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Original Article

Solubility Prediction of Anthracene in Non-Aqueous Solvent Mixtures Using Jouyban-Acree Model

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Abstract

A quanitative structure property relationship was proposed to calculate the binary interaction terms of the Jouyban-Acree model using solubility parameter, boiling point, vapour pressure and density of solvents. The applicability of the proposed method for reproducing solubility data of anthracene in binary solvents has been evaluated using 116 solubility data sets collected from the literature. The mean percentage deviation (MPD) of experimental and calculated solubilities has been computed as a measure of accuracy and the MPD of the proposed method was ~ 6 %. The accuracy of the method was compared with that of a previously reported method where the MPD was ~ 12 % and the mean differences between proposed and previous methods was statistically significant.

Keywords: Jouyban-Acree model; Modeling; Prediction; Solubility; Solvent mixtures.
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1. Introduction

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 potentials [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. 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]. We used anthracene data as model system as very large database have been provided by our group, however, the proposed method could be used for modeling solubility data of a drug in mixed solvents.

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Solubility data is one of the key information in chemical/pharmaceutical areas and it is usually determined in water and many organic solvents. Mixing solvents, cosolvency, is the main solubility enhancement method has been employed in practice. In addition to experimental solubility determinations, a number of equations have been proposed for mathematical representation of solubility data. Solubility of anthracene in non-aqueous mixed solvents has been extensively studied by Acree's group. The experimentally determined data has been correlated using the Jouyban-Acree model. The general form of the model is:

$$\ln X_m = f_1 \ln X_1 + f_2 \ln X_2 + f_1 f_2 \sum_{i=0}^{2} B_i (f_1 - f_2)^i \qquad (1)$$

where X is the mole fraction solubility of the solute, f denotes the volume 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 [3]. 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 [4-5]. It has also been shown that the model is applicable for modeling physicochemical properties other than solubility in solvent mixtures [6].

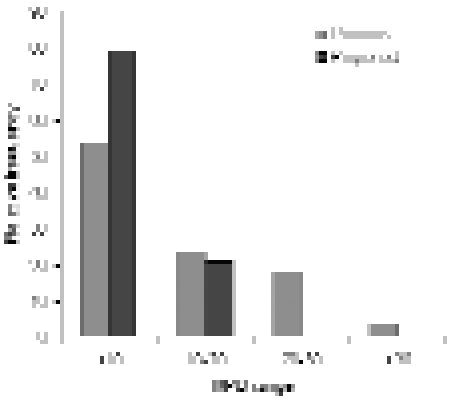

Figure 1. Relative frequency of mean percentage deviation (MPD) values for the previous and proposed methods.

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 [7]. The model has 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. To continue our previous efforts on solubility prediction methods, the aim of this work is to propose an extended form of QSPR models using a larger number of anthracene solubility data in binary solvents. Anthracene data was choosen 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.

2. 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 [7], 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:

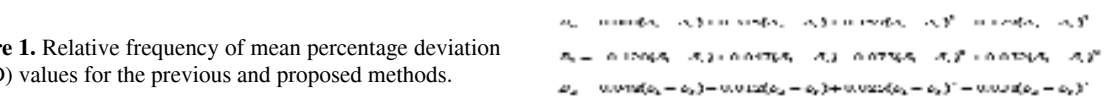

Table 1. List of solvents and the references of solubility data sets and their references.

No.	Solvent 1	Solvent 2	Reference
1	1-Butanol	1,4-Dioxane	[8]
2	1-Butanol	1-Pentanol	[9]
3	1-Butanol	2-Butoxyethanol	[10]
4	1-Butanol	2-Ethyl-1-hexanol	[9]
5	1-Butanol	2-Methoxyethanol	[11]
6	1-Butanol	2-Pentanol	[12]
7	1-Butanol	4-Methyl-2-pentanol	[12]
8	1-Butanol	Dibutyl ether	[13]
9	1-Octanol	1,4-Dioxane	[8]
10	1-Octanol	1-Pentanol	[9]
11	1-Octanol	2-Butoxyethanol	[10]
12	1-Octanol	2-Ethyl-1-hexanol	[9]
13	1-Octanol	2-Methoxyethanol	[11]
14	1-Octanol	2-Pentanol	[12]
15	1-Octanol	4-Methyl-2-pentanol	[12]
16	1-Octanol	Dibutyl ether	[13]
17	1-Pentanol	2-Butoxyethanol	[14]
18	1-Pentanol	2-Pentanol	[12]
19	1-Pentanol	4-Methyl-2-pentanol	[12]
20	1-Propanol	1,4-Dioxane	[8]
21	1-Propanol	1-Pentanol	[9]
22	1-Propanol	2-Ethyl-1-hexanol	[9]
23	1-Propanol	2-Methoxyethanol	[11]
24	1-Propanol	2-Pentanol	[12]
25	1-Propanol	4-Methyl-2-pentanol	[12]
26	1-Propanol	Dibutyl ether	[13]
27	2,2,4-Trimethylpentane	1-Butanol	[15]
28	2,2,4-Trimethylpentane	1-Propanol	[15]
29	2,2,4-Trimethylpentane	2-Butoxyethanol	[14]
30	2,2,4-Trimethylpentane	3-Methyl-1-butanol	[16]
31	2-2-4-Trimethylpentane	1,4-Dioxane	[17]
32	2-2-4-Trimethylpentane	2-Butanol	[18]
33	2-Butanol	1,4-Dioxane	[8]
34	2-Butanol	1-Pentanol	[9]
35	2-Butanol	2-Butoxyethanol	[10]
36	2-Butanol	2-Ethyl-1-hexanol	[9]
37	2-Butanol	2-Methoxyethanol	[11]
38	2-Butanol	2-Pentanol	[12]
39	2-Butanol	4-Methyl-2-pentanol	[12]
40	2-Butanol	Dibutyl ether	[13]
41	2-Butoxyethanol	2-Ethoxyethanol	[19]
42	2-Butoxyethanol	2-Methoxyethanol	[19]
43	2-Methyl-1-propanol	1-Pentanol	[9]
44	2-Methyl-1-butanol	1-Pentanol	[9]
45	2-methyl-1-propanol	1,4-Dioxane	[8]
46	2-Methyl-1-propanol	2-Butoxyethanol	[14]
47	2-Methyl-1-Propanol	2-Ethyl-1-hexanol	[9]
48	2-Methyl-1-propanol	2-Methoxyethanol	[11]
49	2-Methyl-1-propanol	2-Pentanol	[12]
50	2-Methyl-1-propanol	4-Methyl-2-pentanol	[12]
51	2-Methyl-1-propanol	Dibutyl ether	[13]
52	2-Propanol	1,4-Dioxane	[8]
53	2-Propanol	1-Pentanol	[9]
54	2-Propanol	2-Butoxyethanol	[10]
55	2-Propanol	2-Ethyl-1-hexanol	[9]
56	2-Propanol	2-Methoxyethanol	[11]
57	2-Propanol	2-Pentanol	[12]
58	2-Propanol	4-Methyl-2-pentanol	[12]

Table 1. continued

No.	Solvent 1	Solvent 2	Reference
59	2-Propanol	Dibutyl ether	[13]
60	3-Methyl-1-butanol	1,4-Dioxane	[8]
61	3-Methyl-1-butanol	2-Butoxyethanol	[10]
62	3-Methyl-1-butanol	2-Ethyl-1-hexanol	[9]
63	3-Methyl-1-butanol	2-Methoxyethanol	[11]
64	3-Methyl-1-butanol	2-Pentanol	[12]
65	3-Methyl-1-butanol	4-Methyl-2-pentanol	[12]
66	3-Methyl-1-butanol	Dibutyl ether	[13]
67	Benzene	Methylcyclohexane	[20]
68	Benzene	Octane	[20]
69	Cyclohexane	1,4-Dioxane	[17]
70	Cyclohexane	1-Butanol	[15]
71	Cyclohexane	1-Propanol	[15]
72	CycloHexane	2-Butanol	[18]
73	Cyclohexane	2-Butoxyethanol	[14]
74	Cyclohexane	3-Methyl-1-butanol	[16]
75	Dibutyl ether	2,2,4-Trimethylpentane	[21]
76	Dibutyl ether	Cyclohexane	[21]
77	Dibutyl ether	Heptane	[21]
78	Dibutyl ether	Hexane	[21]
79	Dibutyl ether	Methylcyclohexane	[21]
80	Dibutyl ether	Octane	[21]
81	Heptane	1-Butanol	[15]
82	Heptane	1-Propanol	[15]
83	Heptane	2-Butoxyethanol	[14]
84	Heptane	3-Methyl-1-butanol	[16]
85	Hexane	1,4-Dioxane	[17]
86	Hexane	1,4-Dioxane	[17]
87	Hexane	1-Butanol	[15]
88	Hexane	1-Propanol	[15]
89	Hexane	2-Butanol	[18]
90	Hexane	2-Butanol	[18]
91	Hexane	2-Butoxyethanol	[14]
92	Hexane	3-Methyl-1-butanol	[16]
93	Methylcyclohexane	1,4-Dioxane	[17]
94	Methylcyclohexane	1-Butanol	[15]
95	Methylcyclohexane	1-Propanol	[15]
96	Methylcyclohexane	2-Butanol	[18]
97	Methylcyclohexane	2-Butoxyethanol	[14]
98	Methylcyclohexane	3-Methyl-1-butanol	[16]
99	Octane	1,4-Dioxane	[17]
100	Octane	1-Butanol	[15]
101	Octane	1-Propanol	[15]
102	Octane	2-Butanol	[18]
103	Octane	2-Butoxyethanol	[14]
104	Octane	3-Methyl-1-butanol	[16]
105	p-Xylene	2,2,4-Trimethylpentane	[20]
106	p-Xylene	Cyclohexane	[20]
107	p-Xylene	Heptane	[20]
108	p-Xylene	Hexane	[20]
109	p-Xylene	Methylcyclohexane	[20]
110	p-Xylene	Octane	[20]
111	Toluene	2,2,4-Trimethylpentane	[22]
112	Toluene	Cyclohexane	[22]
113	Toluene	Heptane	[22]
114	Toluene	Hexane	[22]
115	Toluene	Methylcyclohexane	[22]
116	Toluene	Octane	[22]

Table 2. Solubility parameter (δ), boiling points (BP), vapour pressure (VP) and density (ρ) of solvents 1 and 2, number of experimental data points in each set (N), and mean percentage deviations (MPD) for the previous [7] and proposed methods.

No.[a]	δ_1 $(Cal/cm^3)^{1/2}$	δ_2 $(Cal/cm^3)^{1/2}$	BP_1 (°C)	BP_2 (°C)	VP_1 (torr)	VP_2 (torr)	ρ_1 (g/cm^3)	ρ_2 (g/cm^3)	N	MPD Previous method	MPD Proposed method
1	11.39	10.02	117.7	101.3	6.180	37.100	0.806	1.028	9	14.4	9.9
2	11.39	11.10	117.7	137.8	6.180	2.350	0.806	0.812	9	9.0	0.3
3	11.39	10.17	117.7	170.2	6.180	0.852	0.806	0.894	9	4.6	4.5
4	11.39	10.17	117.7	184.3	6.180	0.143	0.806	0.829	9	5.2	5.7
5	11.39	12.12	117.7	124.6	6.180	9.700	0.806	0.960	9	4.3	5.3
6	11.39	10.76	117.7	119.0	6.180	5.830	0.806	0.805	9	9.8	0.4
7	11.39	10.31	117.7	131.7	6.180	8.200	0.806	0.804	9	10.2	2.8
8	11.39	7.77	117.7	142.2	6.180	12.500	0.806	0.764	9	28.0	11.4
9	10.32	10.02	195.2	101.3	0.075	37.100	0.822	1.028	9	11.0	7.0
10	10.32	11.10	195.2	137.8	0.075	2.350	0.822	0.812	9	0.5	1.3
11	10.32	10.17	195.2	170.2	0.075	0.852	0.822	0.894	9	1.4	1.2
12	10.32	10.17	195.2	184.3	0.075	0.143	0.822	0.829	9	1.1	0.8
13	10.32	12.12	195.2	124.6	0.075	9.700	0.822	0.960	9	13.1	4.0
14	10.32	10.76	195.2	119.0	0.075	5.830	0.822	0.805	9	4.0	1.9
15	10.32	10.31	195.2	131.7	0.075	8.200	0.822	0.804	9	4.3	1.5
16	10.32	7.77	195.2	142.2	0.075	12.500	0.822	0.764	9	22.4	1.6
17	11.10	10.17	137.8	170.2	2.350	0.852	0.812	0.894	9	3.1	3.8
18	11.10	10.76	137.8	119.0	2.350	5.830	0.812	0.805	9	8.0	0.6
19	11.10	10.31	137.8	131.7	2.350	8.200	0.812	0.804	9	7.9	1.9
20	11.98	10.02	97.2	101.3	20.850	37.100	0.800	1.028	9	16.8	14.4
21	11.98	11.10	97.2	137.8	20.850	2.350	0.800	0.812	9	12.6	0.4
22	11.98	10.17	97.2	184.3	20.850	0.143	0.800	0.829	9	7.5	9.4
23	11.98	12.12	97.2	124.6	20.850	9.700	0.800	0.960	9	2.6	5.0
24	11.98	10.76	97.2	119.0	20.850	5.830	0.800	0.805	9	15.5	1.8
25	11.98	10.31	97.2	131.7	20.850	8.200	0.800	0.804	9	14.9	4.9
26	11.98	7.77	97.2	142.2	20.850	12.500	0.800	0.764	9	29.4	12.6
27	6.84	11.39	99.2	117.7	49.000	6.180	0.688	0.806	9	12.6	14.5
28	6.84	11.98	99.2	97.2	49.000	20.850	0.688	0.800	9	5.6	14.3
29	6.84	10.17	99.2	170.2	49.000	0.852	0.688	0.894	9	6.9	14.1
30	6.84	11.10	99.2	130.5	49.000	2.370	0.688	0.807	9	11.8	11.7
31	6.84	10.02	99.2	101.3	49.000	37.100	0.688	1.028	8	3.6	16.5
32	6.84	10.80	99.2	99.6	49.000	18.290	0.688	0.803	9	5.2	2.0
33	10.80	10.02	99.6	101.3	18.290	37.100	0.803	1.028	9	23.1	16.7
34	10.80	11.10	99.6	137.8	18.290	2.350	0.803	0.812	9	4.3	0.8
35	10.80	10.17	99.6	170.2	18.290	0.852	0.803	0.894	9	12.0	7.4
36	10.80	10.17	99.6	184.3	18.290	0.143	0.803	0.829	9	2.2	4.7
37	10.80	12.12	99.6	124.6	18.290	9.700	0.803	0.960	9	11.3	7.0
38	10.80	10.76	99.6	119.0	18.290	5.830	0.803	0.805	9	5.2	0.8
39	10.80	10.31	99.6	131.7	18.290	8.200	0.803	0.804	9	3.5	0.8
40	10.80	7.77	99.6	142.2	18.290	12.500	0.803	0.764	9	34.6	18.3
41	10.17	11.49	170.2	135.6	0.852	5.300	0.894	0.925	9	1.9	1.1
42	10.17	12.12	170.2	124.6	0.852	9.700	0.894	0.960	9	6.1	1.0
43	11.20	11.10	107.7	137.8	10.220	2.350	0.798	0.812	9	4.0	2.6
44	10.77	11.10	128.7	137.8	3.120	2.350	0.815	0.812	9	4.7	0.6
45	11.20	10.02	107.7	101.3	10.220	37.100	0.798	1.028	9	21.4	16.1
46	11.20	10.17	107.7	170.2	10.220	0.852	0.798	0.894	9	11.6	9.6
47	11.20	10.17	107.7	184.3	10.220	0.143	0.798	0.829	9	3.7	0.6
48	11.20	12.12	107.7	124.6	10.220	9.700	0.798	0.960	9	8.8	7.3
49	11.20	10.76	107.7	119.0	10.220	5.830	0.798	0.805	9	14.1	6.5
50	11.20	10.31	107.7	131.7	10.220	8.200	0.798	0.804	9	6.0	0.7
51	11.20	7.77	107.7	142.2	10.220	12.500	0.798	0.764	9	33.7	18.4
52	11.49	10.02	82.3	101.3	45.160	37.100	0.781	1.028	9	24.3	18.2
53	11.49	11.10	82.3	137.8	45.160	2.350	0.781	0.812	9	3.6	2.3
54	11.49	10.17	82.3	170.2	45.160	0.852	0.781	0.894	9	14.2	8.9

Tabel 2. continued

No.[a]	δ_1 (Cal/cm^3)$^{1/2}$	δ_2 (Cal/cm^3)$^{1/2}$	BP_1 (°C)	BP_2 (°C)	VP_1 (torr)	VP_2 (torr)	ρ_1 (g/cm^3)	ρ_2 (g/cm^3)	N	MPD Previous method	MPD Proposed method
55	11.49	10.17	82.3	184.3	45.160	0.143	0.781	0.829	9	4.6	5.4
56	11.49	12.12	82.3	124.6	45.160	9.700	0.781	0.960	9	8.9	7.3
57	11.49	10.76	82.3	119.0	45.160	5.830	0.781	0.805	9	6.5	1.7
58	11.49	10.31	82.3	131.7	45.160	8.200	0.781	0.804	9	7.1	2.4
59	11.49	7.77	82.3	142.2	45.160	12.500	0.781	0.764	9	35.0	18.8
60	11.10	10.02	130.5	101.3	2.370	37.100	0.807	1.028	9	17.1	11.0
61	11.10	10.17	130.5	170.2	2.370	0.852	0.807	0.894	9	5.2	6.0
62	11.10	10.17	130.5	184.3	2.370	0.143	0.807	0.829	9	2.4	1.5
63	11.10	12.12	130.5	124.6	2.370	9.700	0.807	0.960	9	6.6	5.2
64	11.10	10.76	130.5	119.0	2.370	5.830	0.807	0.805	9	7.4	0.3
65	11.10	10.31	130.5	131.7	2.370	8.200	0.807	0.804	9	5.9	0.2
66	11.10	7.77	130.5	142.2	2.370	12.500	0.807	0.764	9	29.6	12.8
67	9.19	7.82	80.1	100.9	95.200	46.000	0.874	0.765	7	20.0	1.7
68	9.19	7.58	80.1	125.7	95.200	14.000	0.874	0.699	8	16.6	12.3
69	8.21	10.02	80.7	101.3	98.000	37.100	0.774	1.028	10	24.9	15.8
70	8.21	11.39	80.7	117.7	98.000	6.180	0.774	0.806	9	4.0	3.0
71	8.21	11.98	80.7	97.2	98.000	20.850	0.774	0.800	9	10.2	5.2
72	8.21	10.80	80.7	99.6	98.000	18.290	0.774	0.803	9	9.8	12.1
73	8.21	10.17	80.7	170.2	98.000	0.852	0.774	0.894	9	10.7	3.5
74	8.21	11.10	80.7	130.5	98.000	2.370	0.774	0.807	9	3.6	3.3
75	7.77	6.84	142.2	99.2	12.500	49.000	0.764	0.688	7	24.7	1.1
76	7.77	8.21	142.2	80.7	12.500	98.000	0.764	0.774	7	11.4	5.0
77	7.77	7.38	142.2	98.4	12.500	45.700	0.764	0.680	7	17.2	0.9
78	7.77	7.28	142.2	68.7	12.500	151.300	0.764	0.655	7	19.4	3.0
79	7.77	7.82	142.2	100.9	12.500	46.000	0.764	0.765	7	13.9	3.3
80	7.77	7.58	142.2	125.7	12.500	14.000	0.764	0.699	7	14.0	0.5
81	7.38	11.39	98.4	117.7	45.700	6.180	0.680	0.806	9	2.9	7.7
82	7.38	11.98	98.4	97.2	45.700	20.850	0.680	0.800	9	4.2	5.7
83	7.38	10.17	98.4	170.2	45.700	0.852	0.680	0.894	9	3.0	11.6
84	7.38	11.10	98.4	130.5	45.700	2.370	0.680	0.807	9	2.6	5.9
85	7.28	10.02	68.7	101.3	151.300	37.100	0.655	1.028	12	16.4	7.8
86	7.38	10.02	98.4	101.3	45.700	37.100	0.680	1.028	8	10.9	13.0
87	7.28	11.39	68.7	117.7	151.300	6.180	0.655	0.806	9	4.9	4.9
88	7.28	11.98	68.7	97.2	151.300	20.850	0.655	0.800	9	1.4	4.2
89	7.38	10.80	98.4	99.6	45.700	18.290	0.680	0.803	9	3.4	3.7
90	7.28	10.80	68.7	99.6	151.300	18.290	0.655	0.803	9	1.4	5.9
91	7.28	10.17	68.7	170.2	151.300	0.852	0.655	0.894	9	5.2	8.1
92	7.28	11.10	68.7	130.5	151.300	2.370	0.655	0.807	9	3.5	2.4
93	7.82	10.02	100.9	101.3	46.000	37.100	0.765	1.028	10	19.2	8.9
94	7.82	11.39	100.9	117.7	46.000	6.180	0.765	0.806	9	2.7	1.1
95	7.82	11.98	100.9	97.2	46.000	20.850	0.765	0.800	9	8.9	1.9
96	7.82	10.80	100.9	99.6	46.000	18.290	0.765	0.803	9	9.3	10.6
97	7.82	10.17	100.9	170.2	46.000	0.852	0.765	0.894	9	6.5	2.6
98	7.82	11.10	100.9	130.5	46.000	2.370	0.765	0.807	9	2.1	1.7
99	7.58	10.02	125.7	101.3	14.000	37.100	0.699	1.028	9	10.0	10.8
100	7.58	11.39	125.7	117.7	14.000	6.180	0.699	0.806	9	1.3	3.0
101	7.58	11.98	125.7	97.2	14.000	20.850	0.699	0.800	9	8.1	2.7
102	7.58	10.80	125.7	99.6	14.000	18.290	0.699	0.803	9	8.2	7.2
103	7.58	10.17	125.7	170.2	14.000	0.852	0.699	0.894	9	2.3	6.2
104	7.58	11.10	125.7	130.5	14.000	2.370	0.699	0.807	9	2.1	1.2
105	8.85	6.84	138.4	99.2	8.700	49.000	0.857	0.688	7	29.0	6.3
106	8.85	8.21	138.4	80.7	8.700	98.000	0.857	0.774	7	23.4	11.9
107	8.85	7.38	138.4	98.4	8.700	45.700	0.857	0.680	7	23.4	6.6
108	8.85	7.28	138.4	68.7	8.700	151.300	0.857	0.655	7	29.5	3.3
109	8.85	7.82	138.4	100.9	8.700	46.000	0.857	0.765	7	22.4	5.3
110	8.85	7.58	138.4	125.7	8.700	14.000	0.857	0.699	7	21.0	3.5
111	8.90	6.84	110.6	99.2	28.500	49.000	0.862	0.688	12	31.6	9.2
112	8.90	8.21	110.6	80.7	28.500	98.000	0.862	0.774	7	20.8	9.9
113	8.90	7.38	110.6	98.4	28.500	45.700	0.862	0.680	12	26.1	8.3
114	8.90	7.28	110.6	68.7	28.500	151.300	0.862	0.655	7	26.8	0.3
115	8.90	7.82	110.6	100.9	28.500	46.000	0.862	0.765	12	26.9	8.2
116	8.90	7.58	110.6	125.7	28.500	14.000	0.862	0.699	12	20.9	9.5
										11.6±9.0	6.1±5.0

[a] Details of data sets are the same as in Table 1.

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 and the numerical values of the model constants calculated using experimental data of 30 data sets [7]. As a general rule, the more independent variables the more accurate the correlation and the more accurate the predictions. In this work, the experimentally obtained B_i values for 116 data sets of anthracene solubility in non-aqueous binary solvents, were regressed against $(\delta_1-\delta_2)^2$, $(BP_1-BP_2)^2$, $(VP_1-VP_2)^2$ and $(\rho_1-\rho_2)^2$ in which BP, VP and ρ are boiling point, vapour pressure and density of solvents, respectively and subscripts 1 and 2 denote solvents 1 and 2. The back-calculated Bi values, have been used to predict the solubility of anthracene and mean percentage deviation (MPD) have been computed using:

$$MPD(\%) = \frac{100}{N}\sum \frac{\left|(X_m)_{exp} - (X_m)_{calc}\right|}{(X_m)_{exp}}$$

Where N is the number of data points.

3. Results and discussion

The solubilities of anthracene in 116 different binary solvent mixtures (for details see Table 1) were used to compute Bi terms of each binary solvent and the Bi terms were employed to build up a quanitative structure property relationship (QSPR) model using physico-chemical properties of the solvents. Details of the physico-chemical properties were listed in Table 2. The obtained QSPR models for calculating Bi terms are:

$$B_1 = 0.0062(\delta_1-\delta_2)^2 + 0.000009(BP_1-BP_2)^2 - 0.0000269(VP_1-VP_2)^2 + 10.397(\rho_1-\rho_2)^2 \quad (5)$$

$$B_2 = 0.009(\delta_1-\delta_2)^2 + 0.000015(BP_1-BP_2)^2 - 0.000011(VP_1-VP_2)^2 + 3.338(\rho_1-\rho_2)^2 \quad (6)$$

$$B_3 = 0.018(\delta_1-\delta_2)^2 + 0.000039(BP_1-BP_2)^2 - 0.000081(VP_1-VP_2)^2 + 3.374(\rho_1-\rho_2)^2 \quad (7)$$

The back-calculated Bi terms were used to calculate the solubility of anthracene in binary solvent mixtures and MPD values were also listed in Table 2. The lowest and highest MPDs were 0.2 (for solubility of anthracene in 3-methyl-1-butanol + 4-methyl-2-pentanol) and 18.8 (for solubility of anthracene in 2-propanol + dibutyl ether) and the overall MPD (± SD) was 6.1±5.0. 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 systems. The same calculations were done using equations (2-4) taken from a previous work and MPD values were reported in Table 2. The lowest and highest MPDs were 0.5 (for solubility of anthracene in 1-octanol + 1-pentanol) and 35.0 (for solubility of anthracene in 2-propanol + dibutyl ether). The maximum MPD of previous and proposed methods belonged to the same data set. The overall MPD (±SD) was 11.6±9.0 and it was significantly different from the proposed method (paired t-test, $p<0.0005$) revealing that the proposed method provides more accurate results in comparison with previous method.

Figure 1 shows the relative frequency of MPD values sorted in four subgroups, i.e. <10, 10-20, 20-30 and >30 %. All MPD values of the proposed method in this work lied in < 20 % category while it was 78 % for the previous method.

As general conclusion, the proposed method is able to compute solubility of anthracene in mixed solvent systems using experimental data of the solute in mono-solvent systems and the expected prediction error is ~ 6 % which is acceptable error range for prediction purposes. The corresponding prediction error of the previous method is ~ 12 %. Employing BP, VP and ρ of the solvents along with δ values improved the predictability of the method by a factor of 2. This is expected since employing three more physico-chemical properties provides more information from the solvent-solvent interactions and resulted in more accurate predictions.

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