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Predicting Solubility of Anthracene in Non-aqueous Solvent Mixtures Using a Combination of Jouyban–Acree and Abraham Models

Abolghasem Jouyban,*,[a] Maryam Khoubnasabjafari,[b] and William Eugene Acree, Jr.[c]

[a] *Faculty of Pharmacy and Drug Applied Research Centre, Tabriz University of Medical Sciences; Tabriz 51664, Iran:* [b] *Kimia Research Institute; Tabriz, P.O. Box 51665–171, Iran: and* [c] *Department of Chemistry, University of North Texas; Denton, TX 76203–5070, U.S.A.*

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Quantitative structure property relationships were proposed to calculate the binary interaction terms of the Jouyban–Acree model using coefficients of Abraham solvational models. The applicability of the proposed methods for reproducing solubility data of anthracene in binary solvents has been evaluated using 56 solubility data sets collected from the literature. The mean percentage deviation (MPD) of experimental and calculated solubilities, using predicted mole fraction solubility of anthracene in solvents 1 and 2, has been computed as a measure of accuracy and the MPD of the proposed methods were 5.5 and 4.2%. The accuracy of the method was compared with that of a previously reported method where the MPD was 14.4% and the mean differences between proposed and previous methods was statistically significant. To provide a predictive model, solubility of anthracene was computed using Abraham solvational models and employed to predict the solubility in binary solvents using derived model constants of Jouyban–Acree model and the obtained MPDs were 37.9 and 22.2%, respectively.

Key words solubility; prediction; cosolvency; anthracene; Abraham model; Jouyban–Acree model

Polycyclic aromatic hydrocarbons (PAHs) are released to the environment from incomplete combustion of organic materials. They are common constituents of complex mixtures such as automobile exhausts, petroleum refining and crude oil. Most of PAHs are considered dangerous substances because of their toxic and mutagenic or carcinogenic potential.[1)] PAHs are hydrophobic compounds, and they persist in ecosystem because of their poor aqueous solubilities and present in contaminated soil, waters and sediments and play a significant role in the environment safety and human health. Toxicity of PAHs was investigated on different organisms by various research groups.[2—4)] Wurl and Obbard[5)] reviewed the recent reports on the pollutants of sea-surface microlayer (SML) including PAHs from various parts of the world. SML is an essential micro-habitat for a vast diversity of microorganisms (neuston), larvae, and fish eggs. It has been concluded that the total concentration of PAHs in SML increases generally with the size of the port and intensity of shipping traffic. The contamination of SML with pollutants has important implications with respect to the ecology of the wider marine environment, therefore, investigations on different aspects of pollutant fate, transport and ecotoxicological impacts are required. Djomo and coworkers[3)] showed that the toxicity of PAHs on a green alga is strongly influenced by their physico-chemical properties such as aqueous solubility. The alga studied is an important in aquatic food chains and its ecological role as primary producer in transferring energy to the higher trophic levels is well known. Anthracene is a low molecular weight, not acutely toxic, carcinogenic or mutagenic members of PAHs. There is evidence that it is absorbed following oral and dermal exposure.[2)]

Solubility is one of the most important properties of chemicals and it could be altered using mixed solvent systems. A number of models have been presented to calculate a solute solubility in solvent mixtures including the Jouyban–Acree model discussed in this work. Most of the models are based on least square analysis and require a number of experimental data to compute the model cosntants. This is obviously a limiting factor in practical applications of such models where a researcher interested in solubility estimation method without further experimental efforts. Ikeda *et al.*[6)] have employed a fully predictive model namely the Conductor-like Screening Model for Real Solvents (COSMO-RS) to predict the solubility of drugs in different solvent systems including solubility in binary solvents. Although the model is a predictive one, the deviations between experimental versus predicted values are relatively high.

Solubility of anthracene in non-aqueous mixed solvents has been extensively studied by Acree's group.[7—15)] The experimentally determined data has been correlated using a well known solution model, *i.e.* the Jouyban–Acree model. The model was proposed by Acree and co-workers for correlating the solubility of PAHs in non-aqueous solvent mixtures.[16,17)] The general form of the model is:

$$\ln X_{\mathrm{m}} = f_1 \ln X_1 + f_2 \ln X_2 + f_1 f_2 \sum_{j=0}^{2} B_i (f_1 - f_2)^j \qquad (1)$$

where X is the mole fraction solubility of the solute, f denotes the mole fraction of the solvents 1 and 2 in the solvent mixture, subscripts m, 1 and 2 are the mixed solvent and solvents 1 and 2, respectively, and B_i is the model constants which is calculated using a no intercept least square analysis.[18)] Although the model was proposed for modeling of PAHs solubilities in non-aqueous solvent mixtures, it has been shown that the model is applicable for calculating the solubility of polar and/or semi-polar compounds in aqueous solvent mixtures.[19,20)] It has also been shown that the model is applicable for modeling physicochemical properties other than solubility in solvent mixtures.[21)]

The main drawback of the Jouyban–Acree model is that it suffers from the presence of a number of curve-fitting parameters and needs a minimum number of experimental data points for training. In a previous work, a quantitative structure property relationship (QSPR) has been proposed to reduce the number of data points for predicting the solubility of solutes by the Jouyban–Acree model.[22)] The model has

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* To whom correspondence should be addressed. e-mail: ajouyban@hotmail.com

been evaluated using a limited number of anthracene data sets in binary and ternary solvents and the solubility parameters of the solvents and that of anthracene have been used as independent variables.

The Abraham solvational parameter models provide convenient solubility prediction methods for a wide variety of organic solvents. The basic models proposed for processes within condensed phases and processes involving gas to condensed phase transfer as:

$$\log\left(\frac{C_\mathrm{S}}{C_\mathrm{W}}\right)=c+r\cdot R_2+s\cdot\pi_2^\mathrm{H}+a\cdot\sum\alpha_2^\mathrm{H}+b\cdot\sum\beta_2^\mathrm{H}+v\cdot V_\mathrm{X} \tag{2}$$

$$\log\left(\frac{C_\mathrm{S}}{C_\mathrm{G}}\right)=c+r\cdot R_2+s\cdot\pi_2^\mathrm{H}+a\cdot\sum\alpha_2^\mathrm{H}+b\cdot\sum\beta_2^\mathrm{H}+l\cdot\log L^{16} \tag{3}$$

where C_S, C_W are the solute solubility in the organic solvent and water (in mol per liter), respectively, C_G is the gas phase concentration of the solute, R_2 is the excess molar refraction, π_2^H is dipolarity/polarizability of solute, $\sum\alpha_2^\mathrm{H}$ denotes the solute's hydrogen-bond acidity, $\sum\beta_2^\mathrm{H}$ stand for the solute's hydrogen-bond basicity, V_X is the McGowan volume of the solute, $\log L^{16}$ is the logarithm of the solute gas-hexadecane partition coefficient at 298.15 K and c, r, s, a, b, v and l are the model constants depend upon the solvent system under consideration. The numerical values of the Abraham model constants were reported in previous works.[23—26] By replacing numerical values of descriptors, *i.e.* R_2, π_2^H, $\sum\alpha_2^\mathrm{H}$, $\sum\beta_2^\mathrm{H}$, V_X, and $\log L^{16}$ of anthracene taken from a previous paper,[23] in Eqs. 2 and 3, the solubility of anthracene in various organic solvents were calculated using:

$$\log\left(\frac{C_\mathrm{S}}{3.715\times10^{-7}}\right)=c+2.290r+1.340s+0.280b+1.454v \tag{4}$$

$$\log\left(\frac{C_\mathrm{S}}{3.467\times10^{-10}}\right)=c+2.290r+1.340s+0.280b+7.568l \tag{5}$$

where c, r, s, b, v and l values of the solvents were listed in Tables 2 and 3. Average absolute deviation of the solubility of anthracene calculated using Eqs. 4 and 5 for 29 studied organic solvents were 37.1 and 23.0%, respectively.[23]

The aim of this work is to propose a QSPR model using Abraham's solvational parameters to calculate the model constants of the Jouyban–Acree model. The calculated constants were employed to predict solubility of anthracene in binary solvents. Anthracene data was chosen as model system since a large number of its experimental data has been published so far. It is obvious that, this approach could be employed for other solutes in binary solvents. By this extension it is possible to use known Abraham solvational paremeters to predict a solute solubility in mixed solvent systems. The accuracy of the proposed methods has been compared with that of a previously reported method for predicting solubility of anthracene in binary solvent mixtures.

Computational Methods

The model constants of the Jouyban–Acree model represent the extent of solvent–solvent and solvent–solute interactions in the solution and these interactions could be related to the physico-chemical properties of solvents and solutes in order to establish a quantitative structure property relationship approach. In a previous paper,[22] the differences in solubility parameters of the solvents with that of solute and their square values have been used to correlate the binary interaction terms (B_i) of the Jouyban–Acree model as:

$$B_0=0.081(\delta_1-\delta_\mathrm{s})+0.315(\delta_2-\delta_\mathrm{s})+0.159(\delta_1-\delta_\mathrm{s})^2 -0.129(\delta_2-\delta_\mathrm{s})^2 \tag{6}$$

$$B_1=-0.120(\delta_1-\delta_\mathrm{s})+0.047(\delta_2-\delta_\mathrm{s})-0.073(\delta_1-\delta_\mathrm{s})^2 +0.052(\delta_2-\delta_\mathrm{s})^2 \tag{7}$$

$$B_2=0.048(\delta_1-\delta_\mathrm{s})-0.012(\delta_2-\delta_\mathrm{s})+0.025(\delta_1-\delta_\mathrm{s})^2 -0.031(\delta_2-\delta_\mathrm{s})^2 \tag{8}$$

in which δ_1 and δ_2 are the solubility parameters of solvents 1 and 2, respectively, δ_s is the solute's solubility parameter ($=9.9\,(\mathrm{cal/cm^3})^{1/2}$ for anthracene) and the model constants calculated using experimental data of 30 data sets.[22]

In this work, the experimentally obtained B_i values of 56 data sets of anthracene solubility in non-aqueous binary solvents, were regressed against squared differences of coefficients of Abraham's solvational parameters. Using B_i values computed by the developed models, the only unknown parameters to predict the solubility of a solute in a binary solvent system is the numerical values of the solute in solvents 1 and 2, *i.e.* $\ln X_1$ and $\ln X_2$. In order to provide a predictive model (without any experimentally determined parameter), C_S values of anthracene in the solvents under consideration computed using Abraham's model were converted to the mole fraction solubilities using density of the organic solvent and then the computed X_1 and X_2 values were used to predict the solubility in binary solvents using the Jouyban–Acree model. It is obvious that, to convert C_S to mole fraction solubilities, we should use density of saturated solutions, however, since it requires more experimental efforts, we have used density of pure organic solvent and ignored the effect of solute on density of the solution.

The back-calculated B_i values, have been used to predict the solubility of anthracene in binary solvent mixtures and the mean percentage deviation (MPD) of observed and calculated solubilities have been computed using:

$$\mathrm{MPD}=\frac{100}{N}\sum\frac{|(X_\mathrm{m})_\mathrm{cal}-(X_\mathrm{m})_\mathrm{obs.}|}{(X_\mathrm{m})_\mathrm{obs.}}$$

Where N is the number of data points.

Computational Results and Discussion

The solubilities of anthracene in 56 different binary solvent mixtures (for details see Table 1) have been used to compute B_i terms of each binary solvent and the B_i terms were employed to build up QSPR models using coefficients of Abraham model of the solvents. Details of B_i terms and the coefficients were listed in Table 4. The obtained QSPR models using water to solvent coefficients of Abraham model for calculating B_i terms are:

$$B_0=0.128-4.772(c_1-c_2)^2-1.123(r_1-r_2)^2+0.546(s_1-s_2)^2 +0.670(b_1-b_2)^2+1.262(v_1-v_2)^2 \tag{9}$$

$$B_1=0.194-10.404(c_1-c_2)^2-1.746(r_1-r_2)^2+0.133(s_1-s_2)^2 +0.372(b_1-b_2)^2-1.402(v_1-v_2)^2 \tag{10}$$

$$B_2=-0.047-1.340(c_1-c_2)^2-0.934(r_1-r_2)^2+0.140(s_1-s_2)^2 +0.178(b_1-b_2)^2+0.876(v_1-v_2)^2 \tag{11}$$

The corresponding equations for gas to solvent coefficients are:

$$B_0=0.022-2.918(c_1-c_2)^2-2.677(r_1-r_2)^2+0.749(s_1-s_2)^2 +0.756(b_1-b_2)^2+15.191(l_1-l_2)^2 \tag{12}$$

$$B_1=0.160-5.975(c_1-c_2)^2-4.944(r_1-r_2)^2+0.192(s_1-s_2)^2 +0.404(b_1-b_2)^2-6.965(l_1-l_2)^2 \tag{13}$$

$$B_2=-0.089-0.476(c_1-c_2)^2-1.023(r_1-r_2)^2+0.178(s_1-s_2)^2 +0.222(b_1-b_2)^2+6.895(l_1-l_2)^2 \tag{14}$$

In Eqs. 9—14 subscripts 1 and 2 denote solvents 1 and 2, re-

Table 1. List of Solvents and the References of Solubility Data Sets

No.	Solvent 1	Solvent 2	$\ln X_1$	$\ln X_2$	Ref.
1	1-Butanol	1,4-Dioxane	−7.13	−4.79	7
2	1-Butanol	1-Pentanol	−7.13	−6.82	8
3	1-Butanol	Dibutyl ether	−7.13	−5.62	9
4	1-Octanol	1,4-Dioxane	−6.14	−4.79	7
5	1-Octanol	1-Pentanol	−6.14	−6.82	8
6	1-Octanol	Dibutyl ether	−6.14	−5.62	9
7	1-Propanol	1,4-Dioxane	−7.43	−4.79	7
8	1-Propanol	1-Pentanol	−7.43	−6.82	8
9	1-Propanol	Dibutyl ether	−7.43	−5.62	9
10	2,2,4-Trimethyl pentane	1,4-Dioxane	−6.84	−4.78	10
11	2,2,4-Trimethyl pentane	1-Butanol	−6.84	−7.13	11
12	2,2,4-Trimethyl pentane	1-Propanol	−6.84	−7.43	11
13	2,2,4-Trimethyl pentane	2-Butanol	−6.84	−7.44	12
14	2-Butanol	1,4-Dioxane	−7.44	−4.79	7
15	2-Butanol	1-Pentanol	−7.44	−6.82	8
16	2-Butanol	Dibutyl ether	−7.44	−5.62	9
17	2-Methyl-1-propanol	1,4-Dioxane	−7.66	−4.79	7
18	2-Methyl-1-propanol	1-Pentanol	−7.66	−6.82	8
19	2-Methyl-1-propanol	Dibutyl ether	−7.66	−5.62	9
20	2-Propanol	1,4-Dioxane	−7.80	−4.79	7
21	2-Propanol	1-Pentanol	−7.80	−6.82	8
22	2-Propanol	Dibutyl ether	−7.80	−5.62	9
23	Benzene	Methylcyclohexane	−4.90	−6.41	13
24	Benzene	Octane	−4.90	−6.30	13
25	Cyclohexane	1,4-Dioxane	−6.47	−4.78	10
26	Cyclohexane	1-Butanol	−6.47	−7.13	11
27	Cyclohexane	1-Propanol	−6.47	−7.43	11
28	Cyclohexane	2-Butanol	−6.47	−7.44	12
29	Dibutyl ether	2,2,4-Trimethyl pentane	−5.62	−6.84	14
30	Dibutyl ether	Cyclohexane	−5.62	−6.47	14
31	Dibutyl ether	Heptane	−5.62	−6.46	14
32	Dibutyl ether	Hexane	−5.62	−6.67	14
33	Dibutyl ether	Methylcyclohexane	−5.62	−6.41	14
34	Dibutyl ether	Octane	−5.62	−6.30	14
35	Heptane	1,4-Dioxane	−6.46	−4.78	10
36	Heptane	1-Butanol	−6.46	−7.13	11
37	Heptane	1-Propanol	−6.46	−7.43	11
38	Heptane	2-Butanol	−6.46	−7.44	12
39	Hexane	1,4-Dioxane	−6.67	−4.78	10
40	Hexane	1-Butanol	−6.67	−7.13	11
41	Hexane	1-Propanol	−6.67	−7.43	11
42	Hexane	2-Butanol	−6.67	−7.44	12
43	Methylcyclohexane	1,4-Dioxane	−6.41	−4.78	10
44	Methylcyclohexane	1-Butanol	−6.41	−7.13	11
45	Methylcyclohexane	1-Propanol	−6.41	−7.43	11
46	Methylcyclohexane	2-Butanol	−6.41	−7.44	12
47	Octane	1,4-Dioxane	−6.30	−4.78	10
48	Octane	1-Butanol	−6.30	−7.13	11
49	Octane	1-Propanol	−6.30	−7.43	11
50	Octane	2-Butanol	−6.30	−7.44	12
51	Toluene	2,2,4-Trimethyl pentane	−4.91	−6.84	15
52	Toluene	Cyclohexane	−4.91	−6.47	15
53	Toluene	Heptane	−4.91	−6.46	15
54	Toluene	Hexane	−4.91	−6.67	15
55	Toluene	Methylcyclohexane	−4.91	−6.41	15
56	Toluene	Octane	−4.91	−6.30	15

spectively and the model constants were calculated using least squares analysis.

The back-calculated B_i terms using Eqs. 9—11 and 12—14 along with experimental values of $\ln X_1$ and $\ln X_2$ were used to calculate the solubility of anthracene in binary solvent mixtures and MPD values were listed in Table 4. In this analysis, the required information for predicting solubility of anthracene in binary solvents is the numerical values of X_1 and X_2, *i.e.* two points for each binary solvent system. The overall MPDs (±S.D.) were 5.5±4.3 and 4.2±3.1%, respectively. The mean differences between two numerical methods is statistically significant (paired *t*-test, $p<0.0005$) and this means that using gas to solvent Abraham parameters, more accurate calculations could be achieved. This is in agreement with previous finding of Acree and Abraham[23] where the models have been used to calculate solubility of anthracene

Table 2. The Numerical Values of Coefficients of Abraham Model of Water to Solvent

No.	c_1	r_1	s_1	b_1	v_1	c_2	r_2	s_2	b_2	v_2
1	0.152	0.437	−1.175	−3.914	4.119	0.098	0.350	−0.083	−4.826	4.172
2	0.152	0.437	−1.175	−3.914	4.119	0.080	0.521	−1.294	−3.908	4.208
3	0.152	0.437	−1.175	−3.914	4.119	0.203	0.369	−0.954	−5.426	4.508
4	−0.034	0.490	−1.048	−4.229	4.219	0.098	0.350	−0.083	−4.826	4.172
5	−0.034	0.490	−1.048	−4.229	4.219	0.080	0.521	−1.294	−3.908	4.208
6	−0.034	0.490	−1.048	−4.229	4.219	0.203	0.369	−0.954	−5.426	4.508
7	0.148	0.436	−1.098	−3.893	4.036	0.098	0.350	−0.083	−4.826	4.172
8	0.148	0.436	−1.098	−3.893	4.036	0.080	0.521	−1.294	−3.908	4.208
9	0.148	0.436	−1.098	−3.893	4.036	0.203	0.369	−0.954	−5.426	4.508
10	0.288	0.382	−1.668	−5.000	4.461	0.098	0.350	−0.083	−4.826	4.172
11	0.288	0.382	−1.668	−5.000	4.461	0.152	0.437	−1.175	−3.914	4.119
12	0.288	0.382	−1.668	−5.000	4.461	0.148	0.436	−1.098	−3.893	4.036
13	0.288	0.382	−1.668	−5.000	4.461	0.106	0.272	−0.988	−3.805	4.110
14	0.106	0.272	−0.988	−3.805	4.110	0.098	0.350	−0.083	−4.826	4.172
15	0.106	0.272	−0.988	−3.805	4.110	0.080	0.521	−1.294	−3.908	4.208
16	0.106	0.272	−0.988	−3.805	4.110	0.203	0.369	−0.954	−5.426	4.508
17	0.177	0.335	−1.099	−3.570	3.990	0.098	0.350	−0.083	−4.826	4.172
18	0.177	0.335	−1.099	−3.570	3.990	0.080	0.521	−1.294	−3.908	4.208
19	0.177	0.335	−1.099	−3.570	3.990	0.203	0.369	−0.954	−5.426	4.508
20	0.063	0.320	−1.024	−3.824	4.067	0.098	0.350	−0.083	−4.826	4.172
21	0.063	0.320	−1.024	−3.824	4.067	0.080	0.521	−1.294	−3.908	4.208
22	0.063	0.320	−1.024	−3.824	4.067	0.203	0.369	−0.954	−5.426	4.508
23	0.142	0.464	−0.588	−4.625	4.491	0.246	0.782	−1.982	−4.293	4.528
24	0.142	0.464	−0.588	−4.625	4.491	0.223	0.642	−1.647	−5.067	4.526
25	0.159	0.784	−1.678	−4.929	4.577	0.098	0.350	−0.083	−4.826	4.172
26	0.159	0.784	−1.678	−4.929	4.577	0.152	0.437	−1.175	−3.914	4.119
27	0.159	0.784	−1.678	−4.929	4.577	0.148	0.436	−1.098	−3.893	4.036
28	0.159	0.784	−1.678	−4.929	4.577	0.106	0.272	−0.988	−3.805	4.110
29	0.203	0.369	−0.954	−5.426	4.508	0.288	0.382	−1.668	−5.000	4.461
30	0.203	0.369	−0.954	−5.426	4.508	0.159	0.784	−1.678	−4.929	4.577
31	0.203	0.369	−0.954	−5.426	4.508	0.325	0.670	−2.061	−4.733	4.543
32	0.203	0.369	−0.954	−5.426	4.508	0.361	0.579	−1.723	−4.764	4.344
33	0.203	0.369	−0.954	−5.426	4.508	0.246	0.782	−1.982	−4.293	4.528
34	0.203	0.369	−0.954	−5.426	4.508	0.223	0.642	−1.647	−5.067	4.526
35	0.325	0.670	−2.061	−4.733	4.543	0.098	0.350	−0.083	−4.826	4.172
36	0.325	0.670	−2.061	−4.733	4.543	0.152	0.437	−1.175	−3.914	4.119
37	0.325	0.670	−2.061	−4.733	4.543	0.148	0.436	−1.098	−3.893	4.036
38	0.325	0.670	−2.061	−4.733	4.543	0.106	0.272	−0.988	−3.805	4.110
39	0.361	0.579	−1.723	−4.764	4.344	0.098	0.350	−0.083	−4.826	4.172
40	0.361	0.579	−1.723	−4.764	4.344	0.152	0.437	−1.175	−3.914	4.119
41	0.361	0.579	−1.723	−4.764	4.344	0.148	0.436	−1.098	−3.893	4.036
42	0.361	0.579	−1.723	−4.764	4.344	0.106	0.272	−0.988	−3.805	4.110
43	0.246	0.782	−1.982	−4.293	4.528	0.098	0.350	−0.083	−4.826	4.172
44	0.246	0.782	−1.982	−4.293	4.528	0.152	0.437	−1.175	−3.914	4.119
45	0.246	0.782	−1.982	−4.293	4.528	0.148	0.436	−1.098	−3.893	4.036
46	0.246	0.782	−1.982	−4.293	4.528	0.106	0.272	−0.988	−3.805	4.110
47	0.223	0.642	−1.647	−5.067	4.526	0.098	0.350	−0.083	−4.826	4.172
48	0.223	0.642	−1.647	−5.067	4.526	0.152	0.437	−1.175	−3.914	4.119
49	0.223	0.642	−1.647	−5.067	4.526	0.148	0.436	−1.098	−3.893	4.036
50	0.223	0.642	−1.647	−5.067	4.526	0.106	0.272	−0.988	−3.805	4.110
51	0.143	0.527	−0.720	−4.824	4.545	0.288	0.382	−1.668	−5.000	4.461
52	0.143	0.527	−0.720	−4.824	4.545	0.159	0.784	−1.678	−4.929	4.577
53	0.143	0.527	−0.720	−4.824	4.545	0.325	0.670	−2.061	−4.733	4.543
54	0.143	0.527	−0.720	−4.824	4.545	0.361	0.579	−1.723	−4.764	4.344
55	0.143	0.527	−0.720	−4.824	4.545	0.246	0.782	−1.982	−4.293	4.528
56	0.143	0.527	−0.720	−4.824	4.545	0.223	0.642	−1.647	−5.067	4.526

in a number of organic solvents.

The same calculations were done using Eqs. 6—8 taken from a previous work and MPD values were reported in Table 4. The overall MPD (±S.D.) was 14.4±9.8 and it was significantly different from overall MPDs of the proposed methods (paired *t*-test, $p<0.0005$) revealing that the proposed methods provide more accurate results in comparison with the previous method.

As mentioned earlier, three above-mentioned methods require experimental values of X_1 and X_2 as known values. Using Eqs. 4 and 5, it is possible to replace these terms by calculated X_1 and X_2 values. The obtained MPDs using Eqs. 9—11 and 12—14 for computing B_i terms of Jouyban–Acree model and also X_1 and X_2 values derived from Eqs. 4 and 5 were 37.9±30.9 and 22.2±8.0%, respectively. The mean differences between two numerical methods were statistically

Table 3. The Numerical Values of Coefficients of Abraham Model of Gas to Solvent

No.	c_1	r_1	s_1	b_1	l_1	c_2	r_2	s_2	b_2	l_2
1	−0.039	−0.276	0.539	0.995	0.934	−0.034	−0.354	1.674	0.000	0.919
2	−0.039	−0.276	0.539	0.995	0.934	−0.042	−0.277	0.526	0.983	0.932
3	−0.039	−0.276	0.539	0.995	0.934	0.165	−0.421	0.760	−0.664	1.002
4	−0.119	−0.203	0.560	0.702	0.940	−0.034	−0.354	1.674	0.000	0.919
5	−0.119	−0.203	0.560	0.702	0.940	−0.042	−0.277	0.526	0.983	0.932
6	−0.119	−0.203	0.560	0.702	0.940	0.165	−0.421	0.760	−0.664	1.002
7	−0.028	−0.185	0.648	1.043	0.869	−0.034	−0.354	1.674	0.000	0.919
8	−0.028	−0.185	0.648	1.043	0.869	−0.042	−0.277	0.526	0.983	0.932
9	−0.028	−0.185	0.648	1.043	0.869	0.165	−0.421	0.760	−0.664	1.002
10	0.275	−0.244	0.000	0.000	0.972	−0.034	−0.354	1.674	0.000	0.919
11	0.275	−0.244	0.000	0.000	0.972	−0.039	−0.276	0.539	0.995	0.934
12	0.275	−0.244	0.000	0.000	0.972	−0.028	−0.185	0.648	1.043	0.869
13	0.275	−0.244	0.000	0.000	0.972	−0.013	−0.456	0.780	1.064	0.906
14	−0.013	−0.456	0.780	1.064	0.906	−0.034	−0.354	1.674	0.000	0.919
15	−0.013	−0.456	0.780	1.064	0.906	−0.042	−0.277	0.526	0.983	0.932
16	−0.013	−0.456	0.780	1.064	0.906	0.165	−0.421	0.760	−0.664	1.002
17	0.012	−0.407	0.670	1.283	0.895	−0.034	−0.354	1.674	0.000	0.919
18	0.012	−0.407	0.670	1.283	0.895	−0.042	−0.277	0.526	0.983	0.932
19	0.012	−0.407	0.670	1.283	0.895	0.165	−0.421	0.760	−0.664	1.002
20	−0.060	−0.335	0.702	1.040	0.893	−0.034	−0.354	1.674	0.000	0.919
21	−0.060	−0.335	0.702	1.040	0.893	−0.042	−0.277	0.526	0.983	0.932
22	−0.060	−0.335	0.702	1.040	0.893	0.165	−0.421	0.760	−0.664	1.002
23	0.107	−0.313	1.053	0.169	1.020	0.318	−0.215	0.000	0.000	1.012
24	0.107	−0.313	1.053	0.169	1.020	0.215	−0.049	0.000	0.000	0.967
25	0.163	−0.110	0.000	0.000	1.013	−0.034	−0.354	1.674	0.000	0.919
26	0.163	−0.110	0.000	0.000	1.013	−0.039	−0.276	0.539	0.995	0.934
27	0.163	−0.110	0.000	0.000	1.013	−0.028	−0.185	0.648	1.043	0.869
28	0.163	−0.110	0.000	0.000	1.013	−0.013	−0.456	0.780	1.064	0.906
29	0.165	−0.421	0.760	−0.664	1.002	0.275	−0.244	0.000	0.000	0.972
30	0.165	−0.421	0.760	−0.664	1.002	0.163	−0.110	0.000	0.000	1.013
31	0.165	−0.421	0.760	−0.664	1.002	0.275	−0.162	0.000	0.000	0.983
32	0.165	−0.421	0.760	−0.664	1.002	0.292	−0.169	0.000	0.000	0.979
33	0.165	−0.421	0.760	−0.664	1.002	0.318	−0.215	0.000	0.000	1.012
34	0.165	−0.421	0.760	−0.664	1.002	0.215	−0.049	0.000	0.000	0.967
35	0.275	−0.162	0.000	0.000	0.983	−0.034	−0.354	1.674	0.000	0.919
36	0.275	−0.162	0.000	0.000	0.983	−0.039	−0.276	0.539	0.995	0.934
37	0.275	−0.162	0.000	0.000	0.983	−0.028	−0.185	0.648	1.043	0.869
38	0.275	−0.162	0.000	0.000	0.983	−0.013	−0.456	0.780	1.064	0.906
39	0.292	−0.169	0.000	0.000	0.979	−0.034	−0.354	1.674	0.000	0.919
40	0.292	−0.169	0.000	0.000	0.979	−0.039	−0.276	0.539	0.995	0.934
41	0.292	−0.169	0.000	0.000	0.979	−0.028	−0.185	0.648	1.043	0.869
42	0.292	−0.169	0.000	0.000	0.979	−0.013	−0.456	0.780	1.064	0.906
43	0.318	−0.215	0.000	0.000	1.012	−0.034	−0.354	1.674	0.000	0.919
44	0.318	−0.215	0.000	0.000	1.012	−0.039	−0.276	0.539	0.995	0.934
45	0.318	−0.215	0.000	0.000	1.012	−0.028	−0.185	0.648	1.043	0.869
46	0.318	−0.215	0.000	0.000	1.012	−0.013	−0.456	0.780	1.064	0.906
47	0.215	−0.049	0.000	0.000	0.967	−0.034	−0.354	1.674	0.000	0.919
48	0.215	−0.049	0.000	0.000	0.967	−0.039	−0.276	0.539	0.995	0.934
49	0.215	−0.049	0.000	0.000	0.967	−0.028	−0.185	0.648	1.043	0.869
50	0.215	−0.049	0.000	0.000	0.967	−0.013	−0.456	0.780	1.064	0.906
51	0.121	−0.222	0.938	0.099	1.012	0.275	−0.244	0.000	0.000	0.972
52	0.121	−0.222	0.938	0.099	1.012	0.163	−0.110	0.000	0.000	1.013
53	0.121	−0.222	0.938	0.099	1.012	0.275	−0.162	0.000	0.000	0.983
54	0.121	−0.222	0.938	0.099	1.012	0.292	−0.169	0.000	0.000	0.979
55	0.121	−0.222	0.938	0.099	1.012	0.318	−0.215	0.000	0.000	1.012
56	0.121	−0.222	0.938	0.099	1.012	0.215	−0.049	0.000	0.000	0.967

significant (paired *t*-test, $p<0.0005$). These MPDs were similar to those reported in a previous paper[23)] for anthracene solubilities in select organic solvents.

As a general conclusion, the proposed QSPR methods provided accurate solubility predictions using X_1 and X_2 values and the MPD values were improved significantly from a previous method. The extended methods for predicting the solubility of anthracene in binary solvents without employing X_1 and X_2 values, provided reasonable accurate predictions and could be used in solubility estimation methods which are widely required in chemical/pharmaceutical industries.

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Table 4. Number of Data Points in Each Set (N), Numerical Values of B_i Terms Computed Using Experimental Solubility Data and Mean Percentage Deviation (MPD) for Different Numerical Analyses

					MPD values using:				
No.	N	B_0	B_1	B_2	Experimental X_1 and X_2 values and B_i terms computed using Eqs. 6—8	Experimental X_1 and X_2 values and B_i terms computed using Eqs. 9—11	Calculated X_1 and X_2 using Eqs. 4 and 5 and B_i terms computed using Eqs. 9—11	Experimental X_1 and X_2 values and B_i terms computed using Eqs. 12—14	Calculated X_1 and X_2 using Eqs. 4 and 5 and B_i terms computed using Eqs. 12—14
1	9	1.780	1.090	−0.261	14.4	5.3	17.7	1.8	9.8
2	9	0.055	0.033	−0.016	9.0	0.8	31.0	0.7	11.6
3	9	1.746	0.434	0.546	28.0	2.6	22.2	4.5	11.1
4	9	0.957	−0.034	0.227	11.0	3.1	15.4	3.6	19.1
5	9	0.257	0.000	0.040	0.5	1.5	24.5	3.2	25.3
6	9	0.700	−0.149	0.244	22.4	2.9	17.6	6.8	23.3
7	9	2.292	1.298	0.156	16.8	12.3	12.7	8.5	24.5
8	9	0.216	0.089	−0.104	12.6	0.6	33.4	1.8	19.6
9	9	2.211	0.884	0.702	29.4	3.8	20.2	1.1	22.4
10	8	1.483	−0.400	0.309	3.6	2.6	18.1	5.1	24.4
11	9	0.545	0.161	0.101	12.6	8.1	20.0	2.7	14.6
12	9	0.835	−0.082	0.227	5.6	5.4	22.0	2.5	22.0
13	9	1.010	−0.171	0.201	5.2	4.0	16.4	0.7	29.4
14	9	2.207	1.485	0.608	23.1	12.4	9.4	10.3	30.0
15	9	0.106	−0.054	−0.035	4.3	0.8	27.7	1.6	24.3
16	9	2.117	0.842	0.687	34.6	1.6	15.4	3.2	25.2
17	9	2.318	1.188	0.261	21.4	6.7	20.0	3.6	18.9
18	9	0.267	0.044	0.078	4.0	1.2	34.5	3.0	19.2
19	9	2.248	0.903	0.855	33.7	7.5	36.0	11.6	11.3
20	9	2.573	1.707	0.667	24.3	16.9	12.3	13.9	25.0
21	9	0.445	0.111	0.033	3.6	4.1	25.7	5.2	17.6
22	9	2.609	1.198	0.775	35.0	9.0	10.5	5.8	21.6
23	7	0.389	0.004	0.154	20.0	11.6	104.9	5.0	28.8
24	8	−0.129	−0.062	0.212	16.6	14.9	99.0	12.4	35.4
25	10	2.426	0.277	0.372	24.9	11.9	50.1	5.8	20.1
26	9	0.744	0.320	0.203	4.0	5.0	87.0	2.1	3.0
27	9	1.126	0.086	0.244	10.2	2.2	84.8	3.2	9.2
28	9	1.236	0.171	0.078	9.8	1.3	74.9	2.1	18.0
29	7	0.353	−0.022	−0.001	24.7	2.3	19.1	5.3	30.9
30	7	0.466	−0.184	0.008	11.4	1.8	77.4	0.8	18.8
31	7	0.223	−0.009	−0.020	17.2	12.0	13.5	5.7	26.3
32	7	0.346	−0.036	−0.084	19.4	4.2	7.6	3.7	26.5
33	7	0.351	−0.087	−0.050	13.9	16.8	62.4	4.0	21.9
34	7	0.144	0.017	−0.087	14.0	4.0	33.6	4.7	22.2
35	8	1.617	−0.363	0.256	10.9	7.4	14.0	6.7	22.1
36	9	0.723	0.005	0.200	2.9	4.6	16.8	0.4	13.5
37	9	1.103	−0.103	0.294	4.2	1.9	19.5	0.9	21.1
38	9	1.227	−0.313	0.001	3.4	0.7	11.8	3.2	28.3
39	12	1.939	−0.124	0.646	16.4	11.2	11.4	3.4	25.6
40	9	0.731	0.152	−0.091	4.9	1.5	13.3	1.5	12.5
41	9	0.982	−0.072	0.184	1.4	3.3	15.6	1.0	19.1
42	9	1.153	−0.087	0.034	1.4	5.7	11.5	2.6	26.9
43	10	2.062	0.103	0.505	19.2	1.0	39.8	2.9	21.7
44	9	0.855	0.294	0.207	2.7	3.3	39.3	2.7	10.1
45	9	1.229	0.048	0.218	8.9	5.2	39.8	1.5	16.9
46	9	1.361	−0.002	0.299	9.3	9.2	27.7	4.3	24.6
47	9	1.384	−0.488	0.412	10.0	2.6	31.2	4.3	16.7
48	9	0.891	−0.034	0.172	1.3	5.3	41.8	2.9	11.1
49	9	1.264	−0.286	0.304	8.1	2.8	41.4	3.6	19.3
50	9	1.370	−0.525	0.316	8.2	3.7	31.5	8.0	28.1
51	12	0.266	0.086	0.134	31.6	4.2	54.5	6.7	36.9
52	7	0.813	−0.143	−0.027	20.8	3.5	131.9	2.8	31.2
53	12	0.259	0.202	0.008	26.1	12.7	74.1	6.6	35.7
54	7	0.598	0.059	0.090	26.8	2.0	55.5	0.4	33.0
55	12	0.732	0.038	−0.007	26.9	6.7	113.4	2.5	28.3
56	12	0.047	0.215	0.006	20.9	10.1	111.9	10.1	46.6

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