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ARTICLE *in* INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH · FEBRUARY 2012

Impact Factor: 2.59 · DOI: 10.1021/ie2016416

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Application of Neural Networks in the Prediction of Surface Tensions of Binary Mixtures

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ABSTRACT: In this work, an artificial neural network (ANN) has been utilized to predict the surface tension of binary mixtures at different temperatures and concentrations and at atmospheric pressure. It has been shown that a multilayer perceptron network (MLP) can be trained better than other types of ANNs, and it can therefore be used as a predictive tool to predict the thermo-physical properties. In the modeling procedure, 60% of the available experimental data has been selected as the training set; the remaining data has been used to test and validate the network. After training and testing, the artificial neural network has been used for the prediction of the surface tension of a number of other systems, for which a minimum imprecision of 1.8% has been obtained. The results obtained from the trained network have also been compared to those obtained from the Sprow and Prausnitz model [Sprow, F.B., Prausnitz, J.M., Surface tensions of simple liquid mixtures. *Trans. Faraday Soc.* **1966**, *62a* 1097−1104]. It has been shown that the trained MLP network can predict the experimental data better than the r conventional neural network method while only a minimum number of adjustable parameters have been used, compared to the number of adjustable parameters in the thermodynamics models, such as the Sprow and Prausnitz model.

1. INTRODUCTION

Surface tension of pure liquids as well as mixtures is considered an essential thermo-physical property for studying interfacial phenomena. The knowledge regarding the conformation of materials at an interface is useful in understanding the fundamental properties and function of molecules that are present in the interface;[1] surface tension can give the required information in this respect. Furthermore, surface tension is effective in the deposition and transport of colloids in industrial processes, and it also affects the transfer rates of vapor absorption in vapor−liquid contactors. A considerable amount of experimental data has therefore been reported in the literature, and many correlations and theoretical models have also been proposed for the calculation or prediction of surface tension in pure or multicomponent systems (cf. refs 1−7). The proposed models are mostly based on classical and molecular thermodynamic approaches.[5−11] However, we have not been able to find a universal model to predict surface tensions, especially for mixtures. Therefore, it is of interest to find a new method for this ultimate purpose.

Theoretical models can be categorized into two main groups; group one is comprised of correlations and empirical relations which are limited to a few number of compounds. These relations are not applicable for the prediction of surface tension of classes of compounds other than those which have been initially studied, and also for mixtures. The second group consists of thermodynamic-based models. For these types of models, a number of adjustable parameters must usually be specified for each component, making them difficult to use. Most of the time, adjustable parameters must be determined through the fitting of experimental data. Without adjustable parameters, these models do not provide acceptable precision. On the other hand, determination of surface tension through experimental studies is time-consuming and rather expensive. Group-contribution methods have been used extensively for prediction of thermo-physical properties of liquid mixtures by several workers. Li et al.[5] proposed a model based on the corresponding state and group contribution method to estimate the surface tension of pure components; later Anjali et al.[6] extended it to the multicomponent liquid mixtures.

Alternatively, the quantitative structure−property relationship method (QSPR) is a promising tool for the prediction of various thermo-physical properties.[8] This method is based on molecular descriptors which are calculated solely from the molecular structure to fit the experimental data.[9] The method can become quite complex and it may require additional chemical properties and simplifying assumptions in order to perform complete calculations.

Among different models, the model of Sprow and Prausnitz is one of the most applicable methods that have been used extensively to predict the surface tension of mixtures.[7] This method is regarded as a predictive model for the calculation of surface tensions of multicomponent solutions, while it is sensitive to parameters such as molar surface area, pure-component surface tensions, and activity coefficients of the components that are present in the mixture. Considering the above facts, development of an accurate model for the prediction of surface tensions of pure components and mixtures over wide ranges of temperature is still a challenging issue

Recently, more attention has been directed to artificial neural networks (ANNs) as an effective tool for prediction and correlation of thermo-physical properties.[11−20] ANNs can extract the desired information directly from experimental data and do

Received: July 28, 2011
Revised: January 1, 2012
Accepted: January 11, 2012
Published: January 11, 2012

dx.doi.org/10.1021/ie2016416 | *Ind. Eng. Chem. Res.* 2012, 51, 2775−2781

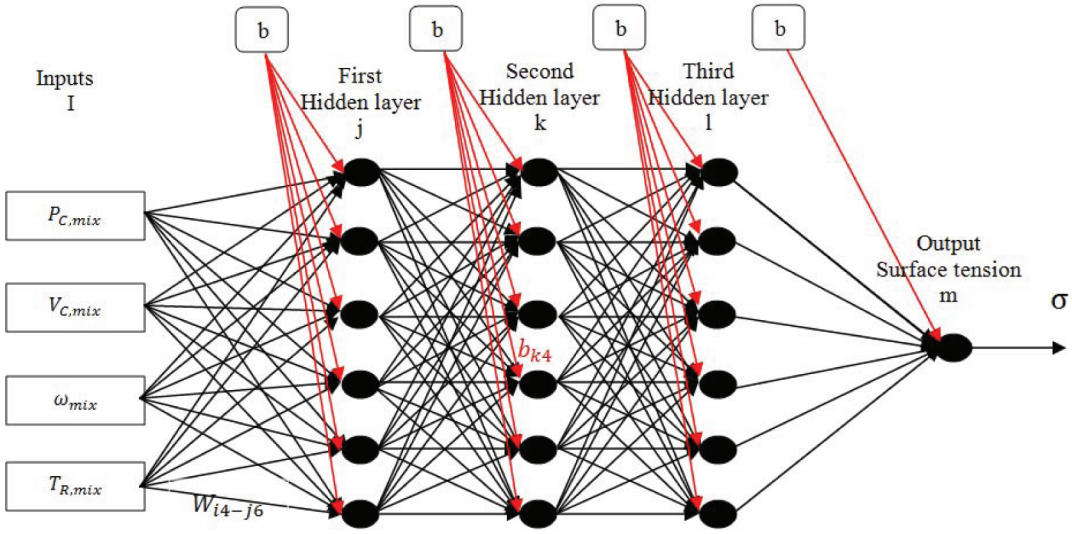

Figure 1. Neural network architecture.

not need to use detailed information of structures and interactions of the studied systems. Also, ANNs can avoid the limitations brought about by the lack of experimental data, and therefore they can improve the prediction accuracy, compared to the thermodynamic models which are based on polynomial correlation fitting. The ability of ANNs to "learn" and "recognize" highly nonlinear and complex relationships, ideally fits them into a wide range of applications in complex systems. ANNs have been applied in various fields of chemical engineering.[10−17] ANNs are also utilized for function estimation, since they are able to estimate any function in a stable and efficient manner. Therefore, the ANN technique creates a platform on which different models can be shaped and constructed. However the ANNs may have problems such as overfitting ones, which in this condition any extrapolations of generated networks are not recommended.[18,19] Gharagheizi et al.[20] used an ANN approach for prediction of the surface tension of pure compounds.

In this work, a new model, based on ANNs, has been proposed for precise prediction of the surface tension of binary mixtures of hydrocarbons. The results have been compared to those obtained from a thermodynamic-based model. Using the ANN method and the critical properties of pure components, the surface tension of 2250 binary mixtures has been predicted. In the first section of the paper modeling with ANN and in the second section the basis of modeling with the Sprow−Prausnitz as a group contribution model has been discussed. Finally, the results of both methods are evaluated and compared.

2. MODELING OF SURFACE TENSION

2.1. Modeling of Surface Tension Using ANNs. The term "neural network" is applied to models of the brain. These models may take the form of mathematical equations or computer simulations. They may also be considered as physical forms, similar to electronic or optoelectronic circuits, which are triggered by the brain's architecture. Neural network models have been created by both scientists and engineers. Artificial neural networks represent a complex configuration, which includes many simple processors (so-called "neurons"), arranged in layers (input, hidden, and output layers). The proper transformation of information is possible as a result of a correctly prepared matrix of weights × numbers attributed to all interneuron connections. In multilayer perceptron (MLP) feedforward networks, which are the most frequently used ones, each neuron simply sums up (properly amplifies or weakens) signals from all neurons of the previous layer, after transforming the data through suitable activation functions. To prepare a network to solve a task, values of the weight of each connection must be adjusted. As a matter of fact, the adjustment of these values is the main and most important part of modeling with ANNs. This step is called the "learning procedure" and is carried out by means of an algorithm. The learning process is executed on the basis of input data sets and associated with the output sets. During the learning process, the computer software compares the calculated values with the expected ones, and adjusts the values of the weights value to reach the best agreement between the two data sets in a step-by-step approach. The optimization is therefore nonlinear and consists of iteratively updating the weights and biases until the output values for each pattern are close to the target values. The error in prediction is then propagated through the system and the interunit connections are changed to minimize the error rate in this precise prediction. This process continues with multiple training sets until the errors dwindle across the sets. After extensive training, the network will eventually establish the input−output relationships through the adjusted weights and biases of the network.

Table 1. 1st Layer Weight Functions ($W_{ip\text{-}jx}$)

x	$p = 1$	$p = 2$	$p = 3$	$p = 4$
1	−0.0204	0.0506	−0.1993	0.0466
2	−1.5113	−2.5421	0.8318	−0.0682
3	0.2979	0.9751	−0.2505	−0.8907
4	2.4046	1.3978	−2.3612	−0.2171
5	−1.2779	−2.2468	0.871	−0.0993
6	−0.2012	−1.0353	0.7998	0.3477

In the first step, the number of inputs and outputs of network must be specified, and the selected inputs must have a theoretical relation to outputs; otherwise there will be problems encountered in the training procedure. In this work, properties such as P_c, V_c, ω (acentric factor), and T_r of pure components and mixtures have been selected as input parameters. To define the critical properties of the mixtures, the following mixing

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Table 2. 2nd Layer Weight Functions ($W_{jx\text{-}ky}$)

X	y = 1	y = 2	y = 3	y = 4	y = 5	y = 6
1	6.2423	29.9841	19.1338	0.4582	−47.715	33.963
2	−18.344	16.6423	0.4937	−0.9466	−21.9669	0.4738
3	−23.4077	21.6413	0.9462	−0.7197	−28.1328	0.7041
4	−7.2078	21.2347	1.1911	2.4159	−23.3425	3.5758
5	0.0977	−0.4678	−0.0431	−0.0929	0.57	−0.121
6	16.1437	−29.1257	−4.2661	1.7288	38.1168	−5.818

Table 3. 3rd Layer Weight Functions ($W_{ky\text{-}ln}$)

n	y = 1	y = 2	y = 3	y = 4	y = 5	y = 6
1	−0.0652	−1.2187	−1.7908	−0.3761	−1.7784	−0.3938
2	2.4035	8.2304	−12.4343	−1.2585	−55.9187	−4.6917
3	−2.0082	−7.0803	10.9037	0.1182	17.6116	4.4122
4	0.1301	−2.2871	−0.3878	−0.894	−10.4426	−2.2871
5	−0.1067	2.0748	0.5793	0.8236	9.3379	2.3167
6	0.0962	0.8512	−0.9081	−0.1238	−6.2498	−0.171

Table 4. 4th Layer Weight Functions ($W_{ln\text{-}m1}$)

n = 1	n = 2	n = 3	n = 4	n = 5	n = 6
5.3916	8.9909	10.4535	−44.6727	−73.8843	57.0184

Table 5. Biases

I	b_{ji}	b_{ki}	b_{li}	.
1	0.2032	−8.6461	−1.7201	−22.1833
2	−1.4812	1.433	27.3914	
3	0.7578	1.5715	−5.3755	
4	0.3959	0.1363	5.3595	
5	−1.396	0.6575	−4.381	
6	−0.4256	2.5137	5.4588	

rules have been applied to define the input data for binary mixtures:

$$T_{R,mix} = \frac{T}{T_{C,mix}} \quad (1)$$

$$T_{C,mix} = \sum_{2}^{j=1}\sum_{2}^{i=1} x_i x_j T_{c_{ij}} \quad (2)$$

$$T_{c_{ij}} = \sqrt{T_{c_i} T_{c_j}} \quad (3)$$

$$V_{C,mix} = \sum_{2}^{j=1}\sum_{2}^{i=1} x_i x_j V_{c_{ij}} \quad (4)$$

$$V_{c_{ij}} = \left(\frac{1}{2}(V_{c_i}^{.3333} + V_{c_j}^{.3333})\right)^3 \quad (5)$$

$$\omega_{mix} = \sum_{2}^{i=1} x_i \omega_i \quad (6)$$

$$P_{C,mix} = \sum_{2}^{i=1} x_i P_{C_i} \quad (7)$$

The surface tension of binary mixtures has been considered as output. A reliable database is critically important for training and testing of an ANN. Large data sets reinforce the validity of the ANN model and improve its performance. Experimental data on the surface tension of binary mixtures were extracted from refs 21−25. To avoid overfitting problems that threaten the generalization capabilities of artificial neural networks, the experimental data have been categorized into training, validating, and testing sets. The first and the second sets have been obtained randomly through a sampling of 60% and 20% of experimental data, respectively. The training set has been used for the determination of weight factors as well as biases leading to minimum error. The validating set has been used to detect overfitting problems. The testing set (20% of remaining experimental data) has been used to gauge the training procedure. To check the prediction ability of the trained ANN, a number of the experimental data have been randomly excluded from the training set.

In the third step, the type of network, the number of layers, neurons, and the activation function of each layer must be defined; this step is the most important and challenging step in designing and training an ANN. Ordinarily, it is done through a trial and error procedure. The Levenberg−Marquart algorithm[26−29] has been used for the training procedure based on the fact that this algorithm has high-speed training capabilities. In the final step, the performance and precision of the trained ANN should be checked. To come up with the best ANN, different structures of the MLP network such as feed forward and cascade forward have been examined, and the accuracy and precision of each network has been evaluated and compared on the basis of rmsd (root-mean-square deviation):

$$\text{rmsd} = \sqrt{\frac{\sum_{n}^{i=1}(\sigma_i^{expt} - \sigma_i^{predict})}{n}} \quad (8)$$

where σ_i^{expt} is the experimental data, $\sigma_i^{predict}$ is the calculated value using the ANN, and n is the number of data sets used in the training step.

The most efficient network has been selected based on the results of the mentioned evaluations. The specification of the selected ANN has been presented in the Results section.

2.2. Modeling of Surface Tension Using the Sprow−Prausnitz Model. The composition of the surface phase usually differs from that of the bulk phase; on this account, the surface composition has a direct relation with surface tension. Usually the mixture surface tension (σ_m) is less than the average value of surface tension of its component, meaning that components with lower values of pure surface tension preferentially concentrate in the surface phase. Sprow and Prausnitz[30] assumed that the bulk and surface phases are in equilibrium, and the partial molar area of component i is the same as the molar area of i. In this study, the UNIFAC group contribution model[31] has been implemented to calculate the activity coefficients in both bulk and surface phases.

To compare the ability of thermodynamic models with the ANN, 21 binary systems have been selected, and their surface tensions have been determined using the Sprow and Prausnitz model. The results have been compared with those obtained using ANN (Table 7).

3. RESULTS

To build an optimum network, different types of ANNs have been examined and finally the MLP feed-forward network with

dx.doi.org/10.1021/ie2016416 | Ind. Eng. Chem. Res. 2012, 51, 2775−2781

Table 6

component 1	component 2	temperature range	AARD %
CCl_4	$CHCl_3$	10−30	2.39
CCl_4	CH_4O	35	1.48
CCl_4	C_2H_3N	25−50	1.35
CCl_4	$C_2H_4O_2$	18	1.54
CCl_4	C_2H_6O	20−80	1.98
CCl_4	C_3H_6O	20−60	0.89
CCl_4	C_3H_8O	30−80	2.52
CCl_4	$C_4H_8O_2$	25	1.19
CCl_4	$C_4H_8O_2$	25−35	2.12
CCl_4	$C_4H_8O_2$	20	1.23
CCl_4	C_5H_{10}	25	1.35
CCl_4	C_6H_5Cl	0−150	1.88
CCl_4	C_6H_6	25−60	1.64
CCl_4	C_6H_{12}	20	1.06
CCl_4	C_7H_8	20−110	0.83
CCl_4	C_7H_{14}	30	1.99
$CHCl_3$	CH_4O	35	1.64
$CHCl_3$	C_2H_6O	0−25	1.63
$CHCl_3$	C_3H_6O	18	0.83
$CHCl_3$	$C_4H_8O_2$	0−35	1.1
$CHCl_3$	C_6H_6	25	1.28
$CHCl_3$	C_6H_7N	0−25	0.86
$CHCl_3$	$C_6H_{12}O$	20	1.06
CH_2O_2	$C_2H_4O_2$	10−80	2.54
CH_2O_2	C_3H_6O	25−45	1.13
CH_2O_2	C_5H_5N	14	1.81
CH_2O_2	$C_5H_{10}O$	35	1.02
CH_2O_2	C_7H_9N	25	2.34
CH_2O_2	$C_8H_{11}N$	25	2.72
CH_4O	$C_2H_4O_2$	35	2.95
CH_4O	C_2H_6O	20−80	1.06
CH_4O	C_3H_6O	0−35	2.25
CH_4O	C_3H_8O	0−95	2.38
CH_4O	$C_4H_8O_2$	25−35	0.91
CH_4O	$C_4H_{10}O$	25	0.7
CH_4O	$C_4H_{10}O$	25	1.47
CH_4O	$C_4H_{10}O$	25	2.08
CH_4O	C_6H_6	25	2.79
CH_4O	$C_6H_{12}O$	20	1.83
CH_4O	C_6H_{14}	20−45	2.07
CH_4O	C_7H_8	20−45	0.82
CH_4O	C_8H_{10}	20−45	1.15
CH_4O	C_9H_{12}	0−40	1.33
C_2H_3N	$C_2H_4O_2$	25−40	0.89
C_2H_3N	C_2H_6O	20	1.37
C_2H_3N	$C_3H_6O_2$	25−45	1.19
C_2H_3N	$C_4H_8O_2$	25−45	1.2
C_2H_4	C_2H_6	−19	0.44
C_2H_4O	C3H6O	20	1.58
$C_2H_4O_2$	C_2H_5NO	60−80	1.7
$C_2H_4O_2$	C_2H_6O	25−30	1.7
$C_2H_4O_2$	C_3H_6O	20−40	1.96
$C_2H_4O_2$	$C_3H_6O_2$	20−60	1.4
$C_2H_4O_2$	$C_4H_6O_2$	20	1.6
$C_2H_4O_2$	$C_4H_6O_3$	20−80	1.56
$C_2H_4O_2$	C_4H_8O	25−45	1.31
$C_2H_4O_2$	$C_4H_8O_2$	25	1.8
$C_2H_4O_2$	$C_5H_{10}O$	25−45	1.86
$C_2H_4O_2$	C_6H_6	20−25	1.27
$C_2H_4O_2$	C_6H_6O	50−90	2.08
$C_2H_4O_2$	C_6H_7N	0−25	0.9
$C_2H_4O_2$	C_6H_{12}	30	4.6
$C_2H_4O_2$	C_6H_6O	60−80	0.91
C_2H_6O	$C_3H_6O_2$	30	0.77
C_2H_6O	$C_5H_{12}O$	0−100	2.65
C_2H_6O	C_6H_6	15−80	3.03
C_2H_6O	C_6H_7N	0−25	1.65
C_2H_6O	C_6H_{12}	22−30	3.4
C_2H_6O	C_6H_{14}	20−25	3.61
C_2H_6O	C_7H_8	25	5.7
C_2H_6O	C_7H_8O	20	2.78
C_2H_6O	C_7H_8O	20	2.47
C_2H_6O	C_7H_8O	20	2.82
C_2H_6O	C_7H_{14}	30	2.68
C_3H_6O	$C_4H_6O_2$	20	0.65
C_3H_6O	$C_4H_8O_2$	25−35	0.93
C_3H_6O	$C_4H_{10}O$	30	2.48
C_3H_6O	C_6H_6	10−50	2.09
C_3H_6O	C_6H_6O	30−50	2.17
C_3H_6O	$C_6H_{12}O$	20	2.92
C_3H_6O	C_7H_8O	20	1.51
C_3H_6O	C_7H_8O	20	2.03
C_3H_6O	C_7H_8O	20	2.3
C_3H_6O	C_8H_{18}	25	2.26
C_3H_6O	$C_{16}H_{34}$	39.85	2.61
$C_3H_6O_2$	$C_4H_6O_3$	20−60	1.28
$C_3H_6O_2$	C_4H_8O	20−40	1.93
$C_3H_6O_2$	$C_4H_8O_2$	11−70	1.9
$C_3H_6O_2$	$C_4H_{11}N$	25	1.5
$C_3H_6O_2$	C_5H_5N	30	1.7
$C_3H_6O_2$	C_5H_{12}	25	1.87
$C_3H_6O_2$	C_6H_{12}	30	2.1
C_3H_7NO	C_7H_8	15−45	1.58
C_3H_7NO	C_7H_{16}	15−45	1.66
C_3H_8O	C_3H_8O	10−50	1.09
C_3H_8O	$C_4H_8O_2$	20−30	1.7
C_3H_8O	C_5H_{12}	25	1.9
C_3H_8O	$C_5H_{12}O$	0−100	2.44
C_3H_8O	C_6H_6	25	2.3
C_3H_8O	C_6H_6	20	2.16
C_3H_8O	C_6H_7N	13−65	2.18
C_3H_8O	C_6H_{14}	25−35	2.77
C_3H_8O	C_7H_8	25	2.5
C_3H_8O	C_7H_{16}	20	2.52
	Average Absolute Deviation		1.84

three hidden layers and a minimum number of neurons (six neurons in each hidden layer) has been selected to model the surface tension of binary mixtures. Modeling has been pursued via changing the activation functions such as tangent sigmoid, log sigmoid, and linear function; finally the tangent sigmoid has been selected as the activation function of input, hidden, and output layers. The topology architecture of the feed forward neural network has been shown in Figure 1.

As it can be seen in Figure 1, i is the input, j, k, and l are the three hidden layers, and m is the output. The subscripts in Figure 1 show the number of neurons in each layer; for example, W_{i3-j2} represents the weight value between input 3

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Table 7. Comparison between Artificial Neural Network and Sprow−Prausnitz Model

component 1	component 2	AARD % (ANN)	AARD% (Sprow−Prausnitz)
C H Cl_3	C Cl_4	2.4	3.1
C H_4 O	C Cl_4	1.5	1.3
C_2 H_3 N	C Cl_4	1.3	2.2
C_2 H_4 O_2	C Cl_4	1.5	4.1
C_3 H_6 O	C Cl_4	2	7.3
C_3 H_6 O	C Cl_4	0.9	2.7
C_3 H_8 O	C Cl_4	1.9	6.2
C_4 H_8 O_2	C Cl_4	3.2	4.5
C_4 H_8 O_2	C Cl_4	1.23	5.5
C_5 H_{10}	C Cl_4	1.4	3.2
C_6 H_5Cl	C Cl_4	1.3	2.3
C_6 H_6	C Cl_4	1.6	1.8
C_6 H_{12}	C Cl_4	1.1	1.5
C_7 H_8	C Cl_4	0.83	2
C_7 H_{14}	C Cl_4	2	2.3
C H_4 O	C H Cl_3	1.6	1.9
C_3 H_6 O	C H_2 O_2	1.1	4
C_2 H_4 O_2	C H_4 O	3	3.6
C_3 H_6 O	C H_4 O	2.2	2.3
C_6 H_6	C H_4 O	2.8	3.9
C_3 H_6 O	C_2 H_4 O_2	2.9	4.4
Average		1.80	3.34

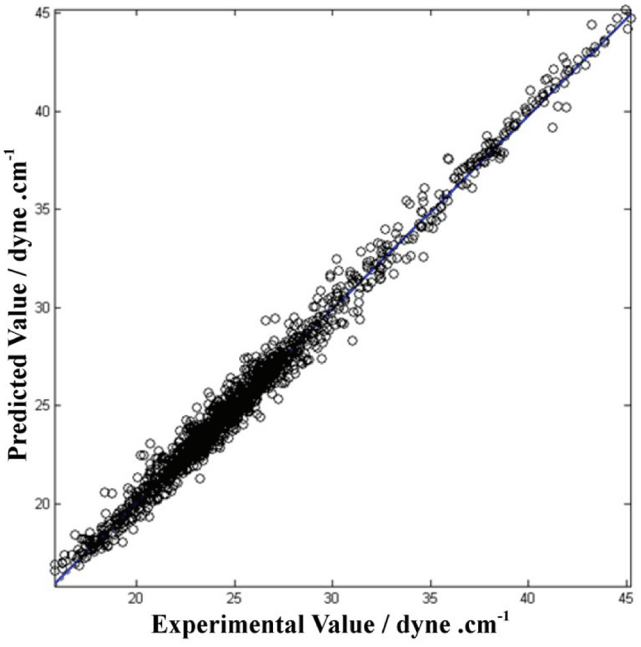

Figure 2. Surface tension predicted by ANN versus experimental data, train data.

(i_3) and neuron 2 in the hidden layer (j_2). According to the above definition, the equations which produce the output in the trained feed-forward network are as follows:

$$\text{output}(\sigma) = \tan\text{sig}\left(\sum_{6}^{n=1} l_n W_{l_n - m_1} + b_{m_1}\right) \quad (12)$$

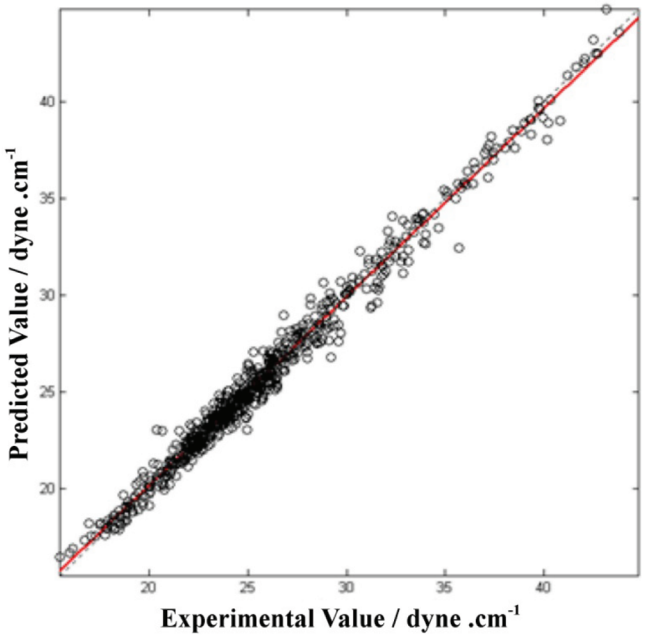

Figure 3. Surface tension predicted by ANN versus experimental data, test data.

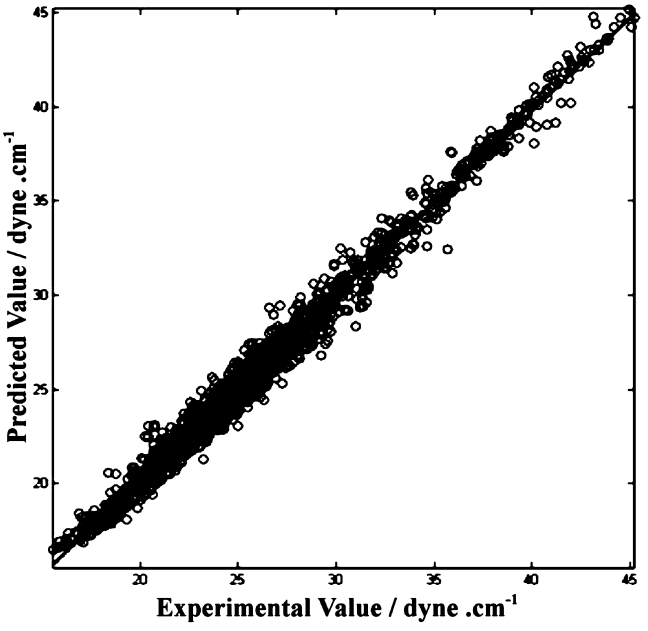

Figure 4. Surface tension predicted by ANN versus experimental data, total data.

$$l_n = \tan\text{sig}\left(\sum_{6}^{y=1} k_y W_{k_y - l_n} + b_{l_n}\right) \quad (13)$$

$$k_y = \tan\text{sig}\left(\sum_{6}^{x=1} j_x W_{j_x - k_y} + b_{k_y}\right) \quad (14)$$

$$j_x = \tan\text{sig}\left(\sum_{4}^{p=1} i_p W_{i_p - j_x} + b_{j_x}\right) \quad (15)$$

dx.doi.org/10.1021/ie2016416 | Ind. Eng. Chem. Res. 2012, 51, 2775−2781

$$\text{tangent sigmoid}\ (x) = \frac{(1 - e^{(-x)})}{(1 + e^{(-x)})}$$

$$x \in [-\infty, +\infty] \quad \text{and}$$

$$\text{tangent sigmoid}\ (x) \in [-1, +1] \tag{16}$$

In the above equations, b_i is the bias. The data of input weight matrix hidden layers and output layer weight matrix have been presented in Tables 1, 2, 3, and 4. Table 5 represents the biases related to activation functions of each layer. In Table 6, the absolute average relative deviation (AARD) of the designed ANN has been compared with experimental data. As it can be deduced, the ANN has managed to predict the experimental data efficiently; the average absolute deviations on the learning set (60% of the database), validation set (20%of the database), and on the test set (remaining 20%) are 1.6, 2, and 2.3, respectively, confirming the high learning ability of the ANN correlations.

Fortunately, the trained network can predict the excluded data with acceptable average absolute relative deviation (AARD); the results have been presented in table 7. The parity plot of experimental and predicted data for the train, test, and total data are given in Figures 2, 3, and 4, respectively.

In Figure.4, experimental data have been compared to results obtained from the artificial neural network for all available data sets. In Table 7, the AARD of results obtained using the Sprow−Prausnitz model in prediction of surface tension for some selected binary mixtures has been compared with those obtained using the ANN. It can be concluded that ANN can predict surface tensions more accurately than the Sprow−Prausnitz model.

4. CONCLUSION

In this research, an artificial neural network has been applied to predict binary mixture surface tensions. It is demonstrated that this model can be used as a general model for the prediction of surface tensions. The results show that ANN has this capability to predict the surface tension of binary mixtures more accurate than the Sprow−Prausnitz model. It is interesting that the trained ANN does not need pure surface tension and density which are necessary in other models; surface tensions of binary mixtures can be predicted using only critical properties of the pure components. Using this model, surface tensions of 96 binary mixtures have been predicted. An MLP feed-forward network with three hidden layers and six neurons in each hidden layer has been proposed. The results proved that ANN can predict the surface tension for binary mixtures efficiently with an AARD of 1.84% using the optimum MLP network. It is also shown that the ANN method has the additional advantage that all the effective parameters on surface tension of the studied mixture can be included in the input data. Therefore, the method is capable of predicting surface tension when the experimental data on physical properties such as pure surface tension and liquid density are not available or there are limitations for the experimental measurements. The results indicate that the ANN method can be applied as an efficient and convenient method as all parameters can be obtained after a single training procedure. It was demonstrated that ANNs may be utilized as a promising way to predict thermodynamic properties in complex systems. By the application of this method, the limitations of conventional thermodynamic methods that are rather complex and usually require determination of "fitting parameters", which are arbitrary in many ways, are prevented. Finally, it is worth concluding that ANNs may also be used to predict the surface tension in multicomponent as well as highly complex systems.

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