Surface Tension Prediction of Hydrocarbon Mixtures Using Artificial Neural Network

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ABSTRACT

In this study, artificial neural network was used to predict the surface tension of 20 hydrocarbon mixtures. Experimental data was divided into two parts (70% for training and 30% for testing). Optimal configuration of the network was obtained with minimization of prediction error on testing data. The accuracy of our proposed model was compared with four well-known empirical equations. The artificial neural network was more accurate as the result showed that while standard deviation of ARD for artificial neural network was 3.63001, the standard deviation of ARD for Brock and Bird, Pitzer, Zuo-Stenby and Sastri-Rao models were 23.77569, 18.44848, 13.00388 and 9.63137 respectively.

1. Introduction

Surface tension is a characteristic property of fluids as scientific and technological researches on many areas need data on surface tension of the materials, such as chemical engineering, materials engineering, oil recovery, environmental protection, etc [1,2]. The surface tension of pure liquids and of liquid mixtures is often required in calculations such as those involving flow through porous media or boiling heat transfer.

In addition to experimental measurements, numerous theoretical researches have been carried out on the surface tension modeling [3-5]. Some of the presented models have a very strong theoretical basis such as those that are based on statistical mechanical theories of liquids and density functional theory [2,6]. Also corresponding state principles have been employed to predict the surface tension of pure materials [7-10]. The experimental data of surface tension for non-polar liquids have been correlated by utilizing the Riedel parameter at the critical point [7]. The critical temperature, pressure and acentric factor have been used as correlation parameters for determining the surface tension [9].

Two-reference corresponding states methods were initially proposed by Rice and Teja [11] in which critical temperature and volume were used to obtain a correlation. Later, Zuo and Stenby employed the same method for calculating surface tensions where critical pressure and temperature were considered as correlation parameters [12]. These equations have not presented satisfactory results for chemical compounds with strong hydrogen-bonding forces. To overcome these hurdles, Sastri and Rao introduced a correlation based on critical pressure and temperature, normal boiling point temperature, reduced temperature and reduced boiling temperature [13]. Although these equations are usually much simpler, their dependency on experimental data for each component limits their application to the cases for which some experimental data exist. These methods usually fail to give accurate predictions for other situations. The surface tension of a liquid mixture is not a simple function of the surface tensions of the pure components. In general, there are several approaches for estimating the surface tension of mixtures (i) based on empirical or semiempirical relations suggested first for pure fluids and (ii) based on statistical mechanical grounds. It is impractical to measure the surface tension for all liquids and liquid mixtures of interest and a method for the prediction of surface tension is therefore of practical importance [11,14,15].

Because of nonlinear nature of surface tension, artificial neural network method may be considered as an alternative tool for the prediction of surface tension. Gharagheizi, et al. applied an artificial neural network-group contribution method to predict the surface tension of pure chemical compounds [16]. Kumar, et al. effectively used parachor, density and refractive indices as input parameters required in the neural network for the prediction of surface tension of various polar and non-polar compounds [17]. Strechan, et al. used artificial neural network for correlations of the surface tension of molecular liquids [10]. Furthermore, artificial neural network has been applied for surface tension prediction of pure liquid metals [18]. To the authors' best knowledge, there has been no study on the application of artificial neural network for the surface tension prediction of hydrocarbon mixtures.

In this study, a feed-forward artificial neural network with Levenberg–Marquardt training algorithm was applied in order to investigate its capability in prediction of the surface tension of 20 hydrocarbon mixtures. The proposed ANN model results were compared with four well-known classical models.

2. Research Method
2.1. Classical models

Numbers of correlations based on the law of corresponding states have been developed for the prediction of surface tension (σ) which relate surface tension to the absolute temperature (T). Brock and Bird [7] proposed Eq. 1 for non-polar liquids.

$$\frac{\sigma}{P_c^{2/3} T_c^{1/3}} = (0.132\alpha_c - 0.279)(1 - T_r)^{11/9} \tag{1}$$

where σ is the surface tension (dyn/cm) and α_c is the Riedel parameter [19] at the critical point and is defined through Eq. 2.

$$\alpha_c = 0.9076\left[1 + \frac{T_{br}\ln(P_c/1.01325)}{1 - T_{br}}\right] \tag{2}$$

where T is the absolute temperature (K), P is pressure (bar) and subscripts c, r and b denote the critical, reduced and boiling values respectively.

Pitzer [20] presented a corresponding state relation for surface tension in terms of critical pressure (P_c), critical temperature (T_c) and acentric factor (ω) as shown in Eq. 3.

$$\sigma = P_c^{2/3} T_c^{1/3} \frac{1.86 + 1.18\omega}{19.05}\left[\frac{3.75 + 0.91\omega}{0.291 - 0.08\omega}\right]^{2/3}(1 - T_r)^{11/9} \tag{3}$$

Zuo and Stenby [12] used a two-reference fluid corresponding state to estimate the surface tensions as was shown in Eq. 4.

$$\sigma_r = \ln\left(1 + \frac{\sigma}{P_c^{2/3} T_c^{1/3}}\right) \tag{4}$$

In this method, the surface tension for the fluid of interest is related to the surface tension of two reference fluids, methane (1) and n-Octane (2) by Eq. 5.

$$\sigma_r = \sigma_r^{(1)} + \frac{\omega - \omega^{(1)}}{\omega^{(2)} - \omega^{(1)}}\left(\sigma_r^{(2)} - \sigma_r^{(1)}\right) \tag{5}$$

where the surface tension of methane is calculated by Eq. 6.

$$\sigma^{(1)} = 40.520(1 - T_r)^{1.287} \tag{6}$$

and the surface tension of n-octane is calculated by Eq. 7.

$$\sigma^{(2)} = 50.095(1 - T_r)^{1.21548} \tag{7}$$

Even though the three above-mentioned corresponding-states methods are satisfactory for the non-polar liquids, they are not suitable for compounds that exhibit strong hydrogen-bonding (e.g. alcohols, acids). To deal with these types of compounds, Sastri and Rao [13] modified the equations as presented in Eq. 8.

$$\sigma = K P_c^x T_b^y T_c^z \left[\frac{1 - T_r}{1 - T_{br}}\right]^m \tag{8}$$

where the values for the constants are presented in Table 1.

Table 1. Values for the constants of Eq. 8.

	K	X	Y	Z	m
Alcohols	2.28	0.25	0.175	0	0.8
Acids	0.125	0.50	-1.5	1.85	1.22
All others	0.158	0.50	-1.5	1.85	1.22

2.2. Artificial neural network (ANN)

Neural networks are composed of simple elements operating in parallel. These elements are inspired by biological nervous systems. As in nature, the network function is determined largely by the connections between elements. One can train a neural network to perform a particular function by adjusting the values of the connections (weights) between elements. Commonly, neural networks are adjusted or trained, so that a particular input leads to a specific target output.

In an ANN, a neuron sums the weighted inputs from several connections and then outputs of neurons are produced by applying transfer function to the sum. There are many transfer functions but the most common one is sigmoid which is used in this study as presented in Eq. 9.

$$\theta_j = \frac{1}{1+e^{-\Psi_j}} \tag{9}$$

where θ_j is the sum of weighted inputs to each neuron and Ψ_j is the output of each neuron which is calculated through Eq. 10.

$$\Psi_j = \left(\sum_{i=1}^{n} w_{ij}.\theta_i\right) + b_j \tag{10}$$

where w_{ij} denotes connection between node *j* of interlayer l to node *i* of interlayer l-1, b_j is a bias term and *n* is the number of neuron in each layer. In any interlayer l and neuron j input values integrate and generate Ψ_j.

In order to minimize the difference between experimental data and the data calculated by neural network, the afore-mentioned process repeats for the total number of training data. After training, validation of neural network can be done by testing the data.

Numerous types of the artificial neural networks exist such as multi-layer perceptron (MLP), radial basis function (RBF) networks and recurrent neural networks (RNN) where the former was used in this study. Multi-layer perceptron networks are one of the most popular and successful neural network architectures which are suited to a wide variety of applications such as the prediction and process modeling [21-23].

2.3. Preparation of dataset

578 datasets for surface tension of 20 hydrocarbon mixtures at different temperature and composition were collected [24] in addition to the critical temperature, critical pressure, critical volume, acentric factor, normal boiling point, molecular weight and ideal liquid density for pure components which were

considered as the input for the ANN. Table 2 shows the list of hydrocarbon mixtures, the number of data point for each mixture and the temperature range. Furthermore, Table 3 shows the values of the physical properties of pure hydrocarbons. In this study, the data sets were divided into three parts: training subset (60% of all data), validation subset (10% of all data) and testing subset (30% of all data). To avoid larger number from overriding smaller number, all data is normalized between [0.1-0.9] using Eq. 11.

$$(Scaled)_{value} = \frac{(Actual)_{value} - \min_{(\text{Actual value})}}{\max_{(\text{Actual value})} - \min_{(\text{Actual value})}} \times 0.8 + 0.1 \tag{11}$$

Table 2. The list of experimental data used in this study [24].

Temperature (K)	Number of data point	Mixtures
288-308	47	Tetrachloromethane - Iodomethane
303-317	33	Tetrachloromethane - Nitromethane
308	12	Tetrachloromethane - Methanol
298-317	44	Tetrachloromethane - Acetonitrile
298-322	33	Tetrachloromethane - Iodo-ethane
303-317	33	Tetrachloromethane - Nitroethane
293-345	18	Tetrachloromethane - Ethanol
303-322	24	Tetrachloromethane - Dimethylsulfoxide
287-349	34	Formic acid - Acetic acid
287-298	27	Formic acid - Pyridine
298	8	Formic acid - 2-methyl-aniline
293-313	33	Iodomethane - Acetic acid
293	11	Nitromethane - Acetic acid
293-303	26	Nitromethane - Benzene
293	6	Nitromethane - Cyclohexane
258-338	46	Methane - Propane
308	11	Methanol - Acetic acid
293-333	50	Methanol - Ethanol
293-323	55	Methanol - Dimethylsulfoxide
273-303	27	Methanol - Benzene

Table 3. Physical properties of pure hydrocarbons used in this study.

Ideal liquid density (kg/m^3)	Molecular weight	Normal boiling point (°C)	Acentric Factor	Critical volume ($m^3/kgmol$)	Critical pressure (bar)	Critical Temperature (°C)	Hydrocarbons
1601	153.8	76.75	0.193	0.2759	45.6	283.3	Tetrachloromethane
1138	61.04	101.1	0.31	0.1732	63.1	313.9	Nitromethane
795.7	32.04	64.65	0.557	0.1270	73.76	239.4	Methanol
782	41.05	81.65	0.327	0.1729	48.2	272.4	Acetonitrile
1961	156	72.45	0.1563	0.2705	47	278.9	Iodo-ethane
1052	75.07	114.8	0.3684	0.2295	51.16	321.8	Nitroethane
796	46.07	78.25	0.6444	0.1671	61.47	240.8	Ethanol
1105	78.14	189.0	0.2806	0.227	56.5	455.9	Dimethylsulfoxide
1225	46.03	100.6	0.3525	0.112	55	296.9	Formic acid
988.8	79.10	115.2	0.243	0.254	56.2	346.9	Pyridine
1002	107.2	200.4	0.438	0.35	37.5	420.9	2- methyl-aniline
2293	141.9	42.55	0.1446	0.1842	65.9	251.9	Iodomethane
1052	60.05	118.0	0.447	0.1710	57.7	319.6	Acetic acid
882.2	78.11	80.09	0.215	0.26	49.24	288.9	Benzene
781.8	84.16	80.73	0.2133	0.308	40.53	280.1	Cyclohexane
299.4	16.04	-161.5	0.0115	0.099	46.41	-82.45	Methane
506.7	44.10	-42.1	0.1524	0.2	42.57	96.75	Propane

2.4. ANN modeling

Programming, validation, training and testing of the ANN model were carried out by MATLAB 7.7.0. To determine the optimized values of weights and biases, the following steps were done:

1. Data sets were divided into three parts, training subset (60% of all data), validation subset (10% of all data) and testing subset (30% of all data).
2. Data was normalized using Eq. 11.

3. The number of neurons in hidden layer was optimized.

3. Results and Analysis

Three layers feeding forward neural network were used for surface tension prediction of 20 hydrocarbon mixtures and all parameters of neural network were determined by trial and error procedure. According to the experimental data and for a fair comparison with the classical models, temperature (T), composition (x), critical temperature (T_c), critical pressure (P_c), critical volume (V_c), acentric factor (ω), normal boiling point (T_b), molecular weight (M) and ideal liquid density (ρ) of mixtures were used as inputs to our proposed neural network.

The physical properties of hydrocarbon mixture were related to the physical properties of pure components, using mixing rules as were shown in Eqs. 12-13 for mixture critical temperature (T_{cm}) and mixture critical pressure (P_{cm}) respectively.

$$T_{c_m} = \sum_i \sum_j \left[x_i x_j \left(\frac{T_{cij}^{\ 2}}{P_{cij}} \right) \right] / \sum_i \sum_j \left[x_i x_j \left(\frac{T_{cij}}{P_{cij}} \right) \right] \tag{12}$$

$$P_{c_m} = \sum_i \sum_j \left[x_i x_j \left(\frac{T_{cij}^{\ 2}}{P_{cij}} \right) \right] / \left\{ \sum_i \sum_j \left[x_i x_j \left(\frac{T_{cij}}{P_{cij}} \right) \right] \right\}^2 \tag{13}$$

where x_i and x_j are the composition of component i and j in the mixture. Binary critical temperature (T_{cij}) and binary critical pressure (P_{cij}) were obtained through Eqs. 14-15, respectively.

$$T_{c_{ij}} = \sqrt{T_{c_i} T_{c_j}} \tag{14}$$

$$P_{c_{ij}} = 8T_{c_{ij}} / \left[\left(T_{c_{ii}} / P_{c_{ii}} \right)^{\frac{1}{3}} + \left(T_{c_{jj}} / P_{c_{jj}} \right)^{\frac{1}{3}} \right]^3 \tag{15}$$

Furthermore, mixture normal boiling point (T_{bm}), mixture critical volume (V_{cm}), mixture acentric factor (ω_m), mixture molecular weight (M_m) and mixture ideal liquid density (ρ_m) were calculated using Eqs. 16-20, respectively.

$$T_{b_m} = \sum_i \sum_j \left[x_i x_j \left(\frac{T_{b_{ij}}^{\ 2}}{P_{c_{ij}}} \right) \right] / \sum_i \sum_j \left[x_i x_j \left(\frac{T_{b_{ij}}}{P_{c_{ij}}} \right) \right] \tag{16}$$

$$V_{c_m} = \sum_i x_i V_{c_i} \tag{17}$$

$$\omega_m = \sum_i x_i \omega_i \tag{18}$$

$$M_m = \sum_i x_i M_i \tag{19}$$

$$1/\rho_m = \sum_i x_i / \rho_i \tag{20}$$

where subscripts *m* and *i* denote the mixture and pure value of each physical property, respectively.

Sigmoid function was used as transfer function in hidden layers and purelin function was used as the transfer function of output layers. Also Levenberg-Marquardt back propagation learning algorithm was used for training. Usually one hidden layer is enough but the numbers of neurons in hidden layers need to be optimized for each problem. In order to optimize the number of neurons in hidden layers, average relative deviation (ARD), (calculated through Eq. 21) of testing data versus the neuron number in hidden layers is plotted, as was shown in Fig. 1. The Results showed that 9-5-1 is the best topology of the neural network (Fig. 2). The cross plot graph which shows the results of training and testing calculations are presented in Fig. 3.

$$ARD = \frac{100}{N} \times \sum_{i=1}^{N} \left| \frac{y^{\exp} - y^{cal}}{y^{\exp}} \right| \tag{21}$$

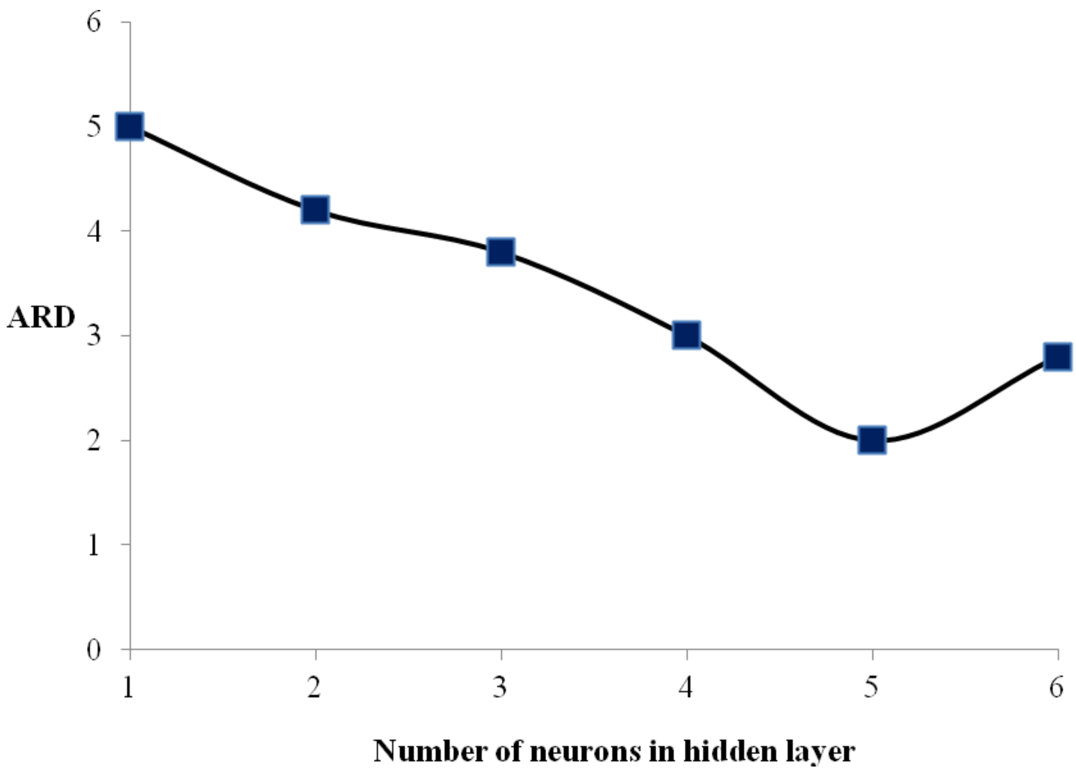

Figure 1. ARD of testing data versus neuron number in hidden layer.

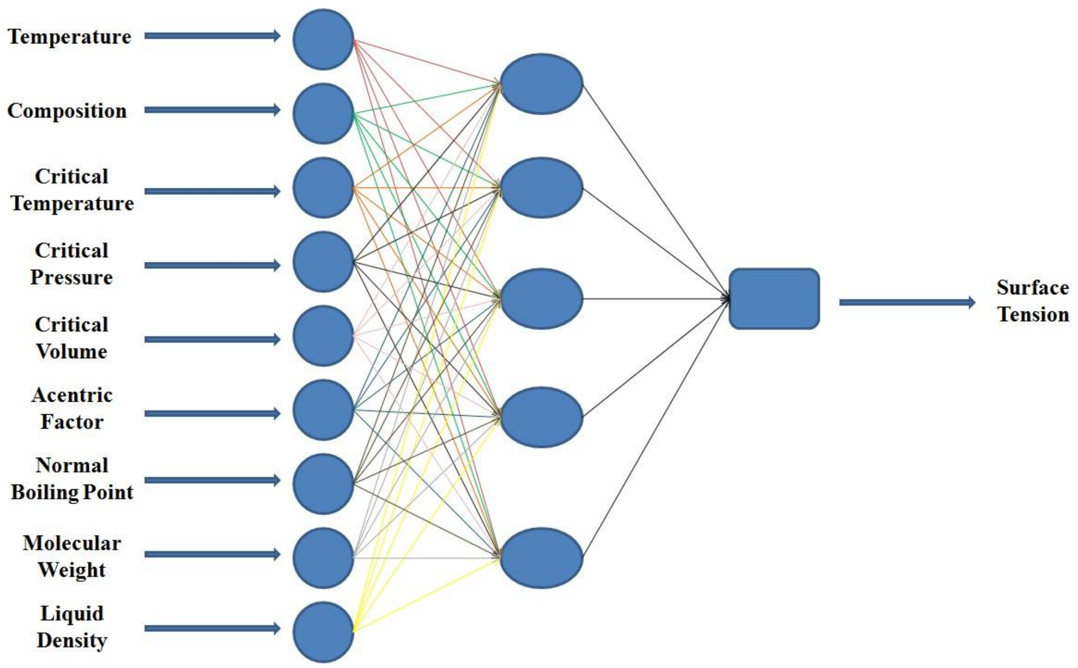

Figure 2. Topology of the proposed neural network.

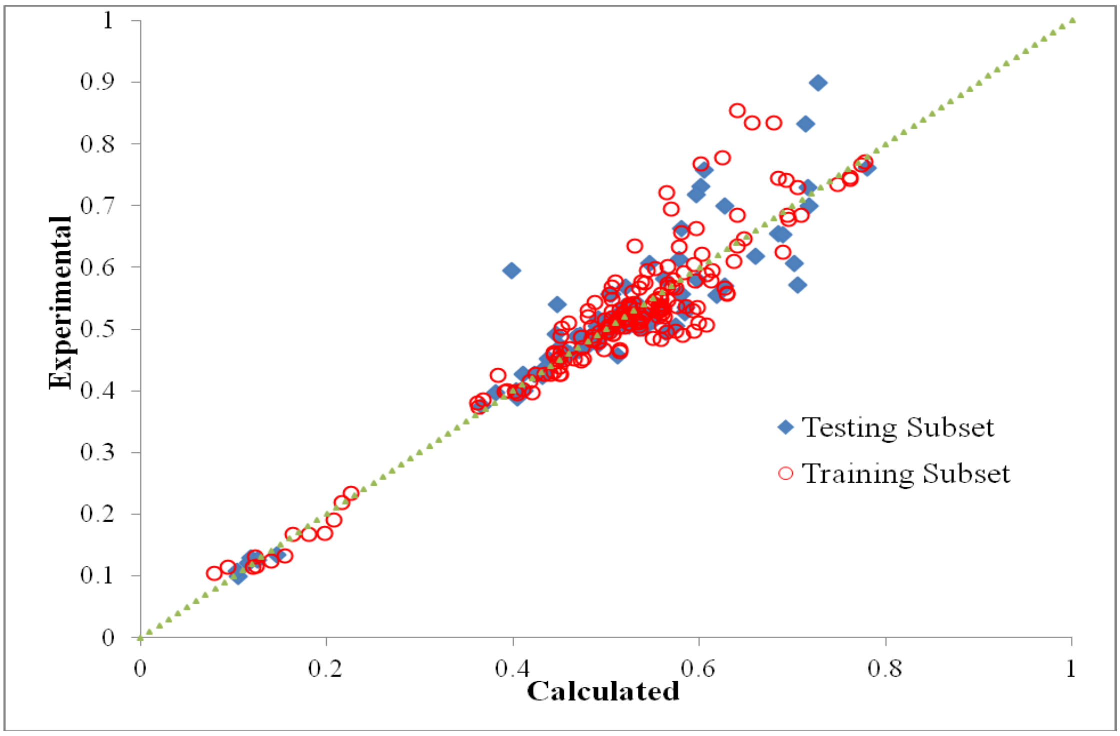

Figure 3. Cross plot graph of the results of training and testing calculations.

Surface tension of each hydrocarbon mixtures was further calculated by four aforementioned classical models: Brock and Bird (Eq. 1), Pitzer (Eq. 3), Zuo-Stenby (Eq. 4) and Sastri-Rao (Eq. 8). The mixing rules used in these four models were the same as the mixing rules used in artificial neural network method.

The accuracy of artificial neural network and four well-known classical models were tabulated in Table 4. They indicate that ARD of artificial neural network is 3.72223% while the ARD of Brock and Bird, Pitzer, Zuo-Stenby and Sastri-Rao models are 28.56102, 25.23901, 25.49967 and 13.58419 respectively.

Table 4. Accuracy of artificial neural network and four well-known classical models.

ANN	**Sastri –Rao [13]**	**Zuo –Stenby [12]**	**Pitzer [20]**	**Brock –Bird [7]**	**Compound**
2.1173	3.538	17.3285	2.0888	2.7273	Tetrachloromethane - iodomethane
2.356	3.4726	19.9798	11.684	10.1782	Tetrachloromethane - nitromethane
2.387	15.6244	50.631	50.483	41.3494	Tetrachloromethane - methanol
9.9893	4.1368	16.5798	4.2103	1.8799	Tetrachloromethane - acetonitrile
1.9742	11.7174	13.0284	10.245	13.3881	Tetrachloromethane - iodo-ethane
1.3618	1.5743	13.6943	10.539	7.4096	Tetrachloromethane - nitroethane
0.9921	7.6215	37.6013	34.576	27.1397	Tetrachloromethane - ethanol
8.077	8.1284	15.0959	17.434	13.8216	Tetrachloromethane - dimethylsulfoxide
1.2466	12.9732	15.0238	30.346	28.1053	formic acid - acetic acid
8.8339	22.2164	19.3833	11.228	12.8345	formic acid - pyridine
0.0213	16.7077	26.2993	3.8937	5.4993	formic acid - 2-methyl-aniline
4.549	15.3109	36.8824	36.558	33.716	Iodomethane - acetic acid
1.2423	9.3977	19.3669	34.451	32.0827	Nitromethane - acetic acid
7.4623	20.7877	10.7804	12.628	92.2474	Nitromethane - benzene
0.8193	2.93	6.8466	7.8804	6.1214	Nitromethane - cyclohexane
2.4441	44.6959	25.4103	41.124	37.3632	Methane - propane
13.4216	19.1128	43.6485	65.399	57.8839	Methanol - acetic acid
1.791	21.9246	48.2051	25.345	71.7885	Methanol - ethanol
1.6447	16.2331	33.2154	56.490	47.1162	Methanol - dimethylsulfoxide
1.7139	13.5803	40.9924	40.259	28.5681	Methanol - benzene
3.72223	13.58419	25.49967	25.239	28.56102	**Average**
3.63001	9.63137	13.00388	18.448	23.77569	**Standard Deviation**

One of the best advantages of artificial neural network is low dependency of accuracy of this method to the type of compounds. Classical methods give quite accurate results for some compounds while their answers for some other compounds may be very inaccurate. To have a quantitative measure of this quality, standard deviation parameter was calculated for each method which is presented in Table 4. The standard deviation of ARD for Brock and Bird, Pitzer, Zuo-Stenby and Sastri-Rao models are 23.77569, 18.44848, 13.00388 and 9.63137 respectively while standard deviation of ARD for artificial neural network is 3.63001.

4. Conclusion

In this study, artificial neural network was used to predict the surface tension of hydrocarbon mixtures. The accuracy of our proposed model was compared to four well-known empirical equations. It showed higher accuracy for the artificial neural network method. Also, results of standard deviation indicated that these empirical relations are so dependent on the type of compounds and some special parameters, while ANN is more independent. The optimized neural network parameters such as inputs and the number of neurons in hidden layers were presented for the calculation of surface tensions for the before mentioned compounds and can be used by other researchers in solving the problems which deal with the surface tension calculations.

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پیش‌بینی کشش سطحی مخلوط‌های هیدروکربنی با استفاده از شبکه عصبی مصنوعی

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چکیده

در مطالعه حاضر، از شبکه عصبی مصنوعی برای پیش‌بینی کشش سطحی ۲۰ مخلوط هیدروکربنی استفاده شده است. داده‌های آزمایشگاهی به دو بخش تقسیم شده است. ساختار بهینه شبکه با حداقل سازی خطای پیش‌بینی حاصل از داده‌های تست حاصل می‌شود. دقت مدل پیشنهادی با چهار معادله تجربی معروف مورد مقایسه قرار گرفته است. بر اساس نتایج حاصله، شبکه عصبی مصنوعی با انحراف استاندارد میانگین ۳/۶۳۰۰۱ بیشترین دقت را داشته است درحالی‌که این مقدار برای مدل‌های Brock and Bird، Pitzer و Sastri-Rao به ترتیب معادل ۲۳/۷۷۵۶۹، ۱۸/۴۴۸۴۸ و ۹/۶۳۱۳۷ می‌باشد.