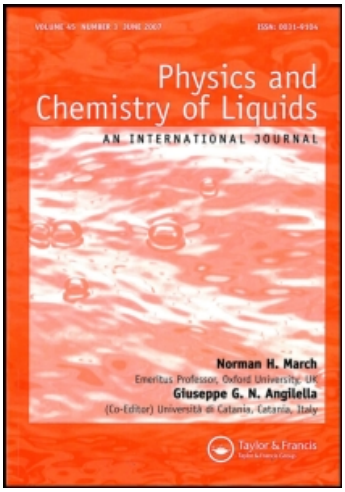

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ESTIMATION OF SOLUBILITY OF PARAFFINS IN WATER BY THE METHOD OF NEURAL NETS

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Water solubilities of paraffins have been estimated by the method of artificial neural nets. The method, using the normal boiling point and temperature as the input parameters could estimate the solubilities of 151 paraffins at the temperatures of 298 K and 372 K with an overall deviation of 3.4%, yielding superior results over those obtained by least squares.

Keywords: Paraffins; water solubilities; neural nets

INTRODUCTION

Solubility of a compound in water is the maximum amount dissolved in water at a specified temperature. Water solubility is one of the most important parameters influencing the fate and transport of chemicals in the environment. Thus, highly soluble chemicals tend to be readily biodegradable by micro organisms in soil, surface water and sewage treatment plants. The information on water solubility of hydrocarbons is also required in the design and operation of stripping processes and chemical spills.

In a recent publication Yaws *et al*, [1] have proposed the cubic equation for the calculation of the aqueous solubility (in wt ppm) of

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151 paraffins in terms of normal boiling point (T_b):

$$\log S = A + BT_b + CT_b^2 + DT_b^3 \tag{1}$$

They have reported different values of the coefficients $A, \ldots, D$ of Eqn (1) for different temperatures of study. This temperature-specific nature of the coefficients implies the lack of generality of the method. It is also found that Eqn (1), while representing the data well at 25°C, has shown large errors over the data set at 99.1°C. Hence, in the present work, we propose a generalized method to provide reasonable estimates of the aqueous solubilities of paraffins using normal boiling point and temperature as inputs.

THE METHOD

The basis of the present method of estimating water solubility of paraffins is the artificial neural net. The neural net architecture comprising of a three layered (input, hidden and output layers) perceptron is illustrated in Figure 1. The neurons constituting the network layers are capable of receiving and transmitting signals simulated by the sigmoid function.

$$y = \frac{1}{1 + e^{-x}} \tag{2}$$

where y and x denote the weighted input function and the input of the neuron respectively. A simulated neuron in given layer, hence, receives the signals from the neurons in the preceding layer and transmits the result to the neurons in the next layer. The weights assigned (e.g. W_{11}) to each of the interconnections are modified until the desired value of the output is attained. The input layer also includes a bias neuron, supplying an invariant output to the neurons in the hidden and output layers. The 'back propagation' procedure [2], where in the errors are propagated back in the learning mode with a simultaneous forward flowing information in the prediction mode is used in this work. The input and output nodes of Figure 1 correspond to the temperature, T, normal boiling point T_b and the solubility S, respectively.

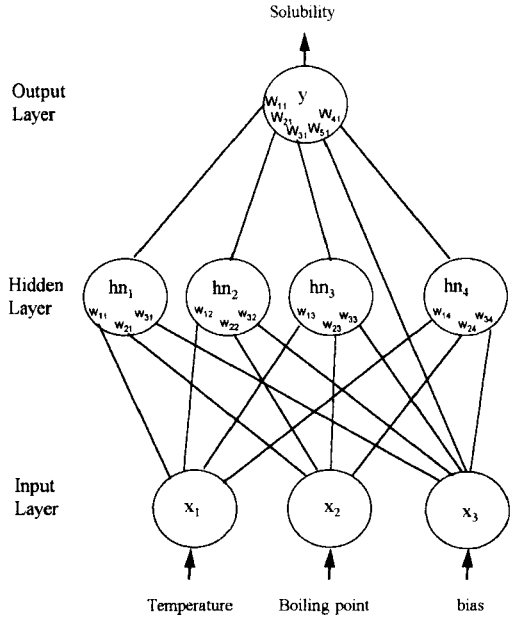

FIGURE 1 Neural Network Configuration for Water Solubility Model.

RESULTS AND DISCUSSION

The two input parameters, the temperature $T(K)$ and boiling Point $T_b(K)$ are normalized into the forms of the variables

$$x'_1 = \frac{T - 335.5}{37.56} \tag{3}$$

$$x'_2 = \frac{T_b - 417.11}{38.23} \tag{4}$$

for feeding into the network. The third variable x'_3 (representing the bias node) is set to unity. The numerical values given in the numerator and denominator of Eqns (3) and (4) are respectively the mean and standard deviations of temperature and boiling point data. The final

form of the network model considered for the prediction of the solubility, S (wt ppm) is given by

$$S = \exp\left[\frac{1}{0.65}\left\{\sum_{j=1}^{4} W_{j1}\left(\frac{1}{1+\exp\left(-\sum_{i=1}^{3} W_{ij}x_i'\right)}\right) + W_{51} - 0.01\right\}\right] \quad (5)$$

In Table I, the solubilities of the compounds studied at the temperatures of relevance and the % deviation (e) between the measured and calculated solubilities using the present neural net method and the method of Yaws *et al*, [1] based on Eqn (1) are reported. The Table also includes the normal boiling points $T_b(K)$ of the paraffins studied.

The coefficients $A,\ldots,D$ of the Eqn (1) used by Yaws *et al* [1] and the optimum values of the weights evolved for the present method are reported in Table II. A glance at Table II reveals that only a single set

TABLE I Representation of the solubility data by the methods of Yaws *et al* [1] and Neural nets

Compound	S_{298} ,wt *ppm*	*Tb* ,*k*	*% deviation (e)**		S_{372} ,wt *ppm*	*% deviation (e)**	
			Yaws et al	*Neural net*		*Yaws et al*	*Neural net*
Pentane	39.5	309.2	1.2	0.6	79.12	−21.4	2.2
i-Pentane	47.80	301.2	−3.8	−7.6	98.87	−23.5	2.1
Hexane	9.47	341.9	−10.3	−7.8	24.12	−6.6	−6.0
i-Hexane	13.00	333.4	−18.5	−15.6	31.56	−20.1	−10.9
3-Methyl pentane	17.91	336.4	24.8	26.6	34.29	3.3	8.5
2,2-Dimethyl butane	23.82	322.9	−0.2	1.8	50.72	−15.8	0.7
2,3-Dimethyl butane	19.10	331.2	11.3	13.4	40.00	−4.3	5.3
Heptane	2.24	371.6	0.1	0.6	7.18	23.3	−5.5
2-Methyl hexane	2.54	363.2	−39.6	−38.1	9.59	9.0	−13.3
3-Methyl hexane	2.64	365.0	−21.9	−20.7	9.29	14.7	−8.4
3-Ethyl pentane	2.95	366.6	0.20	1.0	9.23	21.4	−1.9
2,2-Dimethyl pentane	4.40	352.4	−41.8	−39.3	14.93	−2.8	−13.5
2,3-Dimethyl pentane	5.25	363.1	32.1	32.8	12.13	27.7	10.1
2,4-Dimethyl pentane	4.41	353.8	−31.7	−29.5	14.42	0.9	−11.1
3,3-Dimethyl pentane	5.92	359.2	25.9	26.9	17.67	38.9	27.3
2,2,3-Trimethyl butane	5.74	354.0	−0.2	1.5	15.61	9.4	−1.8
Octane	0.431	398.8	−8.5	−9.0	2.156	46.6	−1.9
2-Methyl heptane	0.747	390.8	0.0	−0.3	3.171	42.0	−0.5
3-Methyl heptane	0.792	392.1	12.5	12.2	3.120	45.4	3.9
4-Methyl heptane	0.742	390.9	−0.1	−0.4	3.156	42.1	−0.5
3-Ethyl hexane	0.709	391.7	0.0	−0.4	3.042	42.6	−0.5
2,2-Dimethyl hexane	1.394	380.0	0.0	−0.1	5.135	33.2	−1.6
2,3-Dimethyl hexane	0.841	388.8	0.1	−0.2	3.471	40.5	−0.7
2,4-Dimethyl hexane	1.187	382.8	−0.1	−0.1	4.535	35.6	−1.3
2,5-Dimethyl hexane	1.261	381.8	0.2	0.2	4.757	34.9	−1.1

TABLE I (Continued)

3,3-Dimethyl hexane	1.039	385.1	−0.2	−0.3	4.097	37.5	−1.4
3,4-Dimethyl hexane	0.703	391.9	−0.3	−0.1	3.025	43.0	−0.1
3-Ethyl-2-Methyl pentane	0.839	388.8	0.1	−0.3	3.469	40.4	−0.7
3-Ethyl-3-Methyl pentane	0.721	391.4	0.1	−0.5	3.083	42.4	−0.5
2,2,3-Trimethyl pentane	1.158	383.3	0.3	0.3	4.447	36.1	−1.0
2,2,4-Trimethyl pentane	2.221	372.4	3.6	4.1	7.276	27.6	−0.5
2,3,3-Trimethyl pentane	0.885	387.9	0.1	−0.2	3.614	39.8	−0.8
2,3,4-Trimethyl pentane	1.360	386.6	29.9	29.7	4.297	45.4	10.1
2,2,3,3-Tetramethyl butane	1.427	379.6	0	0.1	5.233	32.9	−1.5
Nonane	0.122	423.8	11.8	11.3	0.729	63.7	4.4
2-Methyl octane	0.168	416.2	0	−0.5	0.992	58.4	1.2
3-Methyl octane	0.157	417.4	0.2	−0.4	0.942	59.1	1.4
4-Methyl octane	0.115	415.6	−51.1	−51.9	0.894	52.2	−12.7
3-Ethyl heptane	0.168	416.2	0.2	−0.3	0.995	58.5	1.5
4-Ethyl heptane	0.187	414.4	0.2	−0.3	0.108	57.5	1.5
2,2-Dimethyl heptane	0.309	405.9	0.3	−0.2	1.596	52.6	1.2
2,3-Dimethyl heptane	0.195	413.7	0.3	−0.3	1.116	57.2	1.5
2,4-Dimethyl heptane	0.305	406.1	0.3	−0.2	1.583	52.7	1.3
2,5-Dimethyl heptane	0.254	409.2	0.2	−0.3	1.372	54.6	1.4
2,6-Dimethyl heptane	0.266	408.4	0.2	−0.4	1.424	54.1	1.4
3,3-Dimethyl heptane	0.239	410.2	0.2	−0.4	1.310	55.2	1.4
3,4-Dimethyl heptane	0.194	413.8	0.2	−0.3	1.110	57.2	1.4
3,5-Dimethyl heptane	0.254	409.2	0.2	−0.3	1.372	54.6	1.4
4,4-Dimethyl heptane	0.266	408.4	0.2	−0.3	1.424	54.1	1.4
3-Ethyl-2-Methyl hexane	0.226	411.2	0.2	−0.3	1.251	55.7	1.4
4-Ethyl-2-Methyl hexane	0.289	407.0	0.3	−0.3	1.519	53.3	1.4
3-Ethyl-3-Methyl hexane	0.194	413.8	0.2	−0.3	1.110	57.2	1.4
3-Ethyl-4-Methyl hexane	0.196	413.6	0.2	−0.3	1.120	57.2	1.4
2,2,3-Trimethyl hexane	0.293	406.8	0.3	−0.2	1.534	53.2	1.4
2,2,4-Trimethyl hexane	0.444	399.7	0.1	−0.4	2.115	48.4	0.4
2,2,5-Trimethyl hexane	0.540	397.2	4.9	4.4	2.409	47.5	1.8
2,3,3-Trimethyl hexane	0.230	410.8	−0.3	−0.8	1.269	55.3	1.0
2,3,4-Trimethyl hexane	0.212	412.2	0.0	−0.5	1.193	56.2	1.3
2,3,5-Trimethyl hexane	0.334	404.5	0.0	−0.5	1.699	51.6	0.9
2,4,4-Trimethyl hexane	0.348	403.8	−0.1	−0.6	1.755	51.2	0.9
3,3,4-Trimethyl hexane	0.195	413.6	−0.1	−0.6	1.117	57.0	1.2
3,3-Diethyl pentane	0.140	419.3	0.0	−0.5	0.861	60.0	1.1
3-Ethyl-2,2-Dimethyl pentane	0.289	407.0	0.0	−0.5	1.515	53.2	1.1
3-Ethyl-2,3-Dimethyl pentane	0.152	417.9	0.2	−0.3	0.921	59.4	1.5
3-Ethyl-2,4-Dimethyl pentane	0.244	409.9	0.3	−0.2	1.329	55.0	1.5
2,2,3,3-Tetramethyl pentane	0.197	413.4	−0.2	−0.8	1.127	56.8	1.1

TABLE I (Continued)

2,2,3,4-Tetramethyl pentane	0.303	406.2	0.1	−0.4	1.572	52.7	1.1
2,2,4,4-Tetramethyl pentane	0.570	395.4	−0.2	−0.7	2.567	45.3	−0.3
2,3,3,4-Tetramethyl pentane	0.183	414.7	−0.1	−0.6	1.062	57.6	1.1
Decane	0.052	446.9	43.8	45.4	0.298	75.9	17.3
2-Methyl nonane	0.0423	440.2	0.2	0.1	0.333	68.8	−1.9
3-Methyl nonane	0.0405	441.0	0.3	0.4	0.322	69.1	−1.8
4-Methyl nonane	0.0455	438.9	0.2	−0.1	0.353	68.4	−1.9
5-Methyl nonane	0.0471	438.3	0.3	0	0.363	68.2	−1.7
3-Ethyl octane	0.0435	439.7	0.2	0.0	0.341	68.7	−1.9
4-Ethyl octane	0.0511	436.8	0	−0.5	0.388	67.6	−1.8
2,2-Dimethyl octane	0.0749	430.1	0.2	−0.5	0.526	65.0	−0.4
2,3-Dimethyl octane	0.0492	437.5	0.2	−0.3	0.377	67.9	−1.6
2,4-Dimethyl octane	0.0794	429.1	0.3	−0.4	0.551	64.6	−0.2
2,5-Dimethyl octane	0.0684	431.7	0.3	−0.4	0.490	65.8	−0.6
2,6-Dimethyl octane	0.0614	433.5	−0.3	−0.9	0.449	66.3	−1.5
2,7-Dimethyl octane	0.0632	433.0	−0.3	−0.9	0.460	66.1	−1.2
3,3-Dimethyl octane	0.0586	434.4	0.2	−0.5	0.433	66.8	−1.2
3,4-Dimethyl octane	0.0518	436.6	0.3	−0.2	0.392	67.6	−1.7
3,5-Dimethyl octane	0.0650	432.6	0.3	−0.3	0.470	66.1	−0.9
3,6-Dimethyl octane	0.0600	434.0	0.3	−0.4	0.441	66.6	−1.1
4,4-Dimethyl octane	0.0724	430.7	0.2	−0.4	0.512	65.3	−0.5
4.5-Dimethyl octane	0.0556	435.3	0.0	−0.6	0.416	67.1	−1.4
4-Propyl heptane	0.0724	430.7	0.2	−0.4	0.512	65.3	−0.5
4-Isopropyl heptane	0.0668	432.1	0.2	−0.5	0.481	65.9	−0.6
3-Ethyl-2-Methyl heptane	0.0586	434.4	0.2	−0.4	0.433	66.8	−1.2
4-Ethyl-2-Methyl heptane	0.0780	429.4	0.2	−0.4	0.544	64.8	−0.2
5-Ethyl-2-Methyl heptane	0.0639	432.9	0.3	−0.3	0.464	66.2	−0.9
3-Ethyl-3-Methyl heptane	0.0506	437.0	0.2	−0.3	0.385	67.8	−1.6
4-Ethyl-3-Methyl heptane	0.0554	435.4	0.2	−0.4	0.414	67.2	−1.4
3Ethyl-5-Methyl heptane	0.0696	431.4	0.3	−0.4	0.497	65.6	−0.5
3-Ethyl-4-Methyl heptane	0.0530	436.2	0.3	−0.2	0.400	67.5	−1.5
4-Ethyl-4-Methyl heptane	0.0600	434.0	0.3	−0.4	0.441	66.6	−1.1
2,2,3-Trimethyl heptane	0.0720	430.8	0.2	−0.4	0.510	65.4	−0.4
2,2,4-Trimethyl heptane	0.1233	421.5	0.2	−0.3	0.780	61.2	1.1
2,2,5-Trimethyl heptane	0.1070	424.0	0.2	−0.3	0.696	62.4	0.9
2,2,6-Trimethyl heptane	0.1190	422.1	0.1	−0.4	0.758	61.5	0.9
2,3,3-Trimethyl heptane	0.0621	433.4	0.3	−0.3	0.453	66.4	−1.1
2,3,4-Trimethyl heptane	0.0631	433.1	0.2	−0.5	0.459	66.3	−1.0
2,3,5-Trimethyl heptane	0.0603	433.9	0.2	−0.4	0.443	66.6	−1.2

TABLE I (Continued)

2,3,6-Trimethyl heptane	0.0789	429.2	0.2	−0.4	0.549	64.7	−0.1
2,4,4-Trimethyl heptane	0.105	424.2	0.3	−0.3	0.689	62.5	0.7
2,4,5-Trimethyl heptane	0.0767	429.7	0.2	−0.4	0.537	64.9	−0.2
2,4,6-Trimethyl heptane	0.128	420.8	0.2	−0.3	0.805	60.0	1.1
2,5,5-Trimethyl heptane	0.0949	426.0	0.2	−0.4	0.634	63.3	0.4
3,3,4-Trimethyl heptane	0.0564	435.1	0.3	−0.3	0.419	67.0	−1.4
3,3,5-Trimethyl heptane	0.0803	428.9	0.2	−0.4	0.556	64.6	−0.1
3,4,4-Trimethyl heptane	0.0590	434.3	0.3	−0.3	0.435	66.7	−1.2
3,4,5-Trimethyl heptane	0.0545	435.7	0.3	−0.3	0.409	67.3	−1.4
3-Isopropyl-2-Methyl hexane	0.0430	439.9	0.1	0.0	0.338	68.7	−1.9
3,3-Diethyl hexane	0.0440	439.5	0.2	0.0	0.345	68.7	−1.7
3,4-Diethyl hexane	0.0503	437.1	0.1	−0.3	0.383	67.7	−1.8
3-Ethyl-2,2-Dimethyl hexane	0.0785	429.3	0.3	−0.3	0.546	64.7	−0.2
4-Ethyl-2,2-Dimethyl hexane	0.133	420.2	0.2	−0.3	0.829	60.6	1.3
3-Ethyl-2,3-Dimethyl hexane	0.0509	436.9	0.2	−0.3	0.387	67.7	−1.6
4-Ethyl-2,3-Dimethyl hexane	0.0596	434.1	0.1	−0.5	0.439	66.7	−1.1
3-Ethyl-2,4-Dimethyl hexane	0.0624	433.3	0.2	−0.4	0.455	66.3	−1.0
4-Ethyl-2,4-Dimethyl hexane	0.0590	434.3	0.3	−0.3	0.435	66.7	−1.2
3-Ethyl-2,5-Dimethyl hexane	0.0881	427.3	0.3	−0.3	0.598	63.9	0.2
4-Ethyl-3,3-Dimethyl hexane	0.0533	436.1	0.3	−0.3	0.401	67.4	−1.5
3-Ethyl-3,4-Dimethyl hexane	0.0557	435.3	0.2	−0.4	0.416	67.1	−1.4
2,2,3,3-Tetra methyl hexane	0.0616	433.5	0.0	−0.6	0.451	66.4	−1.1
2,2,3,4-Tetra methyl hexane	0.0672	432.0	0.2	−0.4	0.483	65.9	−0.7
2,2,3,5-Tetra methyl hexane	0.123	421.6	0.3	−0.3	0.776	61.2	1.0
2,2,4,4-Tetra methyl hexane	0.0896	427.0	0.2	−0.3	0.607	63.8	0.3
2,2,4,5-Tetra methyl hexane	0.126	421.0	0.2	−0.7	0.795	60.8	0.7
2,2,5,5-Tetra methyl hexane	0.233	410.6	−0.2	−0.7	1.281	55.2	1.0
2,3,3,4-Tetra methyl hexane	0.0484	437.8	0.2	−0.2	0.372	68.0	−1.7
2,3,3,5-Tetra methyl hexane	0.0933	426.3	0.2	−0.3	0.626	63.4	0.4

TABLE I (Continued)

2,3,4,4-Tetra methyl hexane	0.0573	434.8	0.2	−0.4	0.425	66.9	−1.3
2,3,4,5-Tetra methyl hexane	0.0780	429.4	0.2	−0.4	0.544	64.8	−0.2
3,3,4,4-Tetra methyl hexane	0.0358	443.2	0.1	0.9	0.291	69.8	−1.5
2,4-Dimethyl-3-Isopr pentane	0.0743	430.2	−0.1	−0.7	0.524	65.1	−0.5
3,3-Diethyl-2-Methyl pentane	0.0364	442.9	0.1	0.8	0.296	69.7	−1.5
3-Ethyl-223-Trimethyl pentane	0.0368	442.7	0.1	0.7	0.298	69.6	−1.6
3-Ethyl-224-Trimethyl pentane	0.0822	428.5	0.3	−0.3	0.567	64.4	0.1
3-Ethyl-234-Trimethyl pentane	0.0370	442.6	0.1	0.7	0.299	69.6	−1.8
22334-Penta methyl pentane	0.0446	439.2	−0.1	−0.3	0.348	68.4	−2.1
22344-Penta methyl pentane	0.0654	432.5	0.3	−0.3	0.472	66.0	−0.8
Undecane	0.0044	468.7	−117.0	−51.4	0.0752	68.8	3.6
Dodecane	0.0037	488.6	−7.6	14.6	0.0427	77.1	13.0
Tridecane	0.0020	507.8	−2.0	−3.6	0.0219	77.1	−0.7
Tetra decane	0.0022	526.1	40.3	27.6	0.0148	78.2	6.7
Penta decane	0.0011	543.6	3.0	−22.7	0.0082	67.9	−10.4
Hexa decane	0.0009	560.5	−21.7	−34.6	0.0056	51.6	−11.0
Hepta decane	0.0014	576.0	0.2	19.2	0.0049	30.0	8.3

* $e = \dfrac{100(S_{\text{expt}} - S_{\text{calc}})}{S_{\text{expt}}}$

of weights are used in the calculation of solubilities at different temperatures by the present method. On the other hand, Yaws *et al* [1] have used different values of the coefficient A of Eqn (1), while calculating the water solubilities at the temperatures of 298 K and 372 K. From this view point, the present neural net method could be considered generalized enough for being applicable to the temperatures ranging between 298 K and 372 K.

It could be seen from Table II that:

1) The solubility data at 298 K could be represented by both the methods with reasonable and comparable accuracies for the present and Yaws *et al* [1] methods respectively.
2) The accuracy of representation of the data at 372 K by the neural net method is far superior to that of Yaws *et al* ($\bar{e} = 3.4\%$ vs. 54.8%).

TABLE II Parameters/Weights and statistical measures of goodness of fit of Yaws *et al* model and ANN model

	Yaws et al model at		*ANN model*	
	298 K (*Equation* 1)	372 K (*Equation* 1)	(*Equation* 5)	
Parameters/ Weights	$A = -17.652$	$A = -17.261$	$w11 = 0.4989$	$W11 = -1.499$
	$B = 0.177811$	$B = 0.177811$	$w12 = 0.1471$	$W21 = -0.4353$
	$C = -500.907 \times 10^{-6}$	$C = -500.907 \times 10^{-6}$	$w13 = -1.638$	$W31 = -3.210$
	$D = 411.124 \times 10^{-9}$	$D = 411.124 \times 10^{-9}$	$w14 = -0.5085$	$W41 = 3.399$
			$w21 = 1.370$	$W51 = 0.6313$
			$w22 = 6.369$	
			$w23 = 0.6737$	
			$w24 = -0.8620$	
			$w31 = -0.3481$	
			$w32 = -6.825$	
			$w33 = -0.3544$	
			$w34 = -1.179$	
No. of points (np)	151	151	302	

TABLE II (Continued)

Data range:			
T, k	298	372	[298 – 372]
T_b, k	[309.2 – 576]	[309.2 – 576]	[309.2 – 576]
S, wt ppm	[0.0009 – 47.8]	[0.004 – 98.87]	[0.0009 – 98.87]
Coefficient of determination (R^2)	0.9909	0.9516	0.9954
Standard error (s)	0.56	2.68	0.69
Average absolute percentage deviation ($\bar{e}$)	4.3	54.8	3.4

$$R^2 = \frac{\sum S^2_{\text{calc}} - npS^2_{\text{avg}}}{\sum S^2_{\text{expt}} - npS^2_{\text{avg}}} \quad ; S_{\text{avg}} = \text{average of } S \text{ values}$$

$$s = \sqrt{\frac{\sum (S_{\text{expt}} - S_{\text{calc}})^2}{(np-1)}} \quad ; \bar{e} = \frac{\sum |e_i|}{np}$$

$$\sum = \sum_{i=1}^{np}$$

3) The single set of weights of the neural net (reported in Table II) used in the present analysis yielded an average absolute deviation of 3.4% over 302 data points. An analysis of the optimal weights evolved from the computations [3] revealed both the temperature (T) and the normal boiling point (T_b) contribute significantly to the total correlation.

CONCLUSION

The method of neural nets could be used for reasonably good representation of the water solubility data of hydrocarbons.

References

[1] Yaws, C. L., Xiang Pan and Xioyin Lin, (1993). *Chemical Engineering*, 108.
[2] Chitra, S. P. (1993). *Chemical Engineering Progress*, **89**, 44.
[3] Garson, G. D. (1991). *A.I. Expert*, **6**(4), 47.