	21	2.9	1.5
116	Butyl acetate	N,N-dimethylformamide	298.0	[41]	21	4.6	3.7
117	Butyl acetate	Water	298.0	[42]	20	26.7	26.8
118	Carbon tetrachloride	Acetonitrile	298.0	[43]	9	1.0	0.5
119	Carbon tetrachloride	Acetonitrile	303.0	[43]	8	1.2	0.3
120	Carbon tetrachloride	Acetonitrile	308.0	[43]	9	1.7	0.7
121	Carbon tetrachloride	Acetonitrile	313.0	[43]	10	1.3	0.4
122	Carbon tetrachloride	Acetonitrile	318.0	[43]	10	1.4	0.3
123	Carbon tetrachloride	Carbondisulfide	293.0	[44]	10	2.3	2.9
124	Carbon tetrachloride	Carbondisulfide	298.0	[44]	10	2.3	2.9
125	Carbon tetrachloride	Carbondisulfide	303.0	[44]	10	2.2	2.8
126	Carbon tetrachloride	Carbondisulfide	308.0	[44]	10	2.1	2.7
127	Carbon tetrachloride	Carbondisulfide	313.0	[44]	10	2.2	2.7
128	Carbon tetrachloride	Carbondisulfide	318.0	[44]	10	2.1	2.6
129	Carbon tetrachloride	Methyl iodide	288.0	[43]	5	2.0	1.0
130	Carbon tetrachloride	Methyl iodide	293.0	[43]	8	2.4	1.2
131	Carbon tetrachloride	Methyl iodide	298.0	[43]	14	2.9	1.5
132	Carbon tetrachloride	Methyl iodide	303.0	[43]	11	2.9	1.6
133	Carbon tetrachloride	Methyl iodide	308.0	[43]	9	2.8	1.6
134	Cyclohexane	1,4-Dioxane	293.0	[32]	8	0.8	1.3
135	Cyclohexane	1,4-Dioxane	303.0	[32]	8	1.5	0.6
136	Cyclohexane	Benzene	293.0	[32]	8	0.6	0.6
137	Cyclohexane	Benzene	303.0	[32]	11	0.8	1.2
138	Cyclohexane	Nitrobenzene	293.0	[32]	8	2.5	3.0
139	Cyclohexane	Nitrobenzene	303.0	[32]	11	4.8	5.7
140	Dichloromethane	Carbondisulfide	293.0	[45]	9	3.7	4.0
141	Dichloromethane	Carbondisulfide	298.0	[45]	8	2.8	3.1
142	Dichloromethane	Carbondisulfide	303.0	[45]	10	3.3	3.7
143	Dichloromethane	Carbondisulfide	308.0	[45]	10	3.1	3.6
144	Diethanolamine	Water	298.0	[46]	11	8.7	7.2
145	Diethanolamine	Water	303.0	[46]	11	8.3	6.9
146	Diethanolamine	Water	308.0	[46]	11	7.9	6.5
147	Diethanolamine	Water	313.0	[46]	11	7.9	6.7
148	Diethanolamine	Water	318.0	[46]	11	7.1	5.9
149	Diethanolamine	Water	323.0	[46]	11	6.7	5.5
150	Diethylsulfoxide	Water	298.0	[47]	10	2.7	86.8

Table 2 (continued)

No.	Solvent 1	Solvent 2	T	Ref.	N	Eq. (13)	Eq. (14)
151	Diethylsulfoxide	Water	303.0	[47]	10	2.8	86.0
152	Diethylsulfoxide	Water	308.0	[47]	10	2.7	84.0
153	Diethylsulfoxide	Water	313.0	[47]	10	4.3	79.6
154	Diethylsulfoxide	Water	318.0	[47]	10	4.1	78.8
155	Diethylsulfoxide	Water	323.0	[47]	10	4.5	79.7
156	Diethylsulfoxide	Water	328.0	[47]	10	4.3	79.5
157	Diisopropylsulfoxide	Water	298.0	[47]	8	12.8	93.9
158	Diisopropylsulfoxide	Water	303.0	[47]	9	15.1	89.8
159	Diisopropylsulfoxide	Water	308.0	[47]	10	17.4	89.9
160	Diisopropylsulfoxide	Water	313.0	[47]	10	17.4	88.6
161	Diisopropylsulfoxide	Water	318.0	[47]	10	17.1	86.9
162	Diisopropylsulfoxide	Water	323.0	[47]	10	18.2	87.8
163	Diisopropylsulfoxide	Water	328.0	[47]	10	18.7	87.5
164	Dimethylsulfoxide	Water	298.0	[47]	18	8.2	133.9
165	Dimethylsulfoxide	Water	303.0	[47]	18	7.6	131.6
166	Dimethylsulfoxide	Water	308.0	[47]	18	7.3	128.8
167	Dimethylsulfoxide	Water	313.0	[47]	18	6.8	126.4
168	Dimethylsulfoxide	Water	318.0	[47]	18	6.6	123.7
169	Dimethylsulfoxide	Water	323.0	[47]	18	6.0	122.1
170	Dimethylsulfoxide	Water	328.0	[47]	18	5.5	120.4
171	Dimethylsulfoxide	Water	298.0	[39]	13	17.9	15.2
172	Dipropylsulfoxide	Water	298.0	[47]	11	16.8	118.5
173	Dipropylsulfoxide	Water	303.0	[47]	11	17.8	117.5
174	Dipropylsulfoxide	Water	308.0	[47]	11	18.6	116.5
175	Dipropylsulfoxide	Water	313.0	[47]	11	19.5	115.6
176	Dipropylsulfoxide	Water	318.0	[47]	11	20.1	114.6
177	Dipropylsulfoxide	Water	323.0	[47]	11	21.2	114.2
178	Dipropylsulfoxide	Water	328.0	[47]	11	22.1	113.9
179	Ethanol	1,3-Dioxalone	298.0	[23]	16	0.8	4.5
180	Ethanol	1,4-Dioxane	288.0	[28]	24	0.8	2.5
181	Ethanol	1,4-Dioxane	293.0	[28]	25	1.0	2.7
182	Ethanol	1,4-Dioxane	298.0	[28]	24	1.1	2.1
183	Ethanol	1,4-Dioxane	303.0	[28]	26	1.3	2.3
184	Ethanol	1,4-Dioxane	308.0	[28]	23	1.3	2.0
185	Ethanol	2-Methyl-1-butanol	293.0	[48]	14	1.0	2.2
186	Ethanol	2-Methyl-1-butanol	298.0	[48]	14	1.2	2.5
187	Ethanol	2-Methyl-1-butanol	303.0	[48]	14	1.4	2.6
188	Ethanol	2-Methyl-1-butanol	308.0	[48]	14	1.6	2.7
189	Ethanol	2-Methyl-1-butanol	313.0	[48]	14	1.8	3.0
190	Ethanol	2-Methyl-1-butanol	318.0	[48]	14	2.0	3.1
191	Ethanol	2-Methyl-1-butanol	323.0	[48]	14	2.3	3.4
192	Ethanol	2-Methyl-2-butanol	293.0	[48]	14	1.2	2.4
193	Ethanol	2-Methyl-2-butanol	298.0	[48]	14	1.2	2.4
194	Ethanol	2-Methyl-2-butanol	303.0	[48]	14	1.4	2.5
195	Ethanol	2-Methyl-2-butanol	308.0	[48]	14	1.5	2.7
196	Ethanol	2-Methyl-2-butanol	313.0	[48]	14	2.4	3.5
197	Ethanol	2-Methyl-2-butanol	318.0	[48]	14	2.0	3.1
198	Ethanol	2-Methyl-2-butanol	323.0	[48]	14	2.2	3.3
199	Ethanol	3-Methyl-1-butanol	293.0	[48]	14	2.2	3.4
200	Ethanol	3-Methyl-1-butanol	298.0	[48]	14	2.3	3.5
201	Ethanol	3-Methyl-1-butanol	303.0	[48]	14	2.4	3.6
202	Ethanol	3-Methyl-1-butanol	308.0	[48]	14	2.5	3.7
203	Ethanol	3-Methyl-1-butanol	313.0	[48]	14	2.7	3.8
204	Ethanol	3-Methyl-1-butanol	318.0	[48]	14	2.8	3.9
205	Ethanol	3-Methyl-1-butanol	323.0	[48]	14	2.9	4.0
206	Ethanol	Acetonitrile	298.0	[49]	18	0.8	3.1
207	Ethanol	Ethylene glycol	293.0	[50]	8	8.2	11.4
208	Ethanol	Ethylene glycol	298.0	[50]	8	7.8	11.0
209	Ethanol	Ethylene glycol	303.0	[50]	8	7.7	10.8
210	Ethanol	Ethylene glycol	308.0	[50]	8	7.6	10.7
211	Ethanol	Ethylene glycol	313.0	[50]	8	7.8	10.8
212	Ethanol	Ethylene glycol	318.0	[50]	8	7.6	10.6
213	Ethanol	Ethylene glycol	323.0	[50]	8	7.2	10.1
214	Ethanol	N-methyldiethanolamine	288.0	[51]	15	6.1	6.9
215	Ethanol	N-methyldiethanolamine	293.0	[51]	15	6.4	7.1
216	Ethanol	N-methyldiethanolamine	298.0	[51]	15	6.9	7.6
217	Ethanol	N-methyldiethanolamine	303.0	[51]	15	7.4	8.2
218	Ethanol	N-methyldiethanolamine	308.0	[51]	15	7.8	8.5
219	Ethanol	N-methyldiethanolamine	313.0	[51]	15	8.5	9.2
220	Ethanol	Triethanolamine	288.0	[51]	11	6.3	6.7
221	Ethanol	Triethanolamine	293.0	[51]	11	6.5	6.9
222	Ethanol	Triethanolamine	298.0	[51]	11	7.4	7.8
223	Ethanol	Triethanolamine	303.0	[51]	11	7.0	7.5
224	Ethanol	Triethanolamine	308.0	[51]	11	7.2	7.6
225	Ethanol	Triethanolamine	313.0	[51]	11	7.4	7.8
226	Ethanol	Water	293.0	[29]	14	3.4	5.5

Table 2 (continued)

No.	Solvent 1	Solvent 2	T	Ref.	N	Eq. (13)	Eq. (14)
227	Ethanol	Water	298.0	[29]	14	3.2	6.0
228	Ethanol	Water	303.0	[29]	14	3.0	6.5
229	Ethanol	Water	308.0	[29]	14	2.9	6.9
230	Ethanol	Water	313.0	[29]	14	2.9	7.3
231	Ethanol	Water	318.0	[29]	14	2.9	7.9
232	Ethanol	Water	323.0	[29]	14	2.9	8.2
233	Ethyl acetate	Water	298.0	[42]	16	31.0	31.4
234	Ethylene glycol	Water	283.0	[52]	13	12.8	9.5
235	Ethylene glycol	Water	293.0	[52]	13	12.2	9.0
236	Ethylene glycol	Water	303.0	[30]	18	10.8	8.0
237	Ethylene glycol	Water	303.0	[52]	13	11.4	8.3
238	Ethylene glycol	Water	313.0	[52]	13	10.7	7.6
239	Ethylene glycol	Water	323.0	[52]	13	10.4	7.4
240	Formic acid	Water	293.0	[37]	14	8.8	6.8
241	Formic acid	Water	298.0	[37]	14	8.5	5.0
242	Formic acid	Water	303.0	[37]	14	8.1	4.7
243	Formic acid	Water	308.0	[37]	14	7.8	4.5
244	Formic acid	Water	313.0	[37]	14	7.5	4.3
245	Formic acid	Water	318.0	[37]	14	7.1	4.1
246	Formic acid	Water	323.0	[37]	14	6.8	3.9
247	Heptane	1-Butanol	288.0	[53]	13	1.9	4.4
248	Heptane	1-Butanol	293.0	[53]	13	2.1	4.6
249	Heptane	1-Butanol	298.0	[53]	12	2.2	4.5
250	Heptane	1-Butanol	303.0	[53]	13	2.7	5.1
251	Heptane	1-Butanol	308.0	[53]	13	2.6	4.9
252	Heptane	1-Hexanol	288.0	[53]	13	2.1	5.2
253	Heptane	1-Hexanol	293.0	[53]	13	2.5	5.6
254	Heptane	1-Hexanol	298.0	[53]	13	2.6	5.6
255	Heptane	1-Hexanol	303.0	[53]	13	2.8	5.8
256	Heptane	1-Hexanol	308.0	[53]	13	3.2	6.1
257	Heptane	1-Octanol	288.0	[53]	13	2.3	5.2
258	Heptane	1-Octanol	293.0	[53]	13	2.7	5.5
259	Heptane	1-Octanol	298.0	[53]	13	2.9	5.7
260	Heptane	1-Octanol	303.0	[53]	13	3.1	5.9
261	Heptane	1-Octanol	308.0	[53]	13	3.4	6.1
262	Heptane	Cyclohexane	288.0	[54]	11	1.3	5.2
263	Heptane	Cyclohexane	298.0	[54]	11	1.1	4.9
264	Heptane	Cyclohexane	308.0	[54]	11	1.1	4.8
265	Heptane	Cyclohexane	318.0	[54]	11	1.2	4.7
266	Heptane	Cyclohexane	328.0	[54]	11	1.5	5.0
267	Heptane	Decane	293.0	[55]	5	0.9	1.7
268	Heptane	Decane	303.0	[55]	5	1.0	1.5
269	Heptane	Decane	313.0	[55]	5	1.1	1.3
270	Heptane	Decane	323.0	[55]	5	1.4	0.9
271	Heptane	Decane	333.0	[55]	5	1.7	0.5
272	Heptane	Docosane	313.0	[56]	5	5.4	17.8
273	Heptane	Docosane	323.0	[56]	5	5.0	17.1
274	Heptane	Docosane	333.0	[56]	5	5.6	17.3
275	Heptane	Docosane	343.0	[56]	5	6.4	17.7
276	Heptane	Eicosane	313.0	[56]	5	3.8	13.1
277	Heptane	Eicosane	323.0	[56]	5	4.4	13.3
278	Heptane	Eicosane	333.0	[56]	5	4.9	13.5
279	Heptane	Eicosane	343.0	[56]	5	5.6	13.9
280	Heptane	Hexadecane	293.0	[55]	5	2.4	5.4
281	Heptane	Hexadecane	303.0	[55]	5	2.7	5.6
282	Heptane	Hexadecane	313.0	[55]	5	3.1	5.9
283	Heptane	Hexadecane	323.0	[55]	5	3.7	6.4
284	Heptane	Hexadecane	333.0	[55]	5	4.4	6.9
285	Heptane	Tetracosane	323.0	[56]	5	6.4	18.2
286	Heptane	Tetracosane	333.0	[56]	5	6.1	17.7
287	Heptane	Tetracosane	343.0	[56]	5	7.3	18.4
288	Hexyl acetate	1,4-Dioxane	298.0	[41]	21	1.2	0.8
289	Hexyl acetate	N,N-dimethylformamide	298.0	[41]	21	1.2	1.0
290	Methanol	1,3-Dioxalone	298.0	[23]	18	3.1	1.0
291	Methanol	1,4-Dioxane	298.0	[28]	14	3.8	0.8
292	Methanol	Water	293.0	[29]	14	11.4	6.4
293	Methanol	Water	293.0	[57]	9	12.6	13.7
294	Methanol	Water	298.0	[29]	14	11.0	6.1
295	Methanol	Water	298.0	[39]	13	14.4	15.7
296	Methanol	Water	303.0	[29]	14	10.6	5.8
297	Methanol	Water	303.0	[57]	9	12.4	13.5
298	Methanol	Water	308.0	[29]	14	10.3	5.6
299	Methanol	Water	313.0	[29]	14	9.7	5.1
300	Methanol	Water	318.0	[29]	14	9.6	5.1
301	Methanol	Water	323.0	[29]	14	9.2	4.9
302	Methanol	Water	323.0	[57]	9	12.6	13.6
303	Methyl acetate	Water	298.0	[42]	18	6.4	8.4

Table 2 (continued)

No.	Solvent 1	Solvent 2	T	Ref.	N	Eq. (13)	Eq. (14)
304	Monoethanolamine	Water	298.0	[35]	13	10.1	5.7
305	Monoethanolamine	Water	303.0	[35]	13	9.8	5.5
306	Monoethanolamine	Water	308.0	[35]	13	9.4	5.8
307	Monoethanolamine	Water	313.0	[35]	13	9.1	5.1
308	Monoethanolamine	Water	318.0	[35]	13	8.7	5.0
309	Monoethanolamine	Water	323.0	[35]	13	8.4	4.8
310	n-Decane	Hexadecane	293.0	[55]	5	0.8	0.8
311	n-Decane	Hexadecane	303.0	[55]	5	1.0	1.0
312	n-Decane	Hexadecane	313.0	[55]	5	1.3	1.1
313	n-Decane	Hexadecane	323.0	[55]	5	1.3	1.2
314	n-Decane	Hexadecane	333.0	[55]	5	1.3	1.2
315	n-Hexadecane	Eicosane	313.0	[55]	7	0.9	1.6
316	n-Hexadecane	Eicosane	323.0	[55]	7	1.1	1.3
317	n-Hexadecane	Eicosane	333.0	[55]	7	1.0	1.3
318	n-Hexadecane	Eicosane	343.0	[55]	7	1.1	1.0
319	N-methyldiethanolamine	Water	298.0	[58]	14	5.6	5.9
320	N-methyldiethanolamine	Water	303.0	[58]	14	5.5	6.1
321	N-methyldiethanolamine	Water	308.0	[58]	14	5.3	5.9
322	N-methyldiethanolamine	Water	313.0	[58]	14	4.8	5.7
323	N-methyldiethanolamine	Water	318.0	[58]	14	4.5	6.3
324	N-methyldiethanolamine	Water	323.0	[58]	14	4.9	7.4
325	n-Nonane	1-Hexanol	288.0	[59]	13	0.7	3.2
326	n-Nonane	1-Hexanol	298.0	[59]	13	0.9	3.3
327	n-Nonane	1-Hexanol	308.0	[59]	13	1.0	3.4
328	N,N-dimethylformamide	Toluene	288.0	[60]	7	0.8	0.8
329	N,N-dimethylformamide	Toluene	298.0	[60]	7	0.8	0.9
330	N,N-dimethylformamide	Toluene	308.0	[60]	7	0.9	0.9
331	N,N-dimethylformamide	Toluene	318.0	[60]	7	0.6	0.8
332	N,N-dimethylformamide	Toluene	328.0	[60]	7	0.6	0.9
333	Pentyl acetate	1,4-Dioxane	298.0	[41]	21	1.8	0.5
334	Pentyl acetate	N,N-dimethylformamide	298.0	[41]	21	2.9	2.1
335	Propionic acid	Water	293.0	[37]	14	25.1	29.8
336	Propionic acid	Water	298.0	[37]	14	26.4	31.2
337	Propionic acid	Water	303.0	[37]	14	27.0	31.8
338	Propionic acid	Water	308.0	[37]	14	28.0	32.7
339	Propionic acid	Water	313.0	[37]	14	28.9	33.5
340	Propionic acid	Water	318.0	[37]	14	30.0	34.6
341	Propionic acid	Water	323.0	[37]	14	30.9	35.4
342	Propyl acetate	Water	298.0	[42]	28	31.7	31.8
343	Propyl propanoate	m-Xylene	298.0	[61]	14	2.0	4.4
344	Propyl propanoate	o-Xylene	298.0	[61]	19	1.9	4.7
345	Propyl propanoate	p-Xylene	298.0	[61]	20	2.7	4.6
346	Propylene glycol	Water	298.0	[62]	8	3.3	2.4
347	Propylene glycol	Water	303.0	[62]	9	2.5	2.9
348	Propylene glycol	Water	313.0	[62]	9	2.5	3.2
349	Propylene glycol	Water	323.0	[62]	9	2.5	3.5
350	Tetrahydrofuran	1-Decanol	298.0	[27]	16	2.4	2.5
351	Tetrahydrofuran	1-Nonanol	298.0	[27]	14	1.9	1.0
352	Tetrahydrofuran	1-Octanol	298.0	[27]	15	1.4	0.8
353	Tetrahydrofuran	Water	298.0	[39]	13	3.8	10.2
354	Toluene	Heptane	288.0	[60]	6	2.2	2.6
355	Toluene	Heptane	298.0	[60]	7	2.5	3.2
356	Toluene	Heptane	308.0	[60]	7	2.5	3.3
357	Toluene	Heptane	318.0	[60]	7	2.5	3.3
358	Toluene	Heptane	328.0	[60]	7	2.2	2.9
359	Triethanolamine	Water	298.0	[46]	11	5.1	3.9
360	Triethanolamine	Water	303.0	[46]	11	4.7	4.0
361	Triethanolamine	Water	308.0	[46]	11	4.4	4.2
362	Triethanolamine	Water	313.0	[46]	11	4.2	4.5
363	Triethanolamine	Water	318.0	[46]	11	3.9	5.0
364	Triethanolamine	Water	323.0	[46]	11	3.7	5.5

A combination of Eqs. (12) and (13) gives:

$$
\log \sigma_{m,T} = x_1 \left(1.245E_1 + 0.344A_1 + 0.542V_1 + \frac{1}{T}(384.020 - 305.012E_1 + 22.350S_1 - 101.827A_1 + 16.608B_1 - 152.522V_1) \right)
$$

$$
+ x_2 \left(1.245E_2 + 0.344A_2 + 0.542V_2 + \frac{1}{T}(384.020 - 305.012E_2 + 22.350S_2 - 101.827A_2 + 16.608B_2 - 152.522V_2) \right)
$$

$$
+ \frac{x_1 x_2}{T} \left[-11.545 - 23.180(S_1 - S_2)^2 - 3.764(A_1 - A_2)^2 + 6.997(V_1 - V_2)^2 \right] + \frac{x_1 x_2 (x_1 - x_2)}{T} \left[102.261(E_1 - E_2)^2 + 29.458(S_1 - S_2)^2 \right]
$$

$$
+ 26.850(V_1 - V_2)^2 \right] + \frac{x_1 x_2 (x_1 - x_2)^2}{T} \left[52.624 - 310.920(E_1 - E_2)^2 - 13.801(A_1 - A_2)^2 - 69.606(V_1 - V_2)^2 \right].
$$

(14)

Table 3
Details of ternary solvents studied, along with temperature (T), references, number of compositions of the mixtures (N), and mean relative deviation (MRD) of the computations.

No.	Solvent 1	Solvent 2	Solvent 3	T	References	N	Eq. (15)	Eq. (16)
1	1-Amino-2-propanol	Diethanolamine	Water	298.2	[22,45]	4	6.0	7.0
2	1-Amino-2-propanol	Diethanolamine	Water	303.2	[22,45]	4	5.7	6.2
3	1-Amino-2-propanol	Diethanolamine	Water	308.2	[22,45]	4	5.4	5.4
4	1-Amino-2-propanol	Diethanolamine	Water	313.2	[22,45]	4	5.2	4.8
5	1-Amino-2-propanol	Diethanolamine	Water	318.2	[22,45]	4	4.9	4.6
6	1-Amino-2-propanol	Diethanolamine	Water	323.2	[22,45]	4	4.7	4.3
7	1-Amino-2-propanol	Triethanolamine	Water	298.2	[22,45]	4	7.9	8.5
8	1-Amino-2-propanol	Triethanolamine	Water	303.2	[22,45]	4	7.6	8.3
9	1-Amino-2-propanol	Triethanolamine	Water	308.2	[22,45]	4	7.4	8.1
10	1-Amino-2-propanol	Triethanolamine	Water	313.2	[22,45]	4	7.4	8.3
11	1-Amino-2-propanol	Triethanolamine	Water	318.2	[22,45]	4	8.0	9.0
12	1-Amino-2-propanol	Triethanolamine	Water	323.2	[22,45]	4	8.4	9.8
13	1-Propanol	n-Butyl acetate	Water	303.2	[63]	39	19.0	18.5
14	2-(Ethylamino)ethanol	N-methyldiethanolamine	Water	293.2	[34,45]	4	13.3	14.0
15	2-(Ethylamino)ethanol	N-methyldiethanolamine	Water	298.2	[34,45]	4	12.6	13.4
16	2-(Ethylamino)ethanol	N-methyldiethanolamine	Water	303.2	[34,45]	4	12.2	12.5
17	2-(Ethylamino)ethanol	N-methyldiethanolamine	Water	308.2	[34,45]	4	11.6	11.7
18	2-(Ethylamino)ethanol	N-methyldiethanolamine	Water	313.2	[34,45]	4	11.1	10.8
19	2-(Ethylamino)ethanol	N-methyldiethanolamine	Water	318.2	[34,45]	4	10.2	9.9
20	2-(Ethylamino)ethanol	N-methyldiethanolamine	Water	323.2	[34,45]	4	9.6	8.9
21	2-(Ethylamino)ethanol	Triethanolamine	Water	293.2	[34,45]	4	11.0	11.1
22	2-(Ethylamino)ethanol	Triethanolamine	Water	298.2	[34,45]	4	10.4	10.0
23	2-(Ethylamino)ethanol	Triethanolamine	Water	303.2	[34,45]	4	9.9	8.7
24	2-(Ethylamino)ethanol	Triethanolamine	Water	308.2	[34,45]	4	9.4	7.6
25	2-(Ethylamino)ethanol	Triethanolamine	Water	313.2	[34,45]	4	9.1	6.3
26	2-(Ethylamino)ethanol	Triethanolamine	Water	318.2	[34,45]	4	8.5	5.1
27	2-(Ethylamino)ethanol	Triethanolamine	Water	323.2	[34,45]	4	8.2	4.7
28	2-(Methylamino)ethanol	N-methyldiethanolamine	Water	293.2	[34,45]	4	17.0	19.6
29	2-(Methylamino)ethanol	N-methyldiethanolamine	Water	298.2	[34,45]	4	16.1	18.8
30	2-(Methylamino)ethanol	N-methyldiethanolamine	Water	303.2	[34,45]	4	15.6	18.1
31	2-(Methylamino)ethanol	N-methyldiethanolamine	Water	308.2	[34,45]	4	14.7	17.3
32	2-(Methylamino)ethanol	N-methyldiethanolamine	Water	313.2	[34,45]	4	13.9	16.4
33	2-(Methylamino)ethanol	N-methyldiethanolamine	Water	318.2	[34,45]	4	12.8	15.4
34	2-(Methylamino)ethanol	N-methyldiethanolamine	Water	323.2	[34,45]	4	11.9	14.4
35	2-(Methylamino)ethanol	Triethanolamine	Water	293.2	[34,45]	4	15.7	17.7
36	2-(Methylamino)ethanol	Triethanolamine	Water	298.2	[34,45]	4	15.0	16.6
37	2-(Methylamino)ethanol	Triethanolamine	Water	303.2	[34,45]	4	14.4	15.5
38	2-(Methylamino)ethanol	Triethanolamine	Water	308.2	[34,45]	4	13.7	14.5
39	2-(Methylamino)ethanol	Triethanolamine	Water	313.2	[34,45]	4	13.1	13.2
40	2-(Methylamino)ethanol	Triethanolamine	Water	318.2	[34,45]	4	12.3	12.0
41	2-(Methylamino)ethanol	Triethanolamine	Water	323.2	[34,45]	4	11.8	10.7
42	2-Amino-2-methyl-1-pro	1-Amino-2-propanol	Water	298.2	[22,45]	4	14.7	13.9
43	2-Amino-2-methyl-1-pro	1-Amino-2-propanol	Water	303.2	[22,45]	4	15.9	15.3
44	2-Amino-2-methyl-1-pro	1-Amino-2-propanol	Water	308.2	[22,45]	4	17.1	16.7
45	2-Amino-2-methyl-1-pro	1-Amino-2-propanol	Water	313.2	[22,45]	4	18.2	18.3
46	2-Amino-2-methyl-1-pro	1-Amino-2-propanol	Water	318.2	[22,45]	4	19.6	20.0
47	2-Amino-2-methyl-1-pro	1-Amino-2-propanol	Water	323.2	[22,45]	4	20.7	21.8
48	2-Amino-2-methyl-1-pro	3-Amino-1-propanol	Water	298.2	[22,45]	4	9.0	6.4
49	2-Amino-2-methyl-1-pro	3-Amino-1-propanol	Water	303.2	[22,45]	4	9.8	7.3
50	2-Amino-2-methyl-1-pro	3-Amino-1-propanol	Water	308.2	[22,45]	4	10.7	8.3
51	2-Amino-2-methyl-1-pro	3-Amino-1-propanol	Water	313.2	[22,45]	4	11.4	9.3
52	2-Amino-2-methyl-1-pro	3-Amino-1-propanol	Water	318.2	[22,45]	4	12.3	10.4
53	2-Amino-2-methyl-1-pro	3-Amino-1-propanol	Water	323.2	[22,45]	4	13.0	11.7
54	2-Amino-2-methyl-1-pro	N-methyldiethanolamine	Water	298.2	[57]	4	8.5	7.5
55	2-Amino-2-methyl-1-pro	N-methyldiethanolamine	Water	303.2	[57]	4	8.3	6.9
56	2-Amino-2-methyl-1-pro	N-methyldiethanolamine	Water	308.2	[57]	4	8.2	6.4
57	2-Amino-2-methyl-1-pro	N-methyldiethanolamine	Water	313.2	[57]	4	7.7	5.5
58	2-Amino-2-methyl-1-pro	N-methyldiethanolamine	Water	318.2	[57]	4	7.3	5.0
59	2-Amino-2-methyl-1-pro	N-methyldiethanolamine	Water	323.2	[57]	4	7.1	4.3
60	3-Amino-1-propanol	Diethanolamine	Water	298.2	[22,45]	4	11.3	15.5
61	3-Amino-1-propanol	Diethanolamine	Water	303.2	[22,45]	4	11.0	15.1
62	3-Amino-1-propanol	Diethanolamine	Water	308.2	[22,45]	4	10.7	14.6
63	3-Amino-1-propanol	Diethanolamine	Water	313.2	[22,45]	4	10.5	14.1
64	3-Amino-1-propanol	Diethanolamine	Water	318.2	[22,45]	4	10.1	13.6
65	3-Amino-1-propanol	Diethanolamine	Water	323.2	[22,45]	4	9.9	12.9
66	3-Amino-1-propanol	Triethanolamine	Water	298.2	[22,45]	4	9.1	10.5
67	3-Amino-1-propanol	Triethanolamine	Water	303.2	[22,45]	4	9.0	10.2
68	3-Amino-1-propanol	Triethanolamine	Water	308.2	[22,45]	4	8.9	10.2
69	3-Amino-1-propanol	Triethanolamine	Water	313.2	[22,45]	4	8.8	10.1
70	3-Amino-1-propanol	Triethanolamine	Water	318.2	[22,45]	4	8.8	10.1
71	3-Amino-1-propanol	Triethanolamine	Water	323.2	[22,45]	4	8.7	10.1
72	Methanol	n-Butyl acetate	Water	303.2	[62]	48	14.0	13.6
73	Methanol	n-Pentyl acetate	Water	303.2	[62]	26	9.4	8.4
74	N-methyldiethanolamine	Diethanolamine	Water	298.2	[57]	4	14.7	19.2
75	N-methyldiethanolamine	diethanolamine	water	303.2	[57]	4	14.0	18.0

Table 3 (*continued*)

No.	Solvent 1	Solvent 2	Solvent 3	T	References	N	Eq. (15)	Eq. (16)
76	N-methyldiethanolamine	Diethanolamine	Water	308.2	[57]	4	13.8	17.3
77	N-methyldiethanolamine	Diethanolamine	Water	313.2	[57]	4	13.3	16.3
78	N-methyldiethanolamine	Diethanolamine	Water	318.2	[57]	4	12.9	15.7
79	N-methyldiethanolamine	Diethanolamine	Water	323.2	[57]	4	12.6	14.8
					Overall:		11.2	11.7

The above equation provides the possibility of surface tension prediction of binary solvents at various temperatures without the use of any experimental data point. The back-calculated surface tensions resulted in the MRD values of 0.3% (for carbon tetrachloride + acetonitrile at 303 K) and 133.9% (for dimethylsulfoxide + water at 298 K) with the overall MRD ($\pm$SD) of 15.2 ($\pm$27.3) %. By employing Abraham parameters as input data, Eq. (13) predicts the surface tension of binary solvents as a function of temperature and solvent composition. Fig. 2 illustrates the relative frequencies of the IRD for surface tension prediction using Eqs. (13) and (14). It can be seen that Eq. (13) presents the data more accurately than Eq. (14), however it requires two experimental surface tension data of the mono-solvents, whereas Eq. (14) is an ab initio model and does not require any experimental input data in the prediction process.

3.3. Modeling surface tensions of ternary solvents

A further option explored in this study was to extend Eq. (13) as:

$$
\begin{aligned}
\log \sigma_{m,T} = {} & x_1 \log \sigma_{1,T} + x_2 \log \sigma_{2,T} + x_3 \log \sigma_{3,T} + \frac{x_1 x_2}{T}\left[-11.545 - 23.180(S_1 - S_2)^2 - 3.764(A_1 - A_2)^2 + 6.997(V_1 - V_2)^2\right] \\
& + \frac{x_1 x_2 (x_1 - x_2)}{T}\left[102.261(E_1 - E_2)^2 + 29.458(S_1 - S_2)^2 + 26.850(V_1 - V_2)^2\right] \\
& + \frac{x_1 x_2 (x_1 - x_2)^2}{T}\left[52.624 - 310.920(E_1 - E_2)^2 - 13.801(A_1 - A_2)^2 - 69.606(V_1 - V_2)^2\right] \\
& + \frac{x_1 x_3}{T}\left[-11.545 - 23.180(S_1 - S_3)^2 - 3.764(A_1 - A_3)^2 + 6.997(V_1 - V_3)^2\right] \\
& + \frac{x_1 x_3 (x_1 - x_3)}{T}\left[102.261(E_1 - E_3)^2 + 29.458(S_1 - S_3)^2 + 26.850(V_1 - V_3)^2\right] \\
& + \frac{x_1 x_3 (x_1 - x_3)^2}{T}\left[52.624 - 310.920(E_1 - E_3)^2 - 13.801(A_1 - A_3)^2 - 69.606(V_1 - V_3)^2\right] \\
& + \frac{x_2 x_3}{T}\left[-11.545 - 23.180(S_2 - S_3)^2 - 3.764(A_2 - A_3)^2 + 6.997(V_2 - V_3)^2\right] \\
& + \frac{x_2 x_3 (x_2 - x_3)}{T}\left[102.261(E_2 - E_3)^2 + 29.458(S_2 - S_3)^2 + 26.850(V_2 - V_3)^2\right] \\
& + \frac{x_2 x_3 (x_2 - x_3)^2}{T}\left[52.624 - 310.920(E_2 - E_3)^2 - 13.801(A_2 - A_3)^2 - 69.606(V_2 - V_3)^2\right]
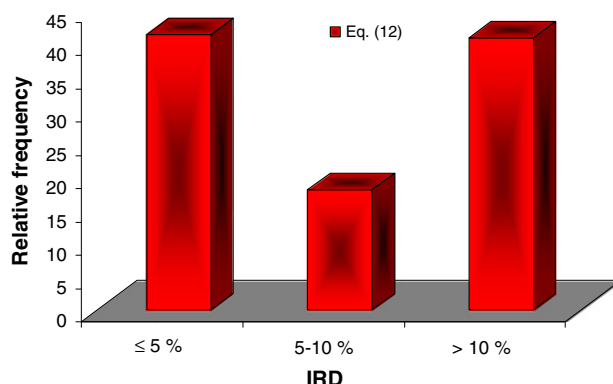\end{aligned}
\tag{15}
$$

Fig. 1. Relative frequency of the individual relative deviations (IRD) of the predicted surface tension of the mono-solvents at various temperatures.
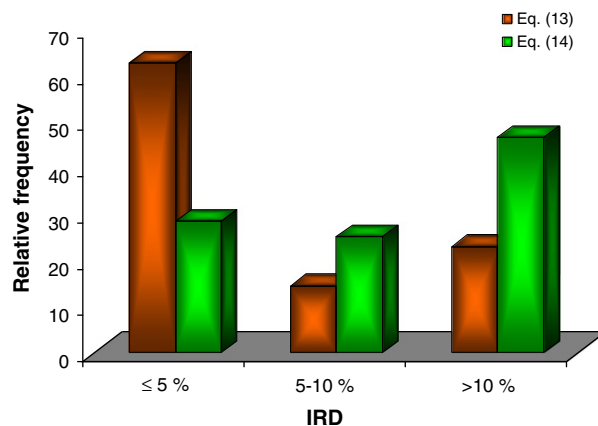
Fig. 2. Relative frequency of the individual relative deviations (IRD) of the predicted surface tension of the binary solvent mixtures at various temperatures.

to calculate the surface tension of ternary solvents at various temperatures. Eq. (14) employs three experimental data of the mono-solvents at each temperature as input data to calculate the surface tension with the MRD of $11.2 \pm 3.5\%$ (N = 79). Combination of Eqs. (12) and (15) provides an ab initio model with the MRD of $11.7 \pm 4.5\%$ as Eq. (15):

$$\log \sigma_{m,T} = \sum_{i=1}^{3} x_i \left(\begin{array}{l} 1.245E_i + 0.344A_i + 0.542V_i \\ + \frac{1}{T}(384.020 - 305.012E_i + 22.350S_i - 101.827A_i + 16.608B_i - 152.522V_i) \end{array} \right)$$
$$\sum_{i=1}^{2} \sum_{j=1+1}^{3} \left(\begin{array}{l} + \frac{x_i x_j}{T} \left[-11.545 - 23.180\left(S_i - S_j\right)^2 - 3.764\left(A_i - A_j\right)^2 + 6.997\left(V_i - V_j\right)^2 \right] \\ + \frac{x_i x_j \left(x_i - x_j\right)}{T} \left[102.261\left(E_i - E_j\right)^2 + 29.458\left(S_i - S_j\right)^2 + 26.850\left(V_i - V_j\right)^2 \right] \\ + \frac{x_i x_j \left(x_i - x_j\right)^2}{T} \left[52.624 - 310.920\left(E_i - E_j\right)^2 - 13.801\left(A_i - A_j\right)^2 - 69.606\left(V_i - V_j\right)^2 \right] \end{array} \right). \tag{16}$$

Applicability of the trained models discussed for ternary solvent mixtures is shown in Table 3. Fig. 3 presents the relative frequencies of the surface tension data predicted using Eqs. (15) and (16), where both models present a similar frequency pattern and IRD values.

4. Conclusion

Jouyban–Acree model is extended through the inclusion of Abraham parameters and yields a new prediction for surface tension calculation. Globally trained versions of the Jouyban–Acree model were presented to calculate the surface tensions of binary and ternary solvent mixtures at various temperatures. Eqs. (13) and (15) employ experimental surface tensions of the mono-solvents at the temperature of interest and produced the overall MRDs of 6.5% and 11.2%, respectively. Eqs. (14) and (16) are ab initio methods used to predict the surface tensions of binary and ternary mixtures using the Abraham solute parameters with the overall MRD of 15.2 and 11.7%. Knowledge of

surface tensions is required in many applications whereas experimental data of most solvent mixtures are not available in the literature. The proposed model is employed to predict the surface tensions of mono-solvents at various temperatures (see Eq. (12)) and its applications could be extended to predict the surface tension of multicomponent solvent systems at various temperatures (Eq. (16)). It is obvious that Eq. (16) could be reduced to Eq. (14) simply by replacing $x_3 = 0$ in the equation. The addition of solvation parameters in this equation yields better prediction for surface tension of multicomponent systems. The proposed model is able to calculate the temperature dependency of surface tension in good agreement with experimental data. It is important however, to recognize the
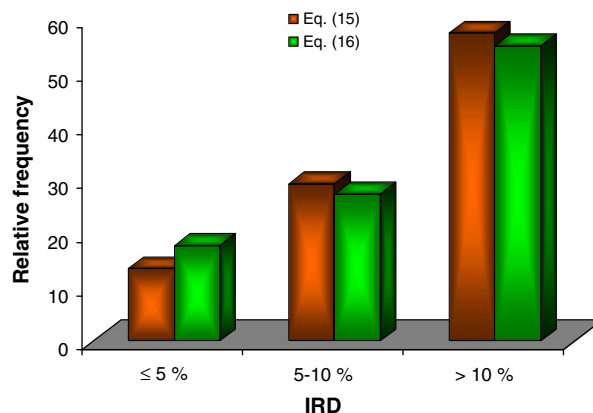

Fig. 3. Relative frequency of the individual relative deviations (IRD) of the predicted surface tension of the ternary solvent mixtures at various temperatures.

limitations associated with the proposed method such as relative complexity of the computation and requirement of mono-solvent data for better prediction of the surface tension of solvent mixtures. The good performance and extreme simplicity of the Jouyban–Acree model have made it a popular method for surface tension calculation of solvent mixtures.

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