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Correlation of Surface Tension of Mono-Solvents at Various Temperatures

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Abstract: Surface tension is among the most important factors in chemical and pharmaceutical processes. Modeling the surface tension of solvents at different temperatures helps to optimize the type of solvent and temperature. The surface tension of solvents at different temperatures with their solvation parameters was used in this study to develop a model based on the van't Hoff equation by multiple linear regression. Abraham solvation parameters, Hansen solubility parameters, and Catalan parameters are among the most discriminating descriptors. The overall MPD of the model was 3.48%, with a minimum and maximum MPD of 0.04% and 11.62%, respectively. The model proposed in this study could be useful for predicting the surface tension of mono-solvents at different temperatures.

Keywords: surface tension; solvation parameters; model; predict

1. Introduction

Surface activity is one of the main physico-chemical properties of liquids. Surface and/or interfacial tension represents the surface and/or interfacial activity of a liquid. Surface tension data is required in many industrial applications, including wettability, dispersibility, and deflocculation of the solid particles in liquids; emulsification of immiscible liquids in emulsion and microemulsion formulations; detergency in sanitary; adsorption of gases and solutes from solutions; solubilization of insoluble drugs in liquid dosage forms; biological activity of drugs and drug absorption from mucosa [1]. Surface tension affects the transformation of heat and mass in solutions which influences many chemical processes [2]. It is a vital step in drug formulation. For example, granulation is a method to improve the falling ability of a powder by adding a binder to the active pharmaceutical ingredient. A crucial step in optimizing granulation performance is wetting the substrate with the binder and spreading the binder over the substrate. Surface tension also acts as an important parameter in controlling the coating process. Suspensions are a dosage form with many pros and cons compared to other dosage forms. One of the disadvantages is related to its instability and cake formation, which could be modified by surface tension control. A comprehensive review of the applications of surface tension in the pharmaceutical sciences was provided in an earlier review paper [3]. Many biological reactions occur at the surface but not in solution. For proper absorption of a drug and efficient function on its active site, it needs to be dissolved properly in the gastric fluids. Surface tension plays a vital role in the function of the respiratory system. A mixture of surface active agents, such as dipalmitoyl lecithin, causes a reduction in the surface tension of alveoli fluid. Increasing the surface tension of alveoli lining fluid results in respiratory distress syndrome and atelectasis, which are two major respiratory disorders. The most important roles of surface tension in clinical sciences have been summarized in a review work [4].

Surface tension reflects the intermolecular interactions and forces between a liquid molecule and the air and depends on many different variables, including viscosity, the existence of ionized compounds in the solution, and temperature [5].

There are various methods for measuring surface tension, including the Du Noüy ring method, Wilhelmy plate method, and spinning drop method, but they all require a lot of cost and energy, and they require an expert to perform the laboratory work. Numerical methods to predict the surface tension of mixed solvents have been proposed, but there are few studies on computational modeling for surface tension prediction of mono-solvents at different temperatures [5].

The aim of this study is to propose a mathematical model for calculating the surface tension of mono-solvents at various temperatures by combining an adopted van't Hoff model with the solvation parameters, including Abraham solvation parameters, Hansen solubility parameters, and Catalan parameters. The applicability of the proposed model is evaluated by using the published surface tension data of several different mono-solvents at various temperatures.

2. Computational Methods

The surface tension of a liquid is decreased by an increase in temperature. An adapted version of the van't Hoff equation is used to represent the temperature effects on the surface tension data ($\sigma_{i,T}$). The van't Hoff type model is:

$$\log \sigma_{i,T} = \alpha_i + \frac{\beta_i}{T} \tag{1}$$

in which α_i and β_i are the model constants [6]. It has been shown that α_i and β_i terms could represent the effects of the physico-chemical properties (PCP) of a given solvent at various temperatures. It is possible to include Abraham solvation parameters (AP_i) [7], Hansen solubility parameters (HP_i) [8], and Catalan parameters (CP_i) [9] to represent the effects of solvent's PCPs on surface tension. To do this, we combined these PCPs with the van't Hoff type model as:

$$\log \sigma_{i,T} = \left(\alpha_0 + \sum_{i=1}^{5} \alpha_{i,AP} AP_i + \sum_{i=1}^{3} \alpha_{i,HP} HP_i + \sum_{i=1}^{4} \alpha_{i,CP} CP_i \right) \\ + \left(\frac{\beta_0 + \sum_{i=1}^{5} \beta_{i,AP} AP_i + \sum_{i=1}^{3} \beta_{i,HP} HP_i + \sum_{i=1}^{4} \beta_{i,CP} CP_i}{T} \right) \tag{2}$$

where α and β terms are the model constants.

Thirty-two solvents with their numerical surface tension ($\sigma_{i,T}$) values at different temperatures were obtained from the literature (Table 1) [10–33]. The tabulated numerical values pertain to a homogeneous liquid system at the specified temperature in equilibrium with its own vapor pressure. The solvents considered in the study contain a wide range of functional groups, and they cannot be classified as belonging to a single type of chemical compound. For each solvent, Abraham solvation parameters [7,34,35], Catalan parameters [9], and Hansen solubility parameters [8] were gathered from different sources. Details of the parameters with their references are listed in Tables 2–4. Parameters for each solvent were divided by temperature to differentiate between the descriptor's numerical values at different temperatures. Repeated data were excluded from the final analyses, and for the data with close reported surface tension data, the average numerical value of surface tension was used for further analysis.

Table 1. Experimental ($\sigma_{i,T}^{Exp}$) and calculated ($\sigma_{i,T}^{Calc}$) surface tension values of the studied mono-solvents at different temperatures (T), the mean percentage deviation (MPD), and the references for $\sigma_{i,T}^{Exp}$ data.

Solvent	T (K)	$\sigma_{i,T}^{Exp}$	$\sigma_{i,T}^{Calc}$	MPD	Ref.
1,4-dioxane	288	33.98	32.40	4.74	[10]
1,4-dioxane	293	33.58	31.70	5.51	[10]
1,4-dioxane	298	32.69	31.10	4.80	[10]
1,4-dioxane	**303**	32.15	30.50	5.01	[10]
1,4-dioxane	308	31.42	30.00	4.52	[10]
1-butanol	**288**	24.68	24.80	0.28	[11]
1-butanol	293	24.21	24.20	0.04	[11]
1-butanol	298	24.10	23.70	1.70	[11,12]
1-butanol	303	23.34	23.20	0.60	[11]
1-butanol	308	22.79	22.70	0.26	[11]
1-hexanol	288	26.08	26.40	1.23	[11]
1-hexanol	**293**	25.61	25.90	1.09	[11]
1-hexanol	298	25.43	25.40	0.08	[11,12]
1-hexanol	303	24.74	25.00	0.89	[11]
1-hexanol	308	24.19	24.50	1.41	[11]
1-octanol	288	27.41	26.80	2.12	[11]
1-octanol	293	26.94	26.30	2.26	[11]
1-octanol	**298**	26.90	25.90	3.90	[11,12]
1-octanol	303	26.07	25.40	2.57	[11]
1-octanol	308	25.52	25.00	2.16	[11]
1-pentanol	**293**	25.69	25.50	1.09	[13,14]
1-pentanol	298	25.00	25.00	0.12	[12,14]
1-pentanol	318	23.67	23.30	1.44	[13,14]
1-propanol	293	23.69	24.20	2.11	[13,14]
1-propanol	298	23.34	23.70	1.37	[12,14]
1-propanol	**303**	22.89	23.20	1.22	[14]
1-propanol	308	22.51	22.70	0.84	[14]
1-propanol	313	22.11	22.30	0.68	[14]
1-propanol	318	21.69	21.80	0.69	[13,14]
1-propanol	323	21.31	21.40	0.56	[14]
2-butanol	**298**	23.01	23.70	2.78	[13]
2-butanone	293	24.70	22.80	7.61	[15]
2-butanone	**298**	24.00	22.20	7.38	[15]
2-methyl–1-propanol	**298**	22.34	23.40	4.52	[16]
2-pentanol	293	23.70	24.20	2.24	[13]
2-pentanol	**298**	23.28	23.70	1.89	[13]
2-pentanol	315	21.60	22.20	2.69	[13]
2-propanol	293	21.74	22.10	1.66	[14]
2-propanol	298	21.03	21.60	2.57	[14]
2-propanol	303	20.72	21.10	1.64	[14]
2-propanol	**308**	20.23	20.60	1.73	[14]
2-propanol	313	19.71	20.10	2.13	[14]
2-propanol	318	19.21	19.70	2.55	[14]
2-propanol	323	18.69	19.30	3.26	[14]
acetone	273	25.17	25.50	1.47	[17]
acetone	287	24.70	23.40	5.22	[17]
acetone	**288**	23.37	23.30	0.39	[17]
acetone	293	23.03	22.60	1.78	[18]
acetone	298	22.50	22.00	2.22	[18]
acetone	303	21.80	21.40	1.79	[17]
acetone	308	21.20	20.90	1.60	[17]
acetone	313	20.80	20.30	2.21	[18]
acetone	318	19.78	19.90	0.35	[17]

Table 1. *Cont.*

Solvent	T (K)	$\sigma_{i,T}^{Exp}$	$\sigma_{i,T}^{Calc}$	MPD	Ref.
acetone	323	19.51	19.40	0.62	[18]
acetone	328	18.60	19.00	1.88	[17]
acetonitrile	298	28.41	28.40	0.21	[19]
acetonitrile	**303**	28.03	27.50	2.07	[19]
acetonitrile	308	27.40	26.60	2.88	[19]
acetonitrile	313	26.76	25.80	3.55	[19]
acetonitrile	318	26.13	25.10	4.06	[19]
benzene	**293**	28.85	32.20	11.61	[20]
benzene	303	27.55	30.80	11.62	[20]
butyl acetate	**298**	24.88	22.80	8.32	[21]
cyclohexane	288	25.34	24.30	4.18	[22]
cyclohexane	**293**	25.00	23.40	6.28	[23]
cyclohexane	298	24.20	22.60	6.49	[23]
cyclohexane	303	23.85	21.90	8.22	[23]
cyclohexane	308	23.02	21.20	7.91	[22,23]
cyclohexane	318	21.84	19.90	8.70	[22,23]
cyclohexane	328	20.71	18.80	9.13	[22,23]
dimethylsulfoxide	288	43.68	45.40	3.94	[24]
dimethylsulfoxide	298	42.18	43.90	4.10	[24]
dimethylsulfoxide	**308**	41.11	42.60	3.55	[24]
dimethylsulfoxide	318	39.99	41.40	3.40	[24]
dimethylsulfoxide	328	38.72	40.20	3.93	[24]
ethanol	288	22.68	24.70	8.86	[14,25]
ethanol	293	22.28	24.10	8.17	[25]
ethanol	298	21.78	23.60	8.13	[12,25]
ethanol	303	21.40	23.00	7.62	[25]
ethanol	308	21.04	22.50	7.13	[25]
ethanol	313	20.66	22.10	6.82	[25]
ethanol	318	20.36	21.60	6.24	[25]
ethanol	**323**	19.91	21.20	6.53	[25]
ethyl acetate	**298**	23.93	21.90	8.32	[20]
ethylene glycol	283	49.76	46.70	6.25	[26,27]
ethylene glycol	293	49.02	45.60	7.04	[26,27]
ethylene glycol	298	48.24	45.10	6.59	[26,27]
ethylene glycol	303	47.67	44.60	6.48	[26,27]
ethylene glycol	**308**	47.50	44.10	7.14	[26,27]
ethylene glycol	313	47.58	43.70	8.22	[26,27]
ethylene glycol	318	46.40	43.30	6.79	[26,27]
ethylene glycol	323	46.68	42.80	8.23	[26,27]
heptane	**288**	20.73	22.20	6.90	[11,22]
heptane	293	20.40	21.30	4.56	[11,28]
heptane	298	19.64	20.60	4.74	[11,22]
heptane	303	19.34	19.90	2.69	[11,22]
heptane	308	18.80	19.20	2.07	[11,22]
heptane	313	18.46	18.60	0.60	[28]
heptane	318	17.76	18.00	1.24	[22]
heptane	323	17.42	17.40	0.06	[28]
heptane	328	16.68	16.90	1.44	[22]
heptane	333	16.46	16.40	0.18	[28]
heptane	343	15.32	15.50	1.44	[28]
methanol	293	22.80	22.80	0.18	[14]
methanol	298	22.27	22.30	0.09	[14]
methanol	303	21.79	21.70	0.46	[14]
methanol	308	21.52	21.20	1.67	[14]
methanol	313	21.13	20.70	2.22	[14]
methanol	318	20.61	20.20	2.04	[14]

Table 1. *Cont.*

Solvent	T (K)	$\sigma_{i,T}^{Exp}$	$\sigma_{i,T}^{Calc}$	MPD	Ref.
methanol	**323**	19.86	19.80	0.55	[14]
methyl acetate	**298**	24.79	22.90	7.62	[29]
N,N-dimethylformamide	288	36.96	36.40	1.41	[22]
N,N-dimethylformamide	298	35.83	35.30	1.40	[22]
N,N-dimethylformamide	**308**	34.65	34.30	0.95	[22]
N,N-dimethylformamide	318	33.37	33.40	0.12	[22]
N,N-dimethylformamide	328	32.03	32.60	1.69	[22]
N-methyl–2-pyrrolidone	239	41.13	44.30	7.80	[22]
N-methyl–2-pyrrolidone	278	42.60	40.80	4.18	[22]
N-methyl–2-pyrrolidone	288	41.35	40.10	3.00	[22]
N-methyl–2-pyrrolidone	298	40.25	39.50	1.99	[22]
N-methyl–2-pyrrolidone	303	40.38	39.10	3.12	[30]
N-methyl–2-pyrrolidone	**308**	39.10	38.80	0.66	[22]
N-methyl–2-pyrrolidone	313	39.99	38.50	3.63	[30]
N-methyl–2-pyrrolidone	318	37.91	38.30	0.98	[22]
N-methyl–2-pyrrolidone	328	36.80	37.80	2.61	[22]
N-methyl–2-pyrrolidone	333	35.90	37.50	4.46	[30]
N-methyl–2-pyrrolidone	338	35.66	37.30	4.54	[22]
propylene glycol	298	35.80	36.30	1.51	[31]
propylene glycol	303	35.70	35.80	0.34	[31]
propylene glycol	**313**	35.00	34.90	0.40	[31]
propylene glycol	323	34.10	34.00	0.35	[31]
toluene	288	28.93	31.90	10.40	[22]
toluene	298	27.76	30.50	9.69	[22]
toluene	**308**	26.60	29.10	9.47	[22]
toluene	318	25.46	27.90	9.66	[22]
toluene	328	24.29	26.80	10.50	[22]
water	283	74.27	77.60	4.42	[32]
water	293	72.72	74.80	2.83	[32]
water	298	71.92	73.50	2.18	[16,32,33]
water	303	71.18	72.30	1.53	[32,33]
water	**308**	70.35	71.10	1.08	[32,33]
water	311	69.91	70.40	0.76	[32]
water	313	69.49	70.00	0.73	[32]
water	318	68.67	69.00	0.41	[32,33]
water	323	67.78	67.90	0.24	[32,33]
water	328	66.60	67.00	0.57	[32,33]

Table 2. Applied solvation parameters of studied solvents for modeling.

Descriptor	Definition
Abraham solvent parameters [7,34,35]	
c	The intercept value in Abraham's solvation model
e	Excess molar refraction
s	Polarity/polarizability
a	Hydrogen-bond acidity
b	Hydrogen-bond basicity
v	McGowan volume characteristic
Hansen solubility parameters [8]	
δ_D	The energy from dispersion forces between molecules
δ_P	The energy from dipolar intermolecular force between molecules
δ_H	The energy from hydrogen bonds between molecules
Catalan parameters [9]	
SdP	Solvent dipolarity
SP	Solvent polarizability
SA	Solvent acidity
SB	Solvent basicity

Table 3. Numerical values of the Abraham solvent parameters.

Solvent	*c*	*e*	*s*	*a*	*b*	*v*
1-butanol	0.17	0.40	−1.01	0.06	−3.96	4.04
1-hexanol	0.12	0.49	−1.16	0.05	−3.98	4.13
1-octanol	−0.03	0.49	−1.04	−0.02	−4.24	4.22
1-pentanol	0.15	0.54	−1.23	0.14	−3.86	4.08
1-propanol	0.14	0.41	−1.03	0.25	−3.77	3.99
1,4-dioxane	0.10	0.35	−0.08	−0.56	−4.83	4.17
2-butanol	0.19	0.35	−1.13	0.02	−3.57	3.97
2-butanone	0.25	0.26	−0.08	−0.77	−4.86	4.15
2-methyl−1-propanol	0.13	0.25	−0.98	0.16	−3.88	4.11
2-pentanol	0.12	0.46	−1.33	0.21	−3.75	4.20
2-propanol	0.10	0.34	−1.05	0.41	−3.83	4.03
acetone	0.31	0.31	−0.12	−0.61	−4.75	3.94
acetonitrile	0.41	0.08	0.33	−1.57	4.39	3.36
benzene	0.14	0.46	−0.59	−3.10	−4.63	4.49
butyl acetate	0.25	0.36	−0.50	−0.87	−4.97	4.28
cyclohexane	0.16	0.78	−1.68	−3.74	−4.93	4.58
dimethylsulfoxide	−0.19	0.33	0.79	−1.26	−4.54	3.36
ethanol	0.22	0.47	−1.04	0.33	−3.60	3.86
ethyl acetate	0.33	0.37	−0.45	−0.70	−4.90	4.15
ethylene glycol	−0.27	0.58	−0.51	0.72	−2.62	2.73
heptane	0.33	0.67	−2.06	−3.32	−4.73	4.54
methanol	0.28	0.33	−0.71	0.24	−3.32	3.55
methyl acetate	0.35	0.22	−0.15	−1.04	−4.53	3.97
N-methyl−2-pyrrolidone	0.15	0.53	0.23	0.84	−4.79	3.67
N,N-dimethylformamide	−0.31	−0.06	0.34	0.36	−4.87	4.49
propylene glycol	−0.15	0.75	−0.97	0.68	−3.13	3.25
toluene	0.14	0.53	−0.72	−3.01	−4.82	4.55
water	−0.99	0.58	2.55	3.81	4.84	−0.87

Multiple linear regression was used in this study to develop a model to calculate the surface tension of different solvents at various temperatures based on the parameters mentioned in Table 1. Surface tension was set as the dependent variable, and solubility parameters as independent variables. Descriptors with *p*-value >0.1 were excluded from the model. The *p*-value shows the statistical significance of the coefficients of each independent variable assessed employing the *t*-test.

The results of the correlations with the proposed model were compared with those of the previously reported model by Freitas et al. [36], which calculates the surface tension of liquids at 20 °C ($\sigma_{i,20\,°C}$):

$$\sigma_{i,20\,°C} = 14.9 + 4.35 A_i^{Exp} - 1.3 B_i^{Exp} + 11.3 S_i^{Exp} + 10.9 E_i + 3.0 V_i + 0.8 N_C \tag{3}$$

and a model based on Abraham solute parameters [37] to compute the surface tensions at various temperatures ($\sigma_{i,T}$):

$$\begin{aligned} \log \sigma_{i,T} = {}& 1.245 E_i + 0.344 A_i + 0.542 V_i \\ & + \frac{1}{T}(384.020 - 305.012 E_i + 22.350 S_i - 101.827 A_i + 16.608 B_i - 152.522 V_i) \end{aligned} \tag{4}$$

where A_i^{Exp}, B_i^{Exp}, S_i^{Exp}, E_i and V_i are the Abraham solute parameters of the liquids. 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 [37], E_i was calculated from refractive index data [38] and V_i was computed using a group contribution method of McGowan and Abraham [39]. N_C is the number of carbons in n-alkanes minus six, i.e., $N_C = 0$ for n-alkanes up to hexane and 1 for heptane [36]. As an informational note, the Abraham solute descriptors used in Equations (3) and (4) are

denoted by capitalized alphabetical characters. These solute descriptors could either be determined from experimental solubility data (denoted by *Exp* as superscript in this work) or could be computed using available software [40]. Abraham solvent parameters, which will be used in later equations, will be denoted by lowercase alphabetical characters.

The accuracy of the models was investigated by computing *MPD* (mean percentage deviation) as follows:

$$MPD = \frac{100}{N} \sum \left(\frac{\left| \sigma_{i,T}^{Calc} - \sigma_{i,T}^{Exp} \right|}{\sigma_{i,T}^{Exp}} \right) \tag{5}$$

where *N* is the number of data points used in the regression analyses.

Table 4. Numerical values of the Hansen and Catalan parameters for the solvents investigated in this work.

solvent	Hansen Parameters			Catalan Parameters			
	δ_D	δ_P	δ_H	SP	SdP	SA	SB
1-butanol	16.00	5.70	15.80	0.67	0.66	0.34	0.81
1-hexanol	15.90	5.80	12.50	0.70	0.55	0.32	0.88
1-octanol	17.00	3.30	11.90	0.71	0.45	0.30	0.92
1-pentanol	13.83	8.82	13.80	0.69	0.59	0.32	0.86
1-propanol	16.00	6.80	17.40	0.66	0.75	0.37	0.78
1,4-dioxane	19.00	1.80	7.40	0.74	0.31	0.00	0.44
2-butanol	13.38	9.53	14.08	0.66	0.71	0.22	0.89
2-butanone	16.00	9.00	5.10	0.67	0.87	0.00	0.52
2-methyl–1-propanol	13.38	9.53	14.08	0.66	0.68	0.31	0.83
2-pentanol	13.65	8.87	12.95	0.67	0.67	0.20	0.92
2-propanol	12.97	10.35	15.68	0.63	0.81	0.28	0.83
acetone	15.50	10.40	7.00	0.65	0.91	0.00	0.48
acetonitrile	11.59	12.95	16.34	0.65	0.97	0.04	0.29
benzene	18.40	0.00	2.00	0.79	0.27	0.00	0.12
butyl acetate	14.49	7.74	6.53	0.67	0.54	0.00	0.53
cyclohexane	16.80	0.00	0.20	0.68	0.00	0.00	0.07
dimethylsulfoxide	18.40	16.40	10.20	0.83	1.00	0.07	0.65
ethanol	15.80	8.80	19.40	0.64	0.78	0.40	0.66
ethyl acetate	15.80	5.30	7.20	0.66	0.60	0.00	0.54
ethylene glycol	17.00	11.00	26.00	0.78	0.91	0.72	0.53
heptane	15.30	0.00	0.00	0.64	0.00	0.00	0.08
methanol	15.10	12.30	22.30	0.61	0.90	0.61	0.55
methyl acetate	12.68	11.42	11.79	0.65	0.64	0.00	0.53
N-methyl–2-pyrrolidone	18.00	12.30	7.20	0.81	0.96	0.02	0.61
N,N-dimethylformamide	17.40	13.70	11.30	0.76	0.98	0.03	0.61
propylene glycol	12.75	14.23	27.95	0.73	0.89	0.48	0.60
toluene	18.00	1.40	2.00	0.78	0.28	0.00	0.13
water	15.50	16.00	42.30	0.68	1.00	1.06	0.03

3. Results and Discussion

The collected surface tension data of the mono-solvents at various temperatures were correlated with three sets of solvation parameters, and the obtained model after excluding non-significant parameters ($p > 0.05$) is:

$$\log \sigma_T = \left(\begin{array}{c} -1.713 - 0.037s + 0.118a + 0.008b + 0.008\delta_D \\ +0.006\delta_P + 0.003\delta_H + 3.636SP - 0.087SdP - 0.089SB \end{array} \right) \\ + \left(\frac{729.913 - 16.509c - 23.369e - 29.450a - 19.611v - 687.155SP - 35.211SA}{T} \right) \tag{6}$$

The correlation coefficient of this equation is 0.992, the F value is 503, and the correlation is statistically significant with a *p*-value of <0.0005. The F value is the Fischer test value revealing the statistical significance of the overall correlation. The minimum and maximum

MPD values for the back-calculated surface tensions belong to 1-butanol at temperature 293 (*MPD* = 0.04%) and benzene at temperature 303 (*MPD* = 11.62%). The overall MPD of the correlated data points was 3.48% (*N* = 146). Equation (6) is valid for interpolation purposes in all temperatures and for extrapolation purposes in a narrow range of temperatures.

Previous studies have shown the importance of Abraham solvation parameters in calculating the surface tension of the mono-solvents [12]. A comparison between surface tension prediction for mono-solvents with our proposed model and Freitas study at 20 °C ($\sigma_{i,20\,°C}$) is shown in Figure 1. Moreover, the MPD for a previous model by our group was 11%. It can be clearly understood that considering the Catalan and Hansen parameters, the prediction ability of the model has been improved in comparison to previous models. An important distinction between the current method and the earlier method of Freitas et al. is that Equation (3) used the solute descriptors of the organic solvents as input parameters. The current treatment uses the Abraham model equation coefficients for each solvent as the input parameters for Equation (2). Solvent coefficients, rather than solute descriptors, are likely the more appropriate parameter to use when dealing with properties such as surface tension. While both types of parameters can be used in describing molecular interactions, their numerical values are determined under a different set of experimental conditions. In the case of solute descriptors, the measurements are normally performed at low concentrations where the dissolved solute is completely surrounded by solvent molecules. Such measurements would not capture the effects of self-association. Solvent parameters, on the other hand, would include effects arising from self-association, as well as any special structural features resulting from "solvent stacking". We recognize that the limited availability of solvent coefficients does make it appealing to use the more readily available solute parameters when developing predictive expressions. Experimental-based solute descriptors are known for more than 8000 different organic and organometallic compounds [40]. Abraham model solvent coefficients, on the other hand, have been determined for only 130 different organic molecules and a few binary aqueous-alcoholic mixtures [41].

In order to validate the model, each solvent was sorted based on the temperature and was divided into training and test sets one by one in order to have different solvents containing various physiochemical properties with different temperatures in both test and training sets. The temperature values of the used training data points are listed in the second column of Table 1 using bold font. The proposed model was trained using the training data points, and the rest of the data points were predicted by the trained model. The obtained overall MPD value was 4.01% (*N* = 118). The results confirm the validity of the model.
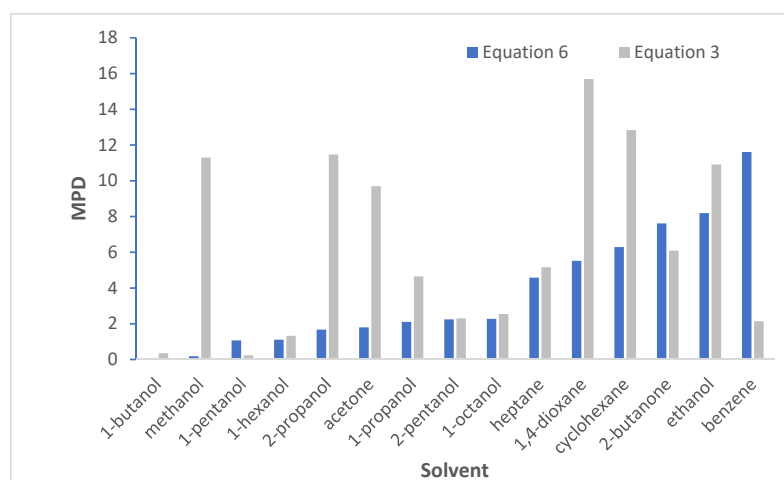
Figure 1. Comparison of MPD values for the calculated surface tension of studied solvents at 293 K by combination of van't Hoff type model and the solvation parameters (Equation (6)) and the reported model by Freitas et al. (Equation (3)).

4. Conclusions

A van't Hoff type-mathematical expression was developed for predicting the surface tension of both water and 27 different organic mono-solvents as a function of temperature using only Abraham solvation parameters, Hansen solubility parameters, and Catalan parameters as input values. The derived mathematical expression described the experimental surface tension data within an overall MPD of the model was 3.48%. The minimum and maximum MPD between predicted and observed values were 0.04% and 11.62%, respectively. The predictive model reported in the current study could help researchers to estimate the surface tension of mono-solvents at different temperatures and identify possible outlier values in need of re-measurement. The availability of needed solvation parameters currently limits the applicability of the proposed model; however, progress is being made to estimate Abraham model solvent coefficients using functional group additivity and machine learning methods [42–44].

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Data Availability Statement: Data used in this study are available from the published literature [16–39].

References

1. Lee, Y.C.; Simamora, P.; Pinsuwan, S.; Yalkowsky, S.H. Review on the systemic delivery of insulin via the ocular route. *Int. J. Pharm.* **2002**, *233*, 1–18. [CrossRef]
2. Khattab, I.S.; Bandarkar, F.; Fakhree, M.A.A.; Jouyban, A. Density, viscosity, and surface tension of water+ ethanol mixtures from 293 to 323K. *Korean J. Chem. Eng.* **2012**, *29*, 812–817. [CrossRef]
3. Fathi Azarbayjani, A.; Jouyban, A.; Chan, S.Y. Impact of surface tension in pharmaceutical sciences. *J. Pharm. Pharm. Sci.* **2009**, *12*, 218–228. [CrossRef] [PubMed]
4. Fathi-Azarbayjani, A.; Jouyban, A. Surface tension in human pathophysiology and its application as a medical diagnostic tool. *Bioimpacts* **2015**, *5*, 29–44. [CrossRef]
5. Jouyban, A.; Fathi Azarbayjani, A. Experimental and computational methods pertaining to surface tension of pharmaceutical. In *Toxicity and Drug Testing*; Acree, W.E., Jr., Ed.; IntechOpen: London, UK, 2012; pp. 47–70.
6. Khoubnasabjafari, M.; Jouyban, V.; Azarbayjani, A.F.; Jouyban, A. Application of Abraham solvation parameters for surface tension prediction of mono-solvents and solvent mixtures at various temperatures. *J. Mol. Liq.* **2013**, *178*, 44–56. [CrossRef]
7. Lee, G.; Che, M.; Qian, E.; Wang, L.; Gupta, A.; Neal, R.; Yue, D.; Downs, S.; Mayes, T.; Rose, O. Determination of Abraham model solute descriptors for o-acetoacetanisidide based on experimental solubility data in organic mono-solvents. *Phys. Chem. Liq.* **2019**, *57*, 528–535. [CrossRef]
8. Hansen, C.M. *Hansen Solubility Parameters: A User's Handbook*; CRC Press: New York, NY, USA, 1998.
9. Catalán, J. Toward a generalized treatment of the solvent effect based on four empirical scales: Dipolarity (SdP, a new scale), polarizability (SP), acidity (SA), and basicity (SB) of the medium. *J. Phys. Chem. B* **2009**, *113*, 5951–5960. [CrossRef]
10. Calvo, E.; Pintos, M.; Amigo, A.; Bravo, R. Thermodynamic analysis of surface formation of {1,4-dioxane + 1-alkanol} mixtures. *J. Colloid Interface Sci.* **2002**, *253*, 203–210. [CrossRef]
11. Vijande, J.; Pineiro, M.M.; García, J.; Valencia, J.L.; Legido, J.L. Density and surface tension variation with temperature for heptane + 1-alkanol. *J. Chem. Eng. Data* **2006**, *51*, 1778–1782. [CrossRef]
12. Segade, L.; Jiménez de Llano, J.; Domínguez-Pérez, M.; Cabeza, Ó.; Cabanas, M.; Jiménez, E. Density, surface tension, and refractive index of octane + 1-alkanol mixtures at T = 298.15 K. *J. Chem. Eng. Data* **2003**, *48*, 1251–1255. [CrossRef]
13. Azizian, S.; Bashavard, N. Surface tension of dilute solutions of linear alcohols in benzyl alcohol. *J. Chem. Eng. Data* **2005**, *50*, 1303–1307. [CrossRef]
14. Vazquez, G.; Alvarez, E.; Navaza, J.M. Surface tension of alcohol water + water from 20 to 50. degree. C. *J. Chem. Eng. Data* **1995**, *40*, 611–614. [CrossRef]
15. Yaws, C.L. *Thermophysical Properties of Chemicals and Hydrocarbons*; William Andrew: Norwich, NY, USA, 2008.
16. Bermúdez-Salguero, C.; Gracia-Fadrique, J.; Calvo, E.; Amigo, A. Densities, refractive indices, speeds of sound, and surface tensions for dilute aqueous solutions of 2-methyl-1-propanol, cyclopentanone, cyclohexanone, cyclohexanol, and ethyl acetoacetate at 298.15 K. *J. Chem. Eng. Data* **2011**, *56*, 3823–3829. [CrossRef]

17. Enders, S.; Kahl, H.; Winkelmann, J. Surface tension of the ternary system water + acetone + toluene. *J. Chem. Eng. Data* **2007**, *52*, 1072–1079. [CrossRef]

18. Howard, K.S.; McAllister, R. Surface tension of acetone–water solutions up to their normal boiling points. *AIChE J.* **1957**, *3*, 325–329. [CrossRef]

19. Jasper, J.J. The surface tension of pure liquid compounds. *J. Phys. Chem. Ref. Data* **1972**, *1*, 841–1010. [CrossRef]

20. Wanchoo, R.; Narayan, J.; Raina, G.; Rattan, V. Excess properties of (2-propanol + ethyl acetate or benzene) binary liquid mixture. *Chem. Eng. Commun.* **1989**, *81*, 145–156. [CrossRef]

21. Washburn, E.R.; Shildneck, C.H. Surface tension studies with n-butyl acetate. *J. Am. Chem. Soc.* **1933**, *55*, 2354–2357. [CrossRef]

22. Kahl, H.; Wadewitz, T.; Winkelmann, J. Surface tension and interfacial tension of binary organic liquid mixtures. *J. Chem. Eng. Data* **2003**, *48*, 1500–1507. [CrossRef]

23. Gómez-Díaz, D.; Mejuto, J.C.; Navaza, J.M. Physicochemical properties of liquid mixtures. 1. Viscosity, density, surface tension and refractive index of cyclohexane + 2, 2, 4-trimethylpentane binary liquid systems from 25 C to 50 C. *J. Chem. Eng. Data* **2001**, *46*, 720–724. [CrossRef]

24. Bagheri, A.; Abolhasani, A.; Moghadasi, A.; Nazari-Moghaddam, A.; Alavi, S. Study of surface tension and surface properties of binary systems of DMSO with long chain alcohols at various temperatures. *J. Chem. Thermodyn.* **2013**, *63*, 108–115.

25. Álvarez, E.; Correa, A.; Correa, J.M.; García-Rosello, E.; Navaza, J.M. Surface tensions of three amyl alcohol + ethanol binary mixtures from (293.15 to 323.15) K. *J. Chem. Eng. Data* **2011**, *56*, 4235–4238. [CrossRef]

26. Azizian, S.; Hemmati, M. Surface tension of binary mixtures of ethanol+ ethylene glycol from 20 to 50 C. *J. Chem. Eng. Data* **2003**, *48*, 662–663. [CrossRef]

27. Tsierkezos, N.G.; Molinou, I.E. Thermodynamic properties of water+ ethylene glycol at 283.15, 293.15, 303.15, and 313.15 K. *J. Chem. Eng. Data* **1998**, *43*, 989–993. [CrossRef]

28. Rolo, L.I.; Caco, A.I.; Queimada, A.J.; Marrucho, I.M.; Coutinho, J.A. Surface tension of heptane, decane, hexadecane, eicosane, and some of their binary mixtures. *J. Chem. Eng. Data* **2002**, *47*, 1442–1445. [CrossRef]

29. Bermúdez-Salguero, C.; Gracia-Fadrique, J.S.; Amigo, A. Surface tension data of aqueous binary mixtures of methyl, ethyl, propyl, and butyl acetates at 298.15 K. *J. Chem. Eng. Data* **2010**, *55*, 2905–2908. [CrossRef]

30. García-Abuín, A.; Gómez-Díaz, D.; Navaza, J.M.; Vidal-Tato, I. Surface tension of aqueous solutions of short n-alkyl-2-pyrrolidinones. *J. Chem. Eng. Data* **2008**, *53*, 2671–2674. [CrossRef]

31. Hoke, B.C., Jr.; Patton, E.F. Surface tensions of propylene glycol + water. *J. Chem. Eng. Data* **1992**, *37*, 331–333. [CrossRef]

32. Vargaftik, N.; Volkov, B.; Voljak, L. International tables of the surface tension of water. *J. Phys. Chem. Ref. Data* **1983**, *12*, 817–820. [CrossRef]

33. Markarian, S.A.; Terzyan, A.M. Surface tension and refractive index of dialkylsulfoxide + water mixtures at several temperatures. *J. Chem. Eng. Data* **2007**, *52*, 1704–1709. [CrossRef]

34. Abraham, M.H.; Smith, R.E.; Luchtefeld, R.; Boorem, A.J.; Luo, R.; Acree, W.E., Jr. Prediction of solubility of drugs and other compounds in organic solvents. *J. Pharm. Sci.* **2010**, *99*, 1500–1515. [CrossRef] [PubMed]

35. Jouyban, A.; Acree, W.E., Jr.; Michael, H. Abraham and his developed parameters: Various applications in medicine, chemistry and biology. *Pharm. Sci.* **2022**, *28*, 170–173. [CrossRef]

36. Freitas, A.A.; Quina, F.H.; Carroll, F.A. A linear free energy analysis of the surface tension of organic liquids. *Langmuir* **2000**, *16*, 6689–6692. [CrossRef]

37. Acree, J.; William, E.; Abraham, M.H. Solubility predictions for crystalline nonelectrolyte solutes dissolved in organic solvents based upon the Abraham general solvation model. *Can. J. Chem.* **2001**, *79*, 1466–1476. [CrossRef]

38. Abraham, M.H.; Ibrahim, A.; Zissimos, A.M. Determination of sets of solute descriptors from chromatographic measurements. *J. Chromatogr. A* **2004**, *1037*, 29–47. [CrossRef]

39. Abraham, M.H.; McGowan, J. The use of characteristic volumes to measure cavity terms in reversed phase liquid chromatography. *Chromatographia* **1987**, *23*, 243–246. [CrossRef]

40. Ulrich, N.; Endo, S.; Brown, T.N.; Watanabe, N.; Bronner, G.; Abraham, M.H.; Goss, K.-U. UFZ-LSER Database v 3.2.1. Available online: http://www.ufz.de/lserd (accessed on 10 October 2022).

41. Sinha, S.; Yang, C.; Wu, E.; Acree, W.E., Jr. Abraham solvation parameter model: Examination of possible intramolecular hydrogen-bonding using calculated solute descriptors. *Liquids* **2022**, *2*, 131–146. [CrossRef]

42. Brown, T.N. Empirical regressions between system parameters and solute descriptors of polyparameter linear free energy relationships (PPLFERs) for predicting solvent-air partitioning. *Fluid Phase Equilib.* **2021**, *540*, 113035. [CrossRef]

43. Grubbs, L.M.; Saifullah, M.; Nohelli, E.; Ye, S.; Achi, S.S.; Acree, W.E., Jr.; Abraham, M.H. Mathematical correlations for describing solute transfer into functionalized alkane solvents containing hydroxyl, ether, ester or ketone solvents. *Fluid Phase Equilib.* **2010**, *298*, 48–53. [CrossRef]

44. Bradley, J.-C.; Abraham, M.H.; Acree, W.E.; Lang, A.S. Predicting Abraham model solvent coefficients. *Chem. Cent. J.* **2015**, *9*, 12. [CrossRef]