Prediction of Dielectric Constants of Binary Solvents at Various Temperatures

Abolghasem Jouyban*,† and Shahla Soltanpour‡

Department of Pharmaceutical and Food Control, Faculty of Pharmacy and Drug Applied Research Center, Tabriz University of Medical Sciences, Tabriz 51664, Iran

A combined form of the Jouyban−Acree model and the Abraham solvation parameters was used for predicting the dielectric constant of binary solvent mixtures at various temperatures. The proposed model was trained with the numbers of the experimental data including aqueous and nonaqueous binary miscible mixtures, and then this trained form of the model was used to predict the dielectric constant of the left-out data. The mean relative deviations (MRDs) between predicted and experimental dielectric constants are used as an accuracy criterion. The overall MRD for all aqueous and nonaqueous mixtures is 22 %, and the corresponding value for aqueous binary mixtures is 9 %. Including the experimental dielectric constants of monosolvents, the prediction capability of the proposed models is improved, and the overall MRDs for all solvent mixtures and aqueous mixtures are 7 % and 3 %, respectively. A reduced form of the proposed model could be used to compute the dielectric constants of monosolvents at various temperatures with the MRD of 26 %.

Introduction

Dielectric constant or relative permittivity (ε) is an important physical property of chemicals which depends on the electronic distribution of the molecule and is influenced by interatomic and intermolecular attractions. The primary importance of the dielectric constant lies in the fact that it is a measure of the ability of a substance to maintain a charge separation. The numerical values of dielectric constants for most of the solvents can be found in the literature, and a number of models have been presented to calculate the dielectric constant.[1] It is also an important physicochemical property in the solvation of ions.[2] The correlation between dielectric constant and other physicochemical properties could be found in the literature including the correlations with the solubility parameter,[3,4] surface tension,[5,6] and index of refraction.[7]

A multiple linear regression model consisting of six descriptors was proposed to correlate the dielectric constants of diverse set of chemicals with the average error of 23 % (for training set, $N = 155$) and 39 % (for test set, $N = 46$).[8] These authors also proposed a neural network model to compute the dielectric constants in which the average errors for train and test sets were 27 % and 35 %, respectively. The Slid−Karelson model has been claimed as the most accurate and generally applicable correlation from the literature[9] and has been improved by developing a four-descriptor model with the mean relative deviation (MRD) of 18 % for the polar compounds with the ε range of 1 to 50. A comparison between the Liu et al. model and the Slid−Karelson model using slightly different test sets showed that the models produced the overall MRDs of 18 % and 39 %, respectively. It should be added that the number of data points as training sets were 519 and 155, and the number of descriptors were 5 and 6, respectively. To provide a better comparison, the common chemicals from two test sets were considered, and the overall MRDs were 20 % and 50 %, respectively. Richardi et al. calculated the dielectric constants of formamide, *N*-methylformamide, and dimethylformamide using Ornstein−Zernike theory.[10] In another report from the same group, a number of functions including the dielectric contant of acetonitrile have been modeled employing a Monte Carlo simulation and Orenstein−Zernike theories.[11]

Mixed solvents have been employed in many chemical and pharmaceutical applications, and using these systems has its own position in the field of analytical and/or pharmaceutical analysis, for example, in separation, quantification, and purification processes.[12,13] The experimental values of dielectric constants of some solvent mixtures (ε_m) are available in the literature; however, a number of computational methods have been presented[14,15] to calculate the ε_m values. For a binary solvent mixture, the ε_m is calculated by

$$\varepsilon_m = x_1\varepsilon_1 + x_2\varepsilon_2 \quad (1)$$

where x is the mole fraction of each solvent in the binary mixture and subscripts 1 and 2 denote the solvents 1 and 2. For data sets reported in other solvent compositions (such as volume or mass fraction), the data have been converted to mole fraction. For a mixture composed of more than two solvents, the dielectric constants are calculated using

$$\varepsilon_m = \sum_{i=1}^{N} x_i\varepsilon_i \quad (2)$$

King and Queen[16] have used a nonlinear relationship to calculate the dielectric constants of binary solvent mixtures as

$$\log \varepsilon_m = \frac{\alpha_0 + \alpha_1 x_1}{\beta_0 + \beta_1 x_1} \quad (3)$$

in which α_0, α_1, β_0, and β_1 are the constant terms.

The Jouyban−Acree model was presented for predicting any physicochemical property of solutes such as the dielectric constant.[17] Its basic form for describing the relationships between the dielectric constants of solvent mixtures at various temperatures of the solvent composition is

* To whom correspondence should be addressed. E-mail: ajouyban@hotmail.com. Fax: +98 411 3363231.
† Faculty of Pharmacy.
‡ Drug Applied Research Center.

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$$\log \varepsilon_{m,T} = x_1 \log \varepsilon_{1,T} + x_2 \log \varepsilon_{2,T} + \frac{x_1 x_2}{T}\left[\sum_{i=0}^{2} J_i (x_1 - x_2)^i\right] \quad (4)$$

in which J_i is the model constant. This model could be used to correlate the dielectric constant of binary solvent mixtures with respect to solvent composition and temperature. Equation 4 provided reasonably accurate results with the overall MRD of 1 % for the fitted data of a binary mixture at a fixed temperature. The corresponding MRD for various temperatures was 1 %. Equation 4 could be trained using a minimum number of three experimental dielectric constants at the lowest and three data at the highest temperature of interest; then the dielectric constants of all solvent compositions and temperatures could be predicted using the interpolation technique, and the expected MRD is around 2 %.[17] Although this numerical method provides good estimation of the dielectric constants, it requires a number of experimental data of the mixed solvent of interest, and this could be considered as a limitation for practical applications. Habibi-Yangjeh[18] reported an artificial neural network with the architecture of 7−16−1 providing reasonable correlation for $\varepsilon_{m,T}$ values.

To provide a more comprehensive model, it is possible to include physicochemical properties of the solvents affecting the dielectric constant in a given binary mixture. Abraham and co-workers proposed the linear solvation energy relationship (LSER) equation to calculate various physicochemical properties (PP) as[19]

$$\log \mathrm{PP} = c + eE + sS + aA + bB + vV \quad (5)$$

in which c, e, s, a, b, and v are the model constants, E is the excess molar refraction, S is 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 J_i terms of eq 4 are due to the various solvent−solvent interactions in the solution; the interactions could be represented by Abraham parameters, and eq 4 could be rewritten as

$$\begin{aligned}\log \varepsilon_{m,T} = {} & x_1 \log \varepsilon_{1,T} + x_2 \log \varepsilon_{2,T} + \frac{x_1 x_2}{T}[W_0 + W_1(c_1 - c_2)^2 + W_2(e_1 - e_2)^2 + W_3(s_1 - s_2)^2 + W_4(a_1 - a_2)^2 + \\ & W_5(b_1 - b_2)^2 + W_6(v_1 - v_2)^2] + \frac{x_1 x_2 (x_1 - x_2)}{T}[W_0' + \\ & W_1'(c_1 - c_2)^2 + W_2'(e_1 - e_2)^2 + W_3'(s_1 - s_2)^2 + W_4'(a_1 - \\ & a_2)^2 + W_5'(b_1 - b_2)^2 + W_6'(v_1 - v_2)^2] + \\ & \frac{x_1 x_2 (x_1 - x_2)^2}{T}[W_0'' + W_1''(c_1 - c_2)^2 + W_2''(e_1 - e_2)^2 + \\ & W_3''(s_1 - s_2)^2 + W_4''(a_1 - a_2)^2 + W_5''(b_1 - b_2)^2 + \\ & W_6''(v_1 - v_2)^2] \end{aligned} \quad (6)$$

where W terms are the model constants representing the two- and three-body interaction energies of the solvents. From a mathematical point of view, they are adjustable curve-fit

Table 1. Abraham Solvation Parameters for the Solvents Investigated in This Work Taken from Literature[16,57]

solvent	c	e	s	a	b	v
1,2-dichloroethane	0.227	0.278	−0.167	−2.816	−4.324	4.205
1,4-dioxane	0.098	0.350	−0.083	−0.556	−4.826	4.172
1-butanol	0.152	0.437	−1.175	0.098	−3.914	4.119
1-decanol	−0.062	0.754	−1.461	0.063	−4.053	4.293
1-heptanol	−0.026	0.491	−1.258	0.035	−4.155	4.415
1-hexanol	0.044	0.470	−1.153	0.083	−4.057	4.249
1-nonanol	0.041	0.562	1.103	0.090	3.540	3.922
1-octanol	−0.034	0.490	−1.048	−0.028	−4.229	4.219
1-pentanol	0.080	0.521	−1.294	0.208	−3.908	4.208
1-propanol	0.148	0.436	−1.098	0.389	−3.893	4.036
2,2,4-trimethylpentane	0.288	0.382	−1.668	−3.639	−5.000	4.461
2-butanol	0.106	0.272	−0.988	0.196	−3.805	4.110
2-methyl-1-propanol	0.177	0.335	−1.099	0.069	−3.570	3.990
2-methyl-2-propanol	0.197	0.136	−0.916	0.318	−4.031	4.113
2-propanol	0.063	0.320	−1.024	0.445	−3.824	4.067
acetone	0.335	0.349	−0.231	−0.411	−4.793	3.963
acetonitrile	0.413	0.077	0.326	−1.566	−4.391	3.364
benzene	0.142	0.464	−0.588	−3.099	−4.625	4.491
carbon tetrachloride	0.361	0.579	−1.723	−3.599	−4.764	4.344
chlorobenzene	0.040	0.246	−0.462	−3.038	−4.769	4.640
cyclohexane	0.159	0.784	−1.678	−3.740	−4.929	4.577
cyclohexanone	0.038	0.225	0.058	−0.976	−4.842	4.315
decane	0.160	0.585	−1.734	−3.435	−5.078	4.582
dibuthyl ether	0.203	0.369	−0.954	−1.488	−5.426	4.508
dichloromethane	0.314	0.001	0.022	−3.238	−4.137	4.259
diethyl ether	0.308	0.377	−0.813	−0.468	−5.012	4.379
dimethyl formamide	−0.438	−0.099	0.670	0.878	−4.970	4.552
dimethyl sulfoxide	−0.194	0.327	0.791	1.260	−4.540	3.361
dodecane	0.114	0.668	−1.644	−3.545	−5.006	4.459
ethanol	0.208	0.409	−0.959	0.186	−3.645	3.928
ethyl acetate	0.358	0.362	−0.449	−0.668	−5.016	4.155
ethylene glycol	0.243	0.695	−0.670	0.726	−2.399	2.670
formamide	−0.171	0.070	0.308	0.589	−3.152	2.432
heptane	0.325	0.670	−2.061	−3.317	−4.733	4.543
hexadecane	0.087	0.667	−1.617	−3.587	−4.869	4.433
hexane	0.361	0.579	−1.723	−3.599	−4.764	4.344
methanol	0.329	0.299	−0.671	0.080	−3.389	3.512
methyl acetate	0.351	0.223	−0.150	−1.035	−4.527	3.972
octane	0.152	0.437	−1.175	0.098	−3.914	4.119
pentane	0.369	0.386	−1.568	−3.535	−5.215	4.514
tetrahydrofuran	0.207	0.372	−0.392	−0.236	−4.934	4.447
toluene	0.143	0.527	−0.720	−3.010	−4.824	4.545
trichloromethane	0.191	0.105	−0.403	−3.112	−3.514	4.395
water	−0.994	0.577	2.549	3.813	4.841	−0.869

parameters[20] determined from regressing ($\log \varepsilon_{m,T} - x_1 \log \varepsilon_{1,T} - x_2 \log \varepsilon_{2,T}$) against ($x_1x_2/T$), (($x_1x_2(c_1 - c_2)^2$)/$T$), (($x_1x_2(e_1 - e_2)^2$)/$T$), (($x_1x_2(s_1 - s_2)^2$)/$T$), (($x_1x_2(a_1 - a_2)^2$)/$T$), (($x_1x_2(b_1 - b_2)^2$)/$T$), (($x_1x_2(\upsilon_1 - \upsilon_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)$)/$T$), (($x_1x_2(x_1 - x_2)(c_1 - c_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(e_1 - e_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(s_1 - s_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(a_1 - a_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(b_1 - b_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(\upsilon_1 - \upsilon_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(c_1 - c_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(e_1 - e_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(s_1 - s_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(a_1 - a_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(b_1 - b_2)^2$)/$T$), and (($x_1x_2(x_1 - x_2)^2(\upsilon_1 - \upsilon_2)^2$)/$T$) using a no-intercept least-squares analysis. The Abraham solvation parameters account for all probable interactions between solvents 1 and 2 in the system. The model can be used to predict the dielectric constant of different binary mixtures at various temperatures by employing the corresponding experimental ε_1 and ε_2 values of the monosolvents at T.

The number of experimental data points required in the computation process of ε_m can be reduced by considering a relationship between temperature and Abraham parameters of the monosolvents, and eq 6 can be written as

$$\log \varepsilon_{m,T} = x_1\gamma_1 + \frac{x_1}{T}\{\alpha_0 + \alpha_1 c_1 + \alpha_2 e_1 + \alpha_3 s_1 + \alpha_4 a_1 + \alpha_5 b_1 + \alpha_6 \upsilon_1\} + x_2\gamma_2 + \frac{x_2}{T}\{\beta_0 + \beta_1 c_2 + \beta_2 e_2 + \beta_3 s_2 + \beta_4 a_2 + \beta_5 b_2 + \beta_6 \upsilon_2\} + \frac{x_1x_2}{T}[W_0 + W_1(c_1 - c_2)^2 + W_2(e_1 - e_2)^2 + W_3(s_1 - s_2)^2 + W_4(a_1 - a_2)^2 + W_5(b_1 - b_2)^2 + W_6(\upsilon_1 - \upsilon_2)^2] + \frac{x_1x_2(x_1 - x_2)}{T}[W_0' + W_1'(c_1 - c_2)^2 + W_2'(e_1 - e_2)^2 + W_3'(s_1 - s_2)^2 + W_4'(a_1 - a_2)^2 + W_5'(b_1 - b_2)^2 + W_6'(\upsilon_1 - \upsilon_2)^2] + \frac{x_1x_2(x_1 - x_2)^2}{T}[W_0'' + W_1''(c_1 - c_2)^2 + W_2''(e_1 - e_2)^2 + W_3''(s_1 - s_2)^2 + W_4''(a_1 - a_2)^2 + W_5''(b_1 - b_2)^2 + W_6''(\upsilon_1 - \upsilon_2)^2] \quad (7)$$

where γ_1, γ_2, α, β, and W terms are the model constants. The numerical values of these terms could be computed by regression $\log \varepsilon_{m,T}$ against x_1, (x_1/T), (x_1e_1/T), (x_1s_1/T), (x_1a_1/T), (x_1b_1/T), ($x_1\upsilon_1/T$), x_2, (x_2/T), (x_2e_2/T), (x_2s_2/T), (x_2a_2/T), (x_2b_2/T), ($x_2\upsilon_2/T$), (x_1x_2/T), (($x_1x_2(e_1 - e_2)^2$)/T), (($x_1x_2(s_1 - s_2)^2$)/T), (($x_1x_2(a_1 - a_2)^2$)/T), (($x_1x_2(b_1 - b_2)^2$)/T), (($x_1x_2(\upsilon_1 - \upsilon_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)$)/$T$), (($x_1x_2(x_1 - x_2)(e_1 - e_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(s_1 - s_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(a_1 - a_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(b_1 - b_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)(\upsilon_1 - \upsilon_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(e_1 - e_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(s_1 - s_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(a_1 - a_2)^2$)/$T$), (($x_1x_2(x_1 - x_2)^2(b_1 - b_2)^2$)/$T$), and (($x_1x_2(x_1 - x_2)^2(\upsilon_1 - \upsilon_2)^2$)/$T$). W terms represent the contribution of different types of interactions in the two-body and three-body interaction terms of the original model.

Experimental Data and Computational Methods

The details of the collected data sets from the literature[21−61] are given in Table 2. These data sets include both aqueous and nonaqueous binary mixtures at various temperatures. In all computations, solvents 1 and 2 are defined as $\varepsilon_1 > \varepsilon_2$.

The fitness of the experimental data to the model was studied by calculating the correlation coefficient and the accuracy criteria. The validity of the proposed model was assessed using cross-validation methods. The model constants calculated using odd set numbers was used to predict the dielectric constants of even set numbers and vice versa.

The accuracy of the dielectric constants was investigated by computing the MRD using

$$\mathrm{MRD} = \frac{1}{N}\sum\left(\frac{|\varepsilon^{\mathrm{Calc}} - \varepsilon^{\mathrm{exp}}|}{\varepsilon^{\mathrm{exp}}}\right) \quad (8)$$

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

Results and Discussion

Modeling Dielectric Constants of All Systems Using Monosolvent Data. All available dielectric constant data of aqueous and nonaqueous mixtures at various temperatures were fitted to eq 6, and the obtained model was

$$\log \varepsilon_{m,T} = x_1 \log \varepsilon_{1,T} + x_2 \log \varepsilon_{2,T} + \frac{x_1x_2}{T}[29.799 + 307.781(c_1 - c_2)^2 - 32.260(s_1 - s_2)^2 + 1.233(a_1 - a_2)^2 - 9.294(b_1 - b_2)^2 + 16.514(\upsilon_1 - \upsilon_2)^2] + \frac{x_1x_2(x_1 - x_2)}{T}[-24.532 - 215.763(e_1 - e_2)^2 + 10.359(a_1 - a_2)^2 - 4.254(b_1 - b_2)^2 + 8.996(\upsilon_1 - \upsilon_2)^2] + \frac{x_1x_2(x_1 - x_2)^2}{T}[-170.280(c_1 - c_2)^2 + 28.419(s_1 - s_2)^2 - 7.893(a_1 - a_2)^2 + 10.123(b_1 - b_2)^2 - 28.228(\upsilon_1 - \upsilon_2)^2] \quad (9)$$

The model was statistically significant with the F value of 279 ($p < 0.0005$) and covered the $\varepsilon_{m,T}$ range of 1.8 to 113.6. The F value represents the statistical significance of the correlation and is a ratio of mean squares due to regression to mean squares about regression. A correlation is considered significant, when the calculated F value is greater than the critical F value obtained from Fisher distribution with the degree of freedom of (number of variables) and (number of observations-number of variables). In eq 9, the degrees of freedom were 16 and 3970, respectively, and the critical F value was 3.1. When the dielectric constant data are back-calculated, the resulted MRDs were in the range of around 0 (i.e., < 0.5) % (for 1-heptanol + cyclohexane at 298 K (set no. 19) or 1-octanol + cyclohexane at 298 K (set no. 37)) and 34 % (for 1,2-dicholoroethane + hexadecane at 293 K (set no. 80)) with the overall MRD (± SD) of 7 (± 6) %. Details of the MRD values for the investigated systems are listed in Table 2.

The cross-validation analyses were performed on the model. The binary systems with even or odd set numbers were used to train the model, and the ε_m of data sets with odd or even numbers were predicted using the trained model. The MRD values were also reported in Table 2. The overall MRDs for these analyses were 7 (± 6) % (number of data sets (NDS) = 136) and 7 (± 6) % (NDS = 136), and the mean difference between these MRDs was not statistically significant ($p > 0.95$).

Ab Initio Modeling of All Systems. The collected ε_m data of aqueous and nonaqueous binary mixtures at various temperatures were fitted to eq 7, and the resulting ab initio model to predict the ε_m value is

Table 2. Details of Binary Solvents, Temperature (*T*), Number of Compositions of the Mixtures (*N*), References, and Mean Percentage Deviations (MRDs) of Equations 9 and 10 for Fitted and Cross-Validated Data

						fitted	fitted	cross-validated	cross-validated
no.	solvent 1	solvent 2	*T*/K	ref	*N*	eq 9	eq 10	eq 9	eq 10
1	1-butanol	benzene	308	21	7	6	41	6	52
2	1-butanol	carbon tetrachloride	296	22	8	7	14	7	13
3	1-butanol	chlorobenzene	307	22	8	4	5	4	5
4	1-butanol	chlorobenzene	318	22	8	4	8	5	9
5	1-butanol	cyclohexane	298	23	26	1	12	1	11
6	1-butanol	decane	298	24	13	17	12	16	10
7	1-butanol	dodecane	298	25	22	2	2	2	3
8	1-butanol	ethanol	295	22	7	4	28	5	32
9	1-butanol	heptane	298	26	14	5	5	5	7
10	1-butanol	heptane	298	27	23	2	5	2	4
11	1-butanol	heptane	308	26	14	20	21	20	23
12	1-butanol	pentane	298	22	13	4	8	4	13
13	1-butanol	toluene	308	21	9	2	9	3	15
14	1-decanol	cyclohexane	298	27	32	1	15	1	16
15	1-decanol	dodecane	298	25	23	1	0	1	2
16	1-decanol	heptane	298	27	35	1	4	1	2
17	1-heptanol	carbon tetrachloride	303	22	9	9	27	10	31
18	1-heptanol	chlorobenzene	303	22	9	4	8	4	10
19	1-heptanol	cyclohexane	298	27	25	0	13	1	12
20	1-heptanol	dodecane	298	25	23	1	1	1	3
21	1-heptanol	heptane	298	27	24	1	5	1	5
22	1-heptanol	heptane	303	28	13	12	17	11	16
23	1-heptanol	heptane	313	28	13	20	29	20	26
24	1-heptanol	hexane	298	29	15	14	29	14	26
25	1-heptanol	hexane	303	28	13	8	24	9	23
26	1-heptanol	hexane	313	28	13	13	32	11	31
27	1-hexanol	1-heptanol	303	22	5	2	15	1	12
28	1-hexanol	cyclohexane	298	27	27	1	12	1	13
29	1-hexanol	dodecane	298	25	22	1	2	2	3
30	1-hexanol	heptane	298	27	24	1	6	1	4
31	1-hexanol	hexane	298	29	15	9	29	10	30
32	1-nonanol	cyclohexane	298	27	24	2	14	1	14
33	1-nonanol	dodecane	298	25	24	2	3	3	3
34	1-nonanol	heptane	298	27	35	2	8	2	9
35	1-octanol	carbon tetrachloride	303	22	9	13	51	14	50
36	1-octanol	chlorobenzene	303	22	9	3	16	3	20
37	1-octanol	cyclohexane	298	27	24	0	13	0	12
38	1-octanol	dodecane	298	25	22	1	3	1	4
39	1-octanol	heptane	298	27	22	1	6	1	6
40	1-pentanol	carbon tetrachloride	303	22	9	8	12	7	9
41	1-pentanol	chlorobenzene	303	22	9	3	12	3	11
42	1-pentanol	cyclohexane	298	27	27	1	13	1	14
43	1-pentanol	dodecane	298	25	22	2	1	2	3
44	1-propanol	heptane	298	26	14	3	2	4	3
45	1-pentanol	heptane	298	27	23	2	5	2	5
46	1-propanol	heptane	308	26	14	17	21	17	19
47	1-pentanol	hexane	298	29	15	9	18	10	21
48	1-propanol	1-hexanol	296	30	5	1	11	1	15
49	1-propanol	1,2-dichloroethane	288	31	11	3	17	3	12
50	1-propanol	1,2-dichloroethane	298	31	11	3	17	3	21
51	1-propanol	1,2-dichloroethane	308	31	11	2	17	2	13
52	1-propanol	1,2-dichloroethane	318	31	11	2	16	2	20
53	1-propanol	benzene	298	23	26	1	76	1	87
54	1-propanol	chlorobenzene	288	32	11	8	20	8	24
55	1-propanol	chlorobenzene	298	32	11	9	19	8	15
56	1-propanol	chlorobenzene	308	32	11	8	19	9	22
57	1-propanol	chlorobenzene	318	32	11	9	18	8	15
58	1-propanol	chlorobenzene	288	31	11	8	20	8	24
59	1-propanol	chlorobenzene	298	31	11	9	19	8	15
60	1-propanol	chlorobenzene	308	31	11	8	19	9	22
61	1-propanol	chlorobenzene	318	31	11	9	18	8	15
62	1-propanol	cyclohexane	298	27	28	1	11	1	12
63	1-propanol	cyclohexane	298	23	27	1	12	1	11
64	1-propanol	dichloromethane	288	31	11	9	11	9	11
65	1-propanol	dichloromethane	298	31	11	10	10	10	10
66	1-propanol	dichloromethane	308	31	11	11	8	11	8
67	1-propanol	dichloromethane	318	31	11	10	7	10	7
68	1-propanol	dodecane	298	25	20	2	4	2	5
69	1-propanol	heptane	298	27	26	2	6	2	6
70	1-propanol	methyl acetate	288	33	11	9	6	8	8
71	1-propanol	methyl acetate	298	33	11	11	6	12	7
72	1,2-dichloroethane	2,2,4-trimethylpentane	293	34	11	15	14	17	14
73	1,2-dichloroethane	2,2,4-trimethylpentane	313	34	11	15	10	13	12

Table 2. Continued

						fitted	fitted	cross-validated	cross-validated
no.	solvent 1	solvent 2	*T*/K	ref	*N*	eq 9	eq 10	eq 9	eq 10
74	1,2-dichloroethane	decane	293	34	11	20	10	22	10
75	1,2-dichloroethane	decane	313	34	11	18	7	16	13
76	1,2-dichloroethane	dodecane	293	34	11	26	14	28	18
77	1,2-dichloroethane	dodecane	313	34	11	24	13	22	8
78	1,2-dichloroethane	heptane	293	34	11	9	18	11	19
79	1,2-dichloroethane	heptane	313	34	11	8	13	6	15
80	1,2-dichloroethane	hexadecane	293	34	11	34	25	36	31
81	1,2-dichloroethane	hexadecane	313	34	11	32	25	30	17
82	2-butanol	benzene	308	21	6	3	47	3	37
83	2-butanol	cyclohexane	308	21	7	5	11	5	12
84	2-butanol	toluene	308	21	6	2	18	3	9
85	2-methyl-1-propanol	benzene	308	21	7	5	43	5	54
86	2-methyl-1-propanol	cyclohexane	308	21	7	3	9	3	10
87	2-methyl-1-propanol	toluene	308	21	6	2	16	2	26
88	2-methyl-2-propanol	2-methyl-1-propanol	307	22	8	20	34	21	25
89	2-methyl-2-propanol	benzene	303	35	15	10	132	10	168
90	2-methyl-2-propanol	benzene	308	21	7	7	79	8	64
91	2-methyl-2-propanol	hexane	303	35	15	22	138	23	168
92	2-methyl-2-propanol	toluene	308	21	6	3	56	3	41
93	2-propanol	2-methyl-2-propanol	303	35	15	1	13	2	17
94	acetonitrile	1-butanol	288	36	21	5	8	6	9
95	acetonitrile	1-butanol	293	36	21	5	8	4	9
96	acetonitrile	1-butanol	298	36	21	5	9	5	9
97	acetonitrile	1-butanol	303	36	21	5	9	5	9
98	acetonitrile	1-butanol	308	36	21	5	9	5	10
99	acetonitrile	1-propanol	288	37	21	3	9	2	8
100	acetonitrile	1-propanol	293	37	21	3	9	3	10
101	acetonitrile	1-propanol	298	37	21	3	10	2	10
102	acetonitrile	1-propanol	303	37	21	3	10	4	11
103	acetonitrile	1-propanol	308	37	21	3	10	2	10
104	acetonitrile	2-butanol	288	36	21	11	11	11	10
105	acetonitrile	2-butanol	293	36	21	10	11	10	12
106	acetonitrile	2-butanol	298	36	21	9	10	10	9
107	acetonitrile	2-butanol	303	36	21	9	9	8	10
108	acetonitrile	2-butanol	308	36	21	8	10	9	9
109	acetonitrile	2-methyl-1-propanol	288	38	21	6	11	5	12
110	acetonitrile	2-methyl-1-propanol	293	38	21	5	10	6	10
111	acetonitrile	2-methyl-1-propanol	298	38	21	5	9	4	9
112	acetonitrile	2-methyl-1-propanol	303	38	21	5	9	6	10
113	acetonitrile	2-methyl-1-propanol	308	38	21	5	8	4	8
114	acetonitrile	2-methyl-2-propanol	293	38	20	8	10	8	6
115	acetonitrile	2-methyl-2-propanol	298	38	20	3	10	3	13
116	acetonitrile	2-methyl-2-propanol	303	38	21	2	11	3	7
117	acetonitrile	2-methyl-2-propanol	308	38	21	2	12	2	14
118	acetonitrile	2-propanol	288	39	21	6	5	7	5
119	acetonitrile	2-propanol	293	39	21	6	5	6	5
120	acetonitrile	2-propanol	298	39	21	6	4	6	5
121	acetonitrile	2-propanol	303	39	21	6	4	5	4
122	acetonitrile	2-propanol	308	39	21	6	4	6	5
123	acetonitrile	benzene	298	40	11	18	9	18	11
124	acetonitrile	benzene	299	41	11	10	23	11	22
125	acetonitrile	chlorobenzene	299	41	11	7	13	8	12
126	acetonitrile	ethanol	298	32	7	1	3	0	3
127	acetonitrile	methanol	288	42	24	2	6	3	7
128	acetonitrile	methanol	298	42	24	2	8	1	8
129	acetonitrile	methanol	308	42	24	2	10	3	11
130	acetonitrile	toluene	299	41	11	8	11	9	12
131	benzene	cyclohexane	298	43	48	4	10	4	13
132	chlorobenzene	benzene	298	23	22	0	69	1	60
133	chlorobenzene	cyclohexane	298	23	26	2	14	2	17
134	cyclohexanone	1,2-dichloroethane	303	44	21	15	31	15	35
135	cyclohexanone	cyclohexane	303	44	19	23	19	23	20
136	cyclohexanone	dichloromethane	303	44	23	10	14	11	18
137	cyclohexanone	trichloromethane	303	44	19	26	21	27	23
138	dibuthyl ether	benzene	298	45	13	1	157	1	172
139	dibuthyl ether	benzene	308	45	13	1	159	1	129
140	dibuthyl ether	toluene	298	45	13	2	134	2	147
141	dibuthyl ether	toluene	308	45	13	2	137	2	108
142	dimethyl formamide	1-propanol	293	46	11	3	12	2	19
143	dimethyl formamide	1-propanol	303	46	11	4	13	5	6
144	dimethyl formamide	1-propanol	313	46	11	6	13	5	19
145	dimethyl formamide	1-propanol	323	46	11	9	16	9	10
146	dimethyl formamide	ethanol	293	46	11	4	10	4	17
147	dimethyl formamide	ethanol	303	46	11	3	11	3	7
148	dimethyl formamide	ethanol	313	46	11	3	12	3	18

Table 2. Continued

						fitted	fitted	cross-validated	cross-validated
no.	solvent 1	solvent 2	*T*/K	ref	*N*	eq 9	eq 10	eq 9	eq 10
149	dimethyl formamide	ethanol	323	46	11	5	14	5	9
150	dimethyl sulfoxide	1-propanol	293	47	11	17	23	16	26
151	dimethyl sulfoxide	1-propanol	303	47	11	15	24	16	23
152	dimethyl sulfoxide	1-propanol	313	47	11	18	26	17	28
153	dimethyl sulfoxide	1-propanol	323	47	11	21	29	22	27
154	dimethyl sulfoxide	ethanol	293	47	11	13	22	12	25
155	dimethyl sulfoxide	ethanol	303	47	11	14	22	15	20
156	dimethyl sulfoxide	ethanol	313	47	11	14	24	14	26
157	dimethyl sulfoxide	ethanol	323	47	11	16	25	17	23
158	ethanol	1,2-dichloroethane	288	48	11	6	28	6	32
159	ethanol	1,2-dichloroethane	298	48	11	5	27	5	22
160	ethanol	1,2-dichloroethane	298	49	12	2	22	2	27
161	ethanol	1,2-dichloroethane	308	48	11	4	26	4	22
162	ethanol	1,2-dichloroethane	318	48	11	3	25	3	30
163	ethanol	1,4-dioxane	298	49	12	19	42	20	48
164	ethanol	2-methyl-2-propanol	303	35	15	3	11	3	14
165	ethanol	benzene	298	50	9	5	25	4	28
166	ethanol	carbon tetrachloride	298	49	12	4	11	5	13
167	ethanol	chlorobenzene	288	32	11	5	26	4	19
168	ethanol	chlorobenzene	298	32	11	5	25	6	29
169	ethanol	chlorobenzene	308	32	11	4	24	4	18
170	ethanol	chlorobenzene	318	32	11	4	22	4	26
171	ethanol	cyclohexane	298	27	28	2	11	2	10
172	ethanol	dichloromethane	288	51	11	15	16	16	18
173	ethanol	dichloromethane	298	51	11	16	16	15	12
174	ethanol	dichloromethane	308	51	11	16	15	16	18
175	ethanol	dichloromethane	318	51	11	15	15	15	12
176	ethanol	diethyl ether	298	49	11	1	20	1	29
177	ethanol	dodecane	298	25	21	3	4	3	4
178	ethanol	ethyl acetate	298	49	12	1	26	0	35
179	ethanol	heptane	298	27	24	2	6	3	7
180	ethanol	methyl acetate	288	33	11	5	14	5	19
181	ethanol	methyl acetate	298	33	11	5	14	5	12
182	ethylene glycol	1-hexanol	293	22	5	20	12	19	16
183	formamide	1-butanol	294	52	7	10	23	11	35
184	formamide	1-propanol	288	53	13	24	44	25	38
185	formamide	1-propanol	298	53	13	24	47	24	55
186	1-butanol	hexane	298	24	16	7	19	7	15
187	carbon tetrachloride	hexane	303	22	18	6	50	7	60
188	hexane	dodecane	298	22	22	6	4	6	4
189	hexane	heptane	298	22	24	4	4	4	5
190	methanol	chlorobenzene	288	54	13	3	19	3	25
191	methanol	1,2-dichloroethane	288	32	11	8	24	8	16
192	methanol	1,2-dichloroethane	298	32	11	8	24	8	29
193	methanol	chlorobenzene	298	54	13	3	17	3	10
194	methanol	1,2-dichloroethane	308	32	11	7	23	8	29
195	methanol	1,2-dichloroethane	318	32	11	7	22	6	17
196	methanol	chlorobenzene	318	54	13	5	19	5	24
197	methanol	1,4-dioxane	288	55	11	3	67	3	83
198	methanol	1,4-dioxane	293	55	11	4	66	5	51
199	methanol	1,4-dioxane	293	55	16	4	69	5	86
200	methanol	1,4-dioxane	298	55	11	5	65	5	50
201	methanol	1,4-dioxane	298	49	15	3	65	2	81
202	methanol	1,4-dioxane	303	55	11	5	64	6	50
203	methanol	1,4-dioxane	308	55	11	6	64	5	77
204	methanol	2-methyl-2-propanol	303	35	15	3	7	3	8
205	methanol	carbon tetrachloride	298	49	15	3	10	2	18
206	methanol	1,2-dichloroethane	288	54	13	3	19	3	25
207	methanol	chlorobenzene	288	32	11	5	14	5	7
208	methanol	chlorobenzene	298	32	11	5	13	4	19
209	methanol	1,2-dichloroethane	298	54	13	2	20	2	13
210	methanol	chlorobenzene	308	32	11	6	13	5	19
211	methanol	chlorobenzene	318	32	11	7	11	7	10
212	methanol	1,2-dichloroethane	318	54	13	4	24	5	29
213	methanol	dodecane	298	25	18	3	5	3	4
214	methanol	ethyl acetate	298	49	12	11	12	12	22
215	methanol	heptane	298	27	26	3	10	4	9
216	methanol	tetrahydrofuran	298	49	14	3	27	3	37
217	1-butanol	octane	298	24	13	14	215	14	229
218	water	1-butanol	288	56	14	3	15	3	15
219	water	1-butanol	293	56	14	3	14	3	14
220	water	1-butanol	298	56	14	26	32	27	33
221	water	1-butanol	303	56	14	27	32	26	31
222	water	1-butanol	308	56	14	27	32	28	34
223	water	1-propanol	293	57	11	7	15	7	15

Table 2. Continued

no.	solvent 1	solvent 2	*T*/K	ref	*N*	fitted eq 9	fitted eq 10	cross-validated eq 9	cross-validated eq 10
224	water	1-propanol	313	57	11	5	15	4	15
225	water	1-propanol	323	57	11	4	15	5	16
226	water	1-propanol	333	57	11	4	15	3	15
227	water	1-propanol	353	57	11	3	14	3	16
228	water	1,4-dioxane	293	58	12	8	33	8	25
229	water	1,4-dioxane	298	58	12	7	32	7	38
230	water	1,4-dioxane	303	58	12	6	30	6	24
231	water	1,4-dioxane	308	58	12	5	29	6	35
232	water	2-butanol	288	59	26	6	13	6	15
233	water	2-butanol	293	59	26	6	12	6	12
234	water	2-butanol	298	59	26	6	11	6	13
235	water	2-butanol	303	59	26	6	11	6	11
236	water	2-butanol	308	59	26	6	11	6	13
237	water	2-methyl-2-propanol	303	35	15	10	37	11	33
238	water	2-propanol	293	57	11	9	9	8	9
239	water	2-propanol	313	57	11	7	9	7	9
240	water	2-propanol	323	57	11	6	10	5	9
241	water	2-propanol	333	57	11	5	10	6	11
242	water	2-propanol	353	57	11	4	9	3	8
243	water	acetone	293	57	11	2	27	3	28
244	water	acetone	298	57	11	2	28	2	28
245	water	acetone	303	57	11	2	28	2	29
246	water	acetone	313	57	11	1	29	1	29
247	water	acetone	323	57	11	1	29	2	31
248	water	acetonitrile	273	60	11	7	13	6	18
249	water	acetonitrile	283	60	11	9	13	10	11
250	water	acetonitrile	298	60	11	7	13	6	14
251	water	acetonitrile	313	60	11	4	16	5	19
252	water	ethanol	293	57	11	9	13	9	13
253	water	ethanol	298	61	11	9	14	9	14
254	water	ethanol	313	57	11	8	15	8	14
255	water	ethanol	323	57	11	7	16	7	17
256	water	ethanol	333	57	11	6	17	6	16
257	water	ethanol	353	57	11	5	17	4	19
258	water	ethylene glycol	293	57	11	5	58	3	74
259	water	ethylene glycol	313	57	11	4	42	5	34
260	water	ethylene glycol	333	57	11	3	32	2	43
261	water	ethylene glycol	353	57	11	2	26	3	18
262	water	ethylene glycol	373	[57]	6	2	32	1	45
263	water	methanol	293	57	11	4	10	4	7
264	water	methanol	303	57	11	4	7	4	11
265	water	methanol	313	57	11	3	5	3	6
266	water	methanol	323	57	11	3	5	3	6
267	water	methanol	333	57	11	3	6	2	8
268	water	*tert*-butanol	293	57	11	6	33	6	35
269	water	*tert*-butanol	313	57	11	10	33	9	30
270	water	*tert*-butanol	323	57	11	12	34	12	37
271	water	*tert*-butanol	333	57	11	13	36	13	32
272	water	*tert*-butanol	353	57	11	17	41	17	43
				Overall 100 MRD		7	22	7	23

$$\log \varepsilon_{m,T} = 0.966x_1 + \frac{x_1}{T}\{335.411 + 116.099c_1 - 110.889e_1 + 21.420s_1 + 60.571a_1 - 50.708b_1 - 99.374v_1\} + \frac{x_2}{T}\{1140.338 - 83.921c_2 - 94.099e_2 + 28.983s_2 + 18.205a_2 + 105.287b_2 - 75.780v_2\} + \frac{x_1x_2}{T}[-36.788 + 438.813(c_1 - c_2)^2 + 367.926(e_1 - e_2)^2 - 27.443(s_1 - s_2)^2 + 5.608(a_1 - a_2)^2 - 14.402(b_1 - b_2)^2 + 22.540(v_1 - v_2)^2] + \frac{x_1x_2(x_1 - x_2)}{T}[135.249 - 183.741(c_1 - c_2)^2 - 421.630(e_1 - e_2)^2 - 50.463(s_1 - s_2)^2 + 30.277(v_1 - v_2)^2] + \frac{x_1x_2(x_1 - x_2)^2}{T}[-128.069 + 113.948(s_1 - s_2)^2 + 9.622(b_1 - b_2)^2 - 78.653(v_1 - v_2)^2] \quad (10)$$

The model was statistically significant with the *F* value of 11590 ($p < 0.0005$). The back-calculated dielectric constant resulted in the MRD values in the range of 0 % (for 1-decanol + dodecane at 298 K (set no. 15)) and 215 % (for 1-butanol + octane at 298 K (set no. 217)) with the overall MRD (± SD) of 22 (± 26) % (for details of the MRD values, see Table 2). Equation 10 predicts the dielectric constant of binary solvents at various temperatures for all mole fraction composition ranges from 0 to 1.

The cross-validation results of MRDs for the developed model using even and odd set numbers were 22 (± 21) % (NDS = 136) and 24 (± 33) % (NDS = 136), and the mean difference between these MRDs was not statistically significant ($p > 0.51$).

Modeling Dielectric Constants of Aqueous Binary Mixtures Using Monosolvent Data. Hydro-organic solvent mixtures play important roles in the field of analytical and biomedical sciences; therefore, any model to predict dielectric constants of such mixtures provides useful information for the researchers. To present such a model, all dielectric constant data of aqueous binary mixtures at various temperatures were fitted to eq 6, and after excluding nonsignificant coefficients from the model ($p > 0.05$), the resulting equation is

Table 3. Details of Binary Solvents, Temperature (*T*), Number of Compositions of the Mixtures (*N*), References, and Mean Percentage Deviations (MRDs) of Equations 11 and 12 for Fitted and Cross-Validated Hydro-organic Solvent Mixtures

						fitted	fitted	cross-validated	cross-validated
no.	solvent 1	solvent 2	*T*/K	ref	*N*	eq 11	eq 12	eq 11	eq 12
1	water	1-butanol	288	56	14	1	23	1	23
2	water	1-butanol	293	56	14	1	23	1	22
3	water	1-propanol	293	57	11	3	4	2	5
4	water	1-propanol	313	57	11	1	4	2	4
5	water	1-propanol	323	57	11	1	5	2	6
6	water	1-propanol	333	57	11	2	5	1	5
7	water	1-propanol	353	57	11	3	7	4	8
8	water	1,4-dioxane	293	58	12	3	13	3	13
9	water	1,4-dioxane	298	58	12	2	14	2	13
10	water	1,4-dioxane	303	58	12	2	15	2	15
11	water	1,4-dioxane	308	58	12	1	16	1	15
12	water	2-butanol	288	59	26	4	8	4	10
13	water	2-butanol	293	59	26	4	7	4	5
14	water	2-butanol	298	59	26	4	6	5	8
15	water	2-butanol	303	59	26	4	5	4	4
16	water	2-butanol	308	59	26	5	4	5	6
17	water	2-methyl-2-propanol	303	35	15	4	17	5	22
18	water	2-propanol	293	57	11	9	20	9	21
19	water	2-propanol	313	57	11	7	18	7	17
20	water	2-propanol	323	57	11	6	17	6	17
21	water	2-propanol	333	57	11	5	15	5	14
22	water	2-propanol	353	57	11	4	11	4	11
23	water	acetone	293	57	11	2	10	3	10
24	water	acetone	298	57	11	3	10	2	9
25	water	acetone	303	57	11	3	10	4	10
26	water	acetone	313	57	11	3	10	2	9
27	water	acetone	323	57	11	3	10	4	11
28	water	acetonitrile	273	60	11	2	3	2	4
29	water	acetonitrile	283	60	11	2	3	2	2
30	water	acetonitrile	298	60	11	3	6	4	6
31	water	acetonitrile	313	60	11	5	9	5	11
32	water	ethanol	293	57	11	4	6	4	5
33	water	ethanol	298	61	11	4	5	4	6
34	water	ethanol	313	57	11	3	5	3	4
35	water	ethanol	323	57	11	2	5	3	6
36	water	ethanol	333	57	11	2	5	2	4
37	water	ethanol	353	57	11	1	4	1	6
38	water	ethylene glycol	293	57	11	1	6	1	5
39	water	ethylene glycol	313	57	11	1	3	1	3
40	water	ethylene glycol	333	57	11	2	2	2	3
41	water	ethylene glycol	353	57	11	3	2	3	2
42	water	ethylene glycol	373	57	6	5	4	5	6
43	water	methanol	293	57	11	3	4	4	5
44	water	methanol	303	57	11	2	3	2	3
45	water	methanol	313	57	11	2	3	2	3
46	water	methanol	323	57	11	2	2	1	2
47	water	methanol	333	57	11	1	2	2	3
48	water	*tert*-butanol	293	57	11	5	10	5	7
49	water	*tert*-butanol	313	57	11	2	12	3	14
50	water	*tert*-butanol	323	57	11	2	15	2	15
51	water	*tert*-butanol	333	57	11	3	18	2	18
52	water	*tert*-butanol	353	57	11	6	27	7	29
				Overall 100 MRD		3	9	3	9

$$\log \varepsilon_{m,T} = x_1 \log \varepsilon_{1,T} + x_2 \log \varepsilon_{2,T} + \frac{x_1 x_2}{T}[94.980 + 270.087(c_1 - c_2)^2 - 971.952(e_1 - e_2)^2 - 29.650(s_1 - s_2)^2 + 5.876(a_1 - a_2)^2 - 8.029(b_1 - b_2)^2 + 11.776(v_1 - v_2)^2] + \frac{x_1 x_2 (x_1 - x_2)}{T}[-230.549(e_1 - e_2)^2 + 14.713(a_1 - a_2)^2 - 7.026(b_1 - b_2)^2 + 14.952(v_1 - v_2)^2] + \frac{x_1 x_2 (x_1 - x_2)^2}{T}[3.173(s_1 - s_2)^2] \quad (11)$$

The model was trained using 656 data points with the $\varepsilon_{m,T}$ range of 2.2 to 87.9, and the correlation was statistically significant with the *F* values of 1509 ($p < 0.0005$). The minimum MRD for the back-calculated data was 1 % (for water + 1-butanol at 288 K (set no. 1), water + 1-butanol at 293 K (set no. 2), and water + 1-propanol at 313 K (set no. 4)), and the maximum values was 9 % (for water + 2-propanol at 293 K (set no. 18)) and the overall MRD (± SD) of 3 (± 2) % (NDS = 52) (for details of the MRD values, see Table 3). The cross-validation results of MRDs for the developed model using even and odd set numbers were 3 (± 2) % (NDS = 26) and 3 (± 2) % (NDS = 26), and the mean difference between these MRDs was not statistically significant ($p > 0.65$).

***Ab Initio* Modeling of Aqueous Binary Mixtures.** The ε_m data of aqueous binary data were fitted to eq 7, and the obtained model was

Table 4. Individual Relative Deviations (IRDs) for Predicted Dielectric Constants of Mono-Solvents at Various Temperatures from Corresponding Experimental Values

no.	solvent	*T*/K	ref	experimental	predicted	100 IRD	no.	solvent	*T*/K	ref	experimental	predicted	100 IRD
1	1-butanol	288	36	19.07	16.78	12	167	benzene	298	45	2.27	3.90	72
2	1-butanol	288	56	18.95	16.78	11	168	benzene	298	50	2.28	3.90	71
3	1-butanol	293	36	18.28	16.61	9	169	benzene	299	41	2.29	3.91	71
4	1-butanol	293	56	18.2	16.61	9	170	benzene	303	35	2.26	3.96	75
5	1-butanol	294	52	19.00	16.58	13	171	benzene	308	21	2.25	4.01	78
6	1-butanol	295	22	19.00	16.56	13	172	benzene	308	45	2.25	4.01	78
7	1-butanol	296	22	18.6	16.51	11	173	carbon tetrachloride	298	49	2.23	2.58	16
8	1-butanol	298	24	17.15	16.45	4	174	chlorobenzene	288	32	5.94	4.14	30
9	1-butanol	298	26	17.51	16.45	6	175	chlorobenzene	288	54	6.26	4.14	34
10	1-butanol	298	36	17.56	16.45	6	176	chlorobenzene	298	32	5.54	4.26	23
11	1-butanol	298	56	17.50	16.45	6	177	chlorobenzene	298	54	5.91	4.26	28
12	1-butanol	298	24	17.33	16.44	5	178	chlorobenzene	299	41	5.91	4.27	28
13	1-butanol	303	36	16.91	16.29	4	179	chlorobenzene	308	32	5.51	4.37	21
14	1-butanol	303	56	16.87	16.29	3	180	chlorobenzene	318	32	5.33	4.47	16
15	1-butanol	308	26	16.56	16.14	3	181	chlorobenzene	318	54	5.07	4.47	12
16	1-butanol	308	36	16.31	16.14	1	182	chlorobenzene	288	31	5.94	4.14	30
17	1-butanol	308	56	16.24	16.14	1	183	chlorobenzene	298	31	5.54	4.26	23
18	1-butanol	308	[21]	17.07	16.14	5	184	chlorobenzene	308	31	5.51	4.37	21
19	1-heptanol	298	29	11.32	11.22	1	185	chlorobenzene	318	31	5.33	4.47	16
20	1-heptanol	303	22	11.07	11.19	1	186	cyclohexane	298	43	2.02	1.97	3
21	1-heptanol	303	28	10.87	11.19	3	187	cyclohexane	308	21	2.02	2.07	2
22	1-heptanol	303	28	10.87	11.19	3	188	cyclohexanone	303	44	17.95	16.19	10
23	1-heptanol	313	28	10.02	11.12	11	189	decane	293	34	2.00	2.76	38
24	1-hexanol	293	22	13.40	13.94	4	190	decane	298	24	2.00	2.82	41
25	1-hexanol	296	30	11.30	13.88	23	191	decane	313	34	1.96	2.98	52
26	1-hexanol	298	29	12.51	13.84	11	192	dibutyl ether	298	45	3.04	12.09	298
27	1-hexanol	303	22	12.04	13.75	14	193	dibutyl ether	308	45	2.96	11.98	304
28	1-pentanol	298	29	15.08	13.80	9	194	dichloromethane	288	31	9.19	6.86	25
29	1-propanol	288	31	21.97	20.67	6	195	dichloromethane	288	51	9.19	6.86	25
30	1-propanol	288	37	21.91	20.67	6	196	dichloromethane	298	31	8.51	6.93	19
31	1-propanol	288	53	21.18	20.67	2	197	dichloromethane	298	51	8.51	6.93	19
32	1-propanol	288	31	21.97	20.66	6	198	dichloromethane	303	44	8.71	6.96	20
33	1-propanol	288	32	21.97	20.66	6	199	dichloromethane	308	31	8.07	6.99	13
34	1-propanol	288	33	20.82	20.66	1	200	dichloromethane	308	51	8.07	6.99	13
35	1-propanol	293	37	21.21	20.39	4	201	dichloromethane	318	31	7.98	7.06	12
36	1-propanol	293	46	20.00	20.39	2	202	dichloromethane	318	51	7.98	7.06	12
37	1-propanol	293	47	20.05	20.39	2	203	diethyl ether	298	49	4.35	20.43	370
38	1-propanol	293	57	20.81	20.39	2	204	dimethyl formamide	293	46	41.30	33.22	20
39	1-propanol	296	30	21.80	20.22	7	205	dimethyl formamide	303	46	38.20	31.85	17
40	1-propanol	298	26	20.33	13.80	32	206	dimethyl formamide	313	46	36.00	30.61	15
41	1-propanol	298	31	20.73	20.12	3	207	dimethyl formamide	323	46	34.50	29.50	14
42	1-propanol	298	37	20.49	20.12	2	208	dimethyl sulfoxide	293	47	48.17	74.77	55
43	1-propanol	298	53	20.13	20.12	0	209	dimethyl sulfoxide	303	47	46.95	69.79	49
44	1-propanol	298	31	20.73	20.11	3	210	dimethyl sulfoxide	313	47	44.95	65.43	46
45	1-propanol	298	32	20.73	20.11	3	211	dimethyl sulfoxide	323	47	43.30	61.59	42
46	1-propanol	298	33	19.37	20.11	4	212	dodecane	293	34	2.04	2.54	24
47	1-propanol	303	37	19.78	19.86	0	213	dodecane	313	34	1.98	2.75	39
48	1-propanol	303	46	18.90	19.86	5	214	ethanol	288	32	25.50	20.47	20
49	1-propanol	303	47	18.96	19.86	5	215	ethanol	288	33	26.31	20.47	22
50	1-propanol	308	26	20.23	13.62	33	216	ethanol	288	48	25.50	20.47	20
51	1-propanol	308	31	19.65	19.62	0	217	ethanol	288	51	25.50	20.47	20
52	1-propanol	308	32	19.65	19.62	0	218	ethanol	293	46	25.70	20.20	21
53	1-propanol	308	37	19.09	19.62	3	219	ethanol	293	47	25.71	20.20	21
54	1-propanol	308	31	19.65	19.61	0	220	ethanol	293	57	25.00	20.20	19
55	1-propanol	313	46	17.30	19.39	12	221	ethanol	295	22	25.40	20.09	21
56	1-propanol	313	47	17.37	19.39	12	222	ethanol	298	48	24.45	19.94	18
57	1-propanol	313	57	18.25	19.39	6	223	ethanol	298	61	24.30	19.94	18
58	1-propanol	318	31	18.09	19.16	6	224	ethanol	298	32	24.40	19.93	18
59	1-propanol	318	32	18.09	19.16	6	225	ethanol	298	33	25.08	19.93	21
60	1-propanol	323	46	15.90	18.95	19	226	ethanol	298	49	24.34	19.93	18
61	1-propanol	323	47	15.92	18.95	19	227	ethanol	298	50	25.13	19.93	21
62	1-propanol	323	57	17.11	18.95	11	228	ethanol	298	51	24.45	19.93	19
63	1-propanol	333	57	15.88	18.54	17	229	ethanol	303	46	23.40	19.68	16
64	1-propanol	353	57	13.86	17.83	29	230	ethanol	303	47	23.42	19.68	16
65	1,2-dichloroethane	288	31	10.88	6.62	39	231	ethanol	303	35	23.60	19.68	17
66	1,2-dichloroethane	288	32	10.88	6.62	39	232	ethanol	308	32	23.40	19.44	17
67	1,2-dichloroethane	288	48	10.88	6.62	39	233	ethanol	308	48	23.31	19.44	17
68	1,2-dichloroethane	288	[54]	11.12	6.62	40	234	ethanol	308	51	23.31	19.44	17
69	1,2-dichloroethane	293	34	10.67	6.66	38	235	ethanol	313	46	22.20	19.21	13
70	1,2-dichloroethane	293	34	10.67	6.66	38	236	ethanol	313	47	22.23	19.21	14
71	1,2-dichloroethane	298	31	10.43	6.69	36	237	ethanol	313	57	22.20	19.21	13
72	1,2-dichloroethane	298	32	10.43	6.69	36	238	ethanol	318	32	22.10	19.00	14
73	1,2-dichloroethane	298	48	10.43	6.69	36	239	ethanol	318	48	22.19	19.00	14
74	1,2-dichloroethane	298	49	10.36	6.69	35	240	ethanol	318	51	22.19	19.00	14
75	1,2-dichloroethane	298	54	10.81	6.69	38	241	ethanol	323	46	20.40	18.78	8

Table 4. Continued

no.	solvent	*T*/K	ref	experimental	predicted	100 IRD	no.	solvent	*T*/K	ref	experimental	predicted	100 IRD
76	1,2-dichloroethane	308	31	10.10	6.76	33	242	ethanol	323	47	20.43	18.78	8
77	1,2-dichloroethane	308	32	10.10	6.76	33	243	ethanol	323	57	20.87	18.78	10
78	1,2-dichloroethane	308	48	10.10	6.76	33	244	ethanol	333	57	19.55	18.39	6
79	1,2-dichloroethane	313	34	9.53	6.80	29	245	ethanol	353	57	17.31	17.69	2
80	1,2-dichloroethane	318	31	9.82	6.83	30	246	ethyl acetate	298	49	6.02	24.90	314
81	1,2-dichloroethane	318	32	9.82	6.83	30	247	ethylene glycol	293	57	38.66	35.87	7
82	1,2-dichloroethane	318	48	9.82	6.83	30	248	ethylene glycol	293	22	40.80	35.85	12
83	1,2-dichloroethane	318	54	9.92	6.83	31	249	ethylene glycol	313	57	34.94	32.89	6
84	1,4-dioxane	288	55	2.23	21.01	844	250	ethylene glycol	333	57	31.58	30.48	3
85	1,4-dioxane	293	55	2.22	20.72	834	251	ethylene glycol	353	57	28.45	28.49	0
86	1,4-dioxane	293	58	2.24	20.72	825	252	ethylene glycol	373	57	25.61	26.82	5
87	1,4-dioxane	298	49	2.21	20.44	825	253	formamide	288	53	110.80	78.86	29
88	1,4-dioxane	298	55	2.21	20.44	825	254	formamide	294	52	110.00	75.48	31
89	1,4-dioxane	298	58	2.21	20.44	825	255	formamide	298	53	109.70	73.39	33
90	1,4-dioxane	303	55	2.20	20.17	817	256	heptane	293	34	1.94	2.68	38
91	1,4-dioxane	303	58	2.20	20.17	817	257	heptane	298	26	1.91	2.73	43
92	1,4-dioxane	308	55	2.19	19.92	809	258	heptane	303	28	1.90	2.79	47
93	1,4-dioxane	308	58	2.19	19.92	810	259	heptane	308	26	1.89	2.85	50
94	2-butanol	288	36	18.45	19.42	5	260	heptane	313	28	1.88	2.90	54
95	2-butanol	288	59	18.28	19.42	6	261	heptane	313	34	1.91	2.90	52
96	2-butanol	293	36	17.54	19.17	9	262	hexadecane	293	34	2.08	2.36	13
97	2-butanol	293	59	17.41	19.17	10	263	hexadecane	313	34	2.03	2.57	27
98	2-butanol	298	36	16.58	18.94	14	264	hexane	298	29	1.92	3.34	74
99	2-butanol	298	59	16.52	18.94	15	265	hexane	298	24	1.89	3.34	77
100	2-butanol	303	36	15.78	18.72	19	266	hexane	303	28	1.87	3.39	81
101	2-butanol	303	59	15.66	18.72	20	267	hexane	303	35	1.87	3.39	82
102	2-butanol	308	36	14.93	18.50	24	268	hexane	313	28	1.86	3.50	88
103	2-butanol	308	59	14.81	18.50	25	269	methanol	288	42	34.84	31.62	9
104	2-butanol	308	21	17.76	18.50	4	270	methanol	288	54	34.64	31.62	9
105	2-methyl-1-propanol	288	38	19.48	18.10	7	271	methanol	288	32	34.64	31.60	9
106	2-methyl-1-propanol	293	38	18.76	17.89	5	272	methanol	288	55	34.64	31.60	9
107	2-methyl-1-propanol	298	38	17.93	17.69	1	273	methanol	293	55	33.66	30.96	8
108	2-methyl-1-propanol	303	38	17.18	17.50	2	274	methanol	293	57	32.35	30.96	4
109	2-methyl-1-propanol	308	38	16.52	17.32	5	275	methanol	298	32	32.57	30.34	7
110	2-methyl-1-propanol	308	21	17.66	17.32	2	276	methanol	298	42	32.66	30.34	7
111	2-methyl-2-propanol	303	35	10.90	26.50	143	277	methanol	298	54	32.55	30.34	7
112	2-methyl-2-propanol	303	38	11.43	26.50	132	278	methanol	298	55	32.63	30.34	7
113	2-methyl-2-propanol	303	35	10.90	26.48	143	279	methanol	298	49	32.66	30.32	7
114	2-methyl-2-propanol	308	38	10.55	26.05	147	280	methanol	303	55	31.62	29.75	6
115	2-methyl-2-propanol	308	21	10.20	26.03	155	281	methanol	303	57	30.68	29.75	3
116	2-propanol	288	39	21.14	20.90	1	282	methanol	303	35	31.70	29.73	6
117	2-propanol	293	39	20.33	20.61	1	283	methanol	308	32	30.91	29.19	6
118	2-propanol	293	57	18.62	20.61	11	284	methanol	308	42	30.56	29.19	4
119	2-propanol	298	39	19.45	20.34	5	285	methanol	308	55	30.64	29.19	5
120	2-propanol	303	39	18.62	20.08	8	286	methanol	313	57	29.03	28.66	1
121	2-propanol	303	35	17.70	20.07	13	287	methanol	318	32	28.91	28.16	3
122	2-propanol	308	39	17.73	19.83	12	288	methanol	318	54	30.91	28.16	9
123	2-propanol	313	57	16.23	19.59	21	289	methanol	323	57	27.44	27.67	1
124	2-propanol	323	57	15.06	19.14	27	290	methanol	333	57	25.97	26.78	3
125	2-propanol	333	57	14.03	18.72	33	291	methyl acetate	288	33	6.91	24.21	250
126	2-propanol	353	57	11.91	17.99	51	292	methyl acetate	298	33	6.74	23.44	248
127	2,2,4-trimethylpentane	293	4	1.95	3.62	86	293	octane	298	24	1.95	16.44	743
128	2,2,4-trimethylpentane	313	34	1.90	3.84	102	294	pentane	298	24	1.82	4.39	142
129	acetone	293	57	19.56	31.26	60	295	*tert*-butanol	293	57	10.03	27.46	174
130	acetone	298	57	19.10	30.63	60	296	*tert*-butanol	313	57	8.44	25.62	204
131	acetone	303	57	18.67	30.03	61	297	*tert*-butanol	323	57	7.67	24.82	224
132	acetone	313	57	17.80	28.92	62	298	*tert*-butanol	333	57	6.96	24.10	246
133	acetone	323	57	16.98	27.91	64	299	*tert*-butanol	353	57	5.90	22.83	287
134	acetonitrile	273	60	42.80	40.57	5	300	tetrahydrofuran	298	49	7.54	20.62	173
135	acetonitrile	283	60	39.20	38.50	2	301	toluene	298	45	2.41	3.92	63
136	acetonitrile	288	42	37.61	37.56	0	302	toluene	299	41	2.38	3.93	65
137	acetonitrile	288	36	37.58	37.53	0	303	toluene	308	21	2.35	4.03	71
138	acetonitrile	288	37	37.58	37.53	0	304	toluene	308	45	2.35	4.03	71
139	acetonitrile	288	38	37.58	37.53	0	305	water	273	60	87.90	100.02	14
140	acetonitrile	288	39	37.58	37.53	0	306	water	283	60	83.90	91.95	10
141	acetonitrile	293	38	36.78	36.67	0	307	water	288	56	82.49	88.36	7
142	acetonitrile	293	39	36.78	36.67	0	308	water	288	59	82.17	88.36	8
143	acetonitrile	293	36	36.78	36.65	0	309	water	293	59	80.31	85.12	6
144	acetonitrile	293	37	36.78	36.65	0	310	water	293	56	80.52	85.02	6
145	acetonitrile	293	38	36.78	36.65	0	311	water	293	57	80.37	85.02	6
146	acetonitrile	298	37	35.97	35.83	0	312	water	293	58	80.38	85.02	6
147	acetonitrile	298	38	35.97	35.83	0	313	water	298	56	78.56	82.01	4
148	acetonitrile	298	39	35.97	35.83	0	314	water	298	59	78.53	82.01	4
149	acetonitrile	298	42	35.96	35.83	0	315	water	298	60	78.30	82.01	5
150	acetonitrile	298	60	37.00	35.83	3	316	water	298	61	78.50	82.01	4
151	acetonitrile	298	32	36.00	35.81	1	317	water	298	57	78.54	81.92	4

Table 4. Continued

no.	solvent	*T*/K	ref	experimental	predicted	100 IRD	no.	solvent	*T*/K	ref	experimental	predicted	100 IRD
152	acetonitrile	298	36	35.97	35.81	0	318	water	298	58	78.48	81.92	4
153	acetonitrile	298	38	35.97	35.81	0	319	water	303	35	76.60	79.11	3
154	acetonitrile	298	40	36.00	35.81	1	320	water	303	56	76.73	79.11	3
155	acetonitrile	299	41	36.40	35.65	2	321	water	303	59	76.79	79.11	3
156	acetonitrile	303	37	35.09	35.04	0	322	water	303	57	76.73	79.02	3
157	acetonitrile	303	38	35.09	35.04	0	323	water	303	58	76.73	79.02	3
158	acetonitrile	303	39	35.09	35.04	0	324	water	308	56	75.00	76.40	2
159	acetonitrile	303	36	35.09	35.02	0	325	water	308	59	74.97	76.40	2
160	acetonitrile	308	37	34.25	34.29	0	326	water	308	58	74.97	76.32	2
161	acetonitrile	308	38	34.25	34.29	0	327	water	313	60	73.10	73.86	1
162	acetonitrile	308	39	34.25	34.29	0	328	water	313	57	73.12	73.79	1
163	acetonitrile	308	42	34.25	34.29	0	329	water	323	57	69.85	69.20	1
164	acetonitrile	308	36	34.25	34.27	0	330	water	333	57	66.62	65.14	2
165	acetonitrile	313	60	33.10	33.58	1	331	water	353	57	60.58	58.32	4
166	benzene	298	40	2.30	3.90	70	332	water	373	57	55.10	52.84	4
												Overall	55

$$\log \varepsilon_{m,T} = 1.153x_1 - 254.576\frac{x_1 v_1}{T} + 0.432x_2 + \frac{x_2}{T}\{760.636 + 344.451c_2 - 85.369e_2 - 314.315s_2 - 112.658a_2 - 41.477b_2 - 244.958v_2\} + \frac{x_1x_2}{T}[-495.976 + 326.004(c_1 - c_2)^2 - 1482.432(e_1 - e_2)^2 + 14.232(a_1 - a_2)^2 - 2.968(b_1 - b_2)^2] + \frac{x_1x_2(x_1 - x_2)}{T}[-705.339 - 619.698(e_1 - e_2)^2 + 35.456(s_1 - s_2)^2 + 25.735(a_1 - a_2)^2] + \frac{x_1x_2(x_1 - x_2)^2}{T}[1983.817 - 101.905(s_1 - s_2)^2 - 35.786(b_1 - b_2)^2 + 83.278(v_1 - v_2)^2] \quad (12)$$

Equation 12 was a significant ($p < 0.0005$) correlation with the *F* value of 18325. The minimum (2 %) and maximum (27 %) of MRDs were observed for water + methanol at 333 K (set no. 47) and water + *tert*-butanol at 353 K (set no. 52) and the overall MRD (± SD) of 9 (± 6) % (NDS = 52) (for details of the MRD values, see Table 3). The cross-validation results of MRDs for eq 12 using even and odd set numbers were 9 (± 7) % (NDS = 26) and 9 (± 6) % (NDS = 26), and the mean difference between these MRDs was not statistically significant ($p > 0.95$).

Prediction of Dielectric Constants for Monosolvents. Considering $x_1 = 1$, eq 10 is reduced to

$$\log \varepsilon_T = 0.966 + \frac{1}{T}\{335.411 + 116.099c - 110.889e + 21.420s + 60.571a - 50.708b - 99.374v\} \quad (13)$$

which could be used to predict dielectric constants of monosolvents at various temperatures (ε_T). The calculated MRD value for 332 data points is 50 %, and as listed in Table 4, a number of solvents, such as 1,4-dioxane, diethyl ether, dibutyl ether, methyl acetate, and ethyl acetate produced very large prediction errors. By excluding these solvents, the MRD reduces to 26 %, which is comparable with similar results from the literature[8,9] and possesses an advantage of predicting dielectric constants at various temperatures.

Conclusion

Four trained versions of the Jouyban−Acree model were presented for the calculation of dielectric constants of solvent mixtures. Equations 9 and 11 employ two experimental dielectric constants of monosolvents at the temperature of interest and produced the overall MRDs of 7 % and 3 %. Equations 10 and 12 are the ab initio methods and predict the dielectric constants of solvent mixtures using the Abraham solvent parameters with the overall MRDs of 22 % and 9 %, respectively. As briefly discussed in the Introduction, knowledge of dielectric constants is required in many applications, and data of most of the solvent mixtures are not available in the literature. The proposed model is employed to predict dielectric constants of monosolvents at various temperatures (see eq 13), and its applications could be extended to predict the dielectric constant of multicomponent solvent systems at various temperatures and provide useful information for researchers. The disadvantages of the proposed method are the following: (1) Abraham solvation parameters for some solvents are not available, (2) required computations are a little bit complex (we tried to solve this by providing Excel sheet to compute dielectric constants), and (3) to provide better predictions (i.e., with an MRD of ~7), dielectric constants of monosolvents are required.

Supporting Information Available:

Four developed equations in this work are included in an Excel file; by including the required input data, one can predict the dielectric constant of the mixture. The required input data (temperature, the Abraham solvent parameters, etc.) for predicting the dielectric constants using these Excel sheets (one sheet for each equation) are noticed using red font, and by adding the data, the dielectric constants will be computed, reported as blue font and graphically represented on the screen. This material is available free of charge via the Internet at http://pubs.acs.org.

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