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The Prediction of Surface Tension of Ternary Mixtures at Different Temperatures Using Artificial Neural Networks

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Abstract

In this work, artificial neural network (ANN) has been employed to propose a practical model for predicting the surface tension of multi-component mixtures. In order to develop a reliable model based on the ANN, a comprehensive experimental data set including 15 ternary liquid mixtures at different temperatures was employed. These systems consist of 777 data points generally containing hydrocarbon components. The ANN model has been developed as a function of temperature, critical properties, and acentric factor of the mixture according to conventional corresponding-state models. 80% of the data points were employed for training ANN and the remaining data were utilized for testing the generated model. The average absolute relative deviations (AARD%) of the model for the training set, the testing set, and the total data points were obtained 1.69, 1.86, and 1.72 respectively. Comparing the results with Flory theory, Brok-Bird equation, and group contribution theory has proved the high prediction capability of the attained model.

Keywords: Surface Tension, Mixtures, Artificial Neural Network

1. Introduction

Surface tension is one of the important characteristics of liquids which influences various surface phenomena such as creating bubbles, foams, droplets, emulsion, and heterogeneous liquid phases (Brocos et al., 2005; Gharagheizi et al., 2011c; Mohsen-Nia et al., 2010; Poling et al., 2000; Roosta et al., 2011; Tahery et al., 2005). Certainly, the determination of physical and chemical properties of liquids is unattainable without considering surface tension. In chemical and petroleum engineering operations such as separation, distillation, extraction, and adsorption, the surface tension of the mixtures (σ_m) is an essential parameter (Bainbridge and Sawistowski, 1964; El-Bourawi et al., 2006; Rosen and Kunjappu, 2012; Syeda et al., 2004; Zuiderweg and Harmens, 1958). Moreover, the surface tension of the reservoir fluid plays a key role in enhancing oil recovery (EOR) and it has different effects on capillary pressure, residual oil saturation, and relative permeability (Dake, 2001; Donaldson et al., 1985; Sheng, 2010; Tarek Ahmed, 2010).

The surface tension of mixtures depends on surface composition and temperature. However, it is not a linear function of the surface tension of ingredients because the surface composition is different from bulk and cannot easily be defined. Consequently, simple and linear models for the prediction of the

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surface tension in multi-component systems are inapplicable (Poling et al., 2000).

In the past years, several methods, which are usually derived from thermodynamic definitions, have been presented to calculate the surface tension of the mixtures. Butler (1932) proposed an equation to predict surface tension which has widely been applied to developing other methods such as Redlich-Kister (1948) correlation for binary systems. Sprow and Prausnitz (1967) proposed a model for non-ideal mixtures similar to Butler's model. Jufu et al. (1986) developed a correlation based on the local composition model using Wilson's equation as an activity model. Suarez et al. (1989) used the modified UNIFAC group-contribution method—developed by Larsen et al. (1987)—to compute the activity coefficients in the surface and bulk phases. Zhibao et al. (1990) combined the UNIFAC model with Butler's equation for calculating the surface tension of both binary and multicomponent systems. Furthermore, several approaches have been proposed for predicting the surface tension of multicomponent systems in recent years. Sonawane and Kumar (1999) correlated the surface tension of binary liquid mixtures based on Butler's equation. Chunxi et al. (2000) presented a two-parameter surface tension equation for binary and multicomponent systems based on thermodynamic definitions and an expression for Gibbs free energy. Pineiro et al. (2001) proposed a model using Kretschmer and Wiebe (1954) results for estimating the composition of the surface layer in binary liquid mixtures. Santos et al. (2003) presented a new equation to correlate the excess surface tension of binary mixtures obtained from Butler's equation for calculating surface tension in the binary and ternary liquid mixtures. Miqueu et al. (2004) used the gradient theory of fluid interfaces to compute the surface tension of binary and ternary hydrocarbon mixtures. Brocos et al. (2005) employed the extended Langmuir model to define the behavior of binary systems as a function of bulk concentration. Tahery et al. (2005) correlated the surface tensions of aqueous and non-aqueous binary solutions utilizing the excess number of molecular layers and free energy change in the surface region (Shereshefsky, 1967). Ramirez-Verduzcoet al. (2006) obtained a method based on the UNIFAC group contribution model for the prediction of the surface tension. In this method, the analogy between bubble point pressure and vapor composition was used for calculations. Lin et al. (2007) applied the gradient theory to estimating the surface tension of pure fluids and binary mixtures. In this technique, the Helmholtz free energy density and the bulk properties were calculated using volume-translated Peng–Robinson (VTPR) and Soave Redlich–Kwong (VTSRK) equations of state. Gardas and Coutinho (2008) used quantitative structure–property relationship (QSPR) for predicting the surface tensions of ionic liquids. Bitaab et al. (2008) proposed a model based on the perturbation theory of fluids to correlate the surface tension of pure and binary hydrocarbon mixtures. Mohsen-Nia et al. (2010) correlated the surface tension of mixtures by a new model obtained from coupling scaled particle theory (SPT) and the MMM equation of state.

Recently, artificial neural network (ANN) has extensively been taken into consideration for the prediction of thermo-physical properties. Gharagheizi et al. (2011) utilized artificial neural network−group contribution (ANN-GC) method to calculate the surface tension of pure compounds. Roosta et al. (2012) applied ANN for modeling the surface tension of pure organic compounds. They used critical pressure, acentric factor, reduced temperature, reduced normal boiling temperature, and specific gravity at the normal boiling point as the input parameters to the ANN. In our previous work, (Parhizgar et al., 2012) we proposed a new model based on the ANN for the prediction of the surface tension of binary mixtures. 105 binary mixtures containing 2250 data points were applied to generate the new model using critical pressure, critical volume, reduced temperature, and acentric factor of pure component as the inputs.

Although there are varied approaches to the prediction of the surface tension, they have some limitations. Most of the mentioned methods have inherent complexity and require lots of input parameters. Additionally, the majority of them do not offer a precise estimation for new systems. On this account, it is inferred that an effective practical method with a high prediction capability would be required (Eslamimanesh et al., 2011; Mohammadi et al., 2010; Mohammadi and Richon, 2010). In this work, an ANN method has been applied to generate a new comprehensive model for the prediction of the surface tension of ternary mixtures. In fact, the current work is a complementary study for our previous investigations (Parhizgar et al., 2012). For the evaluation of the accuracy of the obtained model, the results have been compared with some well-known theories.

2. Artificial neural networks

In recent years, artificial neural network (ANN) has widely been employed for modeling complex nonlinear systems, especially for the prediction of thermodynamic properties (Boozarjomehry et al., 2005; Dehghani et al., 2006; Eslamimanesh et al., 2011; Eslamloueyan and Khademi, 2009; Eslamloueyan and Khademi, 2010; Gharagheizi et al., 2010; Gharagheizi et al., 2011a; Gharagheizi et al., 2011b; Moghadassi et al., 2010; Mohammadi et al., 2010; Mohammadi and Richon, 2010). ANN is known as a powerful approach among black box modeling approaches. This method does not involve detailed theories and trains the functionality of the presented input-output data automatically (Eslamimanesh et al., 2011; Mohammadi et al., 2010; Mohammadi and Richon, 2010).

There are different types of ANN methods such as feed forward, radial basis function, and auto associative network. Feed forward network (FF) has been frequently applied to engineering studies, especially in chemical engineering because of its simple structure and mathematical analysis. Back propagation (BP) is the most common type of FF network because it has a straight instruction procedure (Boozarjomehry et al., 2005; Dehghani et al., 2006; Eslamimanesh et al., 2011; Eslamloueyan and Khademi, 2010; Gharagheizi et al., 2010; Gharagheizi et al., 2011a).

The network of ANN is composed of an input layer, some hidden layers (at least one), and one output layer. Layers contain one or more simple internal units named neuron. The number of neurons in the input and output layers are consistent with the number of input and output variables. It has emphasized that a network with appropriate hidden layers and neurons is capable to predict any functionality. Neurons are associated to each other by weight functions; each neuron receives signals from previous layers proportional to the weight functions and generates an output spreading to forward layers. In each layer, the neuron value (a^i_j) is calculated by Equation 1 (Boozarjomehry et al., 2005; Eslamloueyan and Khademi, 2009; Eslamloueyan and Khademi, 2010).

$$a^i_j = f^i_j\left(\sum_{k=1}^{n_{i-1}} w^i_{jk} \times a^{i-1}_k + b^i_j\right) \tag{1}$$

where, *i*, *j*, *w*, and *b* are layer number, neuron number in layer *i*, weight function and bias respectively. The biases are added to the neurons for adjusting the outputs; it makes the simulation be performed faster and more accurate. In Equation 1, *f* is the transfer function including linear and nonlinear algebraic expressions changing the input of each layer to the output. Classically, log sigmoid, tangent sigmoid, and linear transfer functions are implemented in the networks (Boozarjomehry et al., 2005; Dehghani et al., 2006; Gharagheizi et al., 2010; Gharagheizi et al., 2011a; Gharagheizi et al., 2011b; Gharagheizi et al., 2011c; Parhizgar et al., 2012; Roosta et al., 2011). After defining the structure of the network, i.e. the number of hidden layers, neurons, and transfer functions, unknown parameters (the weight functions and biases) would be adjusted to reach the outputs of the experimental values.

Network structure should be in the lowest possible volume; Understanding the best structure for acceptable results is a challenging step and is usually performed through trial and error procedure. There are two major steps in the process of ANN construction, namely training and testing. In the training step, the input data and the corresponding outputs are presented to the network and the weight functions and biases are accordingly adjusted to attain the minimum imprecision. In the BP network, deviations are returned back to the network for readjusting the weight functions and biases. To develop an acceptable network, a suitable dispersion of the training data is required (Boozarjomehry et al., 2005; Eslamloueyan and Khademi, 2009; Eslamloueyan and Khademi, 2010). After the training step, the network will be able to predict new data points (test). There are different algorithms to adjust weights and biases in training step; for instance, Levenberg-Marquardt is a frequently used algorithm. Detailed definitions about ANN can be found in the literature (Braspenning et al., 1995; Haykin, 1999; Kwok et al., 2010; Murray, 1994; Priddy and Keller, 2005).

3. Modeling and results

3.1. Developing an ANN model

The first step to develop an ANN model for the current study is the investigation of the parameters affecting the surface tension of multicomponent systems; these parameters organize the inputs of the network. Through an extensive literature review, it was inferred that the corresponding-state models have more competency to be followed for defining the input parameters. The corresponding-state models constitute a significant sub-group of predictive thermodynamic models and have more available and easy-to-use inputs. In this regard, critical pressure and volume, reduced temperature, and an acentric factor of the mixture were selected as the input parameters. Considering the linear mixing rules used in Brok-Bird model (Brock and Bird, 1955; Pandey et al., 2004), the input parameters including the mixture reduced temperature ($T_{R,\,m}$), critical pressure ($P_{c,m}$), critical volume ($V_{c,m}$), and the acentric factor (ω_m) were defined as follows (Equations 2-6):

$$T_{R,m} = \frac{T}{T_{c,m}} \tag{2}$$

$$T_{c,m} = \sum_{i=1}^{3} x_i \times T_{c,i} \tag{3}$$

$$P_{c,m} = \sum_{i=1}^{3} x_i \times P_{c,i} \tag{4}$$

$$V_{c,m} = \sum_{i=1}^{3} x_i \times V_{c,i} \tag{5}$$

$$\omega_{c,m} = \sum_{i=1}^{3} x_i \times \omega_{c,i} \tag{6}$$

where, $T_{c,i}$, $P_{c,i}$, $V_{c,i}$, ω_i, and x_i are critical temperature, critical pressure, critical volume, the acentric factor, and the mole fraction of component *i* in the mixture respectively. Critical properties and the acentric factor of the components were quoted from *Perry's Chemical Engineers' Handbook* (Green and Perry, 2007).

15 ternary liquid systems containing 777 experimental data points were utilized to create the ANN model. Table 1 presents the selected mixtures generally composed of hydrocarbons. It should be noted that the data related to the surface tension of ternary mixtures are so restricted. We have tried to

collect relatively all of the accessible data in the literature, considering that ionic liquids or refrigerants are studied in this work. As it is shown in Table 1, the selected data lies in a diverse temperature range (287.81 to 328.15 K).

Table 1
Selected ternary mixtures; the number of data points and temperature range.

Compound 1	Compound 2	Compound 3	Number of data points	Temperature range (K)	Reference
Water	Ethyl Butyrate	Methanol	43	303.15	Kijevcanin et al., 2003
Diethyl Carbonate	p-Xylene	Decane	73	298.15	Mosteiro et al., 2009
Sulfuric Acid	Dimethylamine	Water	131	297.35	Hyvärinen et al., 2004
Heptane	Toluene	N,N-Dimethyl formamide	73	287.81-317.86	Kahl et al., 2004
Water	Acetone	Toluene	158	288.15-328.15	Enders et al., 2007
Water	n-Butyl Acetate	1-Propanol	68	303.15	Johnson et al., 2008
n-Hexane	Cyclohexane	Benzene	10	298.15	Pandey et al., 2001
Cyclohexane	n-Heptane	Toluene	10	298.15	Pandey et al., 2008
n-Pentane	n-Hexane	Benzene	10	298.15	Pandey et al., 2008
2,2,4-Trimethyl Pentane	Cyclohexane	Decane	44	298.15	Pandey et al., 2008
Hexane	Decane	Hexadecane	24	303.16	Pandey and Pant, 1982
Nitromethane	Benzene	1-Propanol	31	296.15-299.95	Michaels et al., 1950
2-Propanol	Toluene	Furfural	30	293.65-300.85	Michaels et al., 1950
Toluene	Benzyl Alcohol	Ethyl Acetate	31	295.45-302.85	Michaels et al., 1950
Water	Ethyl Propionate	Methanol	41	303.15	Kijevcanin et al., 2004

Due to the frequent usage of back propagation feed forward networks in the field of thermodynamics, this type of ANN was utilized. Furthermore, the average absolute relative deviation (AARD%) was chosen to evaluate the errors. The AARD% equation is defined by the following equation:

$$AARD\% = 100 \times \frac{1}{n} \times \sum_{i=1}^{n} \frac{|\sigma_{i,\exp} - \sigma_{i,prd}|}{\sigma_{i,\exp}} \tag{7}$$

where, $\sigma_{i,exp}$, $\sigma_{i,prd}$, and n are the experimental data, predicted data, and the number of data set used in the training step respectively. In the training step, Levenberg-Marquardt algorithm was utilized for

analyzing the errors and adjusting the network parameters. To design ANN, 80% of the data were randomly selected for network training and the rest were applied to testing.

For keeping away from over-fitting, the lowest number of adjustable parameters should be considered. To meet such a requirement, the network structure was developed based on a trial and error investigation; at the first step, the minimum number of hidden layers and neurons were selected and the procedure was then pursued by the examination of different networks with various transfer functions, the number of hidden layers, and neurons to attain satisfactory results. Eventually, the network with 2 hidden layers composed of 6 and 5 neurons was selected as the most excellent network. The topology architecture of the designed ANN is depicted in Figure 1. Log sigmoid, tangent sigmoid and linear transfer functions have been selected for the input, hidden, and output layers respectively.

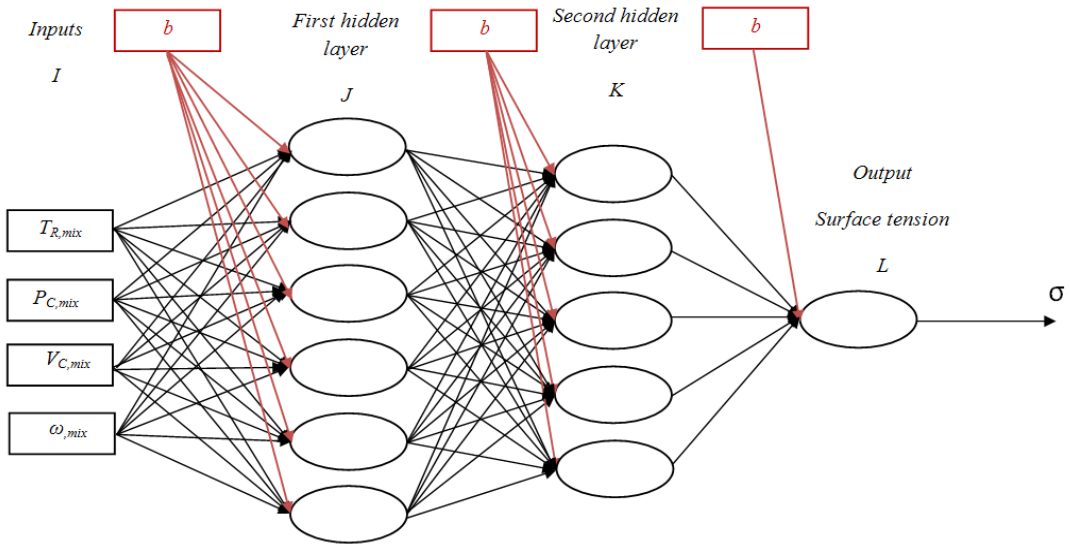

Figure 1
Neural network architecture.

As it is indicated in Figure 1, *i* is the input layer, *j* and *k* are the two hidden layers, and *l* is the output layer. According to the above definitions, the equations generating the outputs in the trained ANN are as follows:

$$output(\sigma_m) = \sum_{n=1}^{5} k_n \times w_{k_n - l_1} + b_{l_1} \tag{8}$$

$$k_n = \text{tangent}\, sigmoid\left(\sum_{x=1}^{6} j_x \times w_{j_x - k_n} + b_{k_n}\right) \tag{9}$$

$$j_x = \log sigmoid\left(\sum_{p=1}^{4} i_p \times w_{i_p - j_x} + b_{j_x}\right) \tag{10}$$

For instance, $w_{j_4-k_1}$ represents the weight value between neuron 4 in the first hidden layer (J_4) and neuron 1 in the second hidden layer (k_1). Log-sigmoid and tangent sigmoid functions are defined by:

$$\log sigmoid(x) = \frac{1}{1+e^{-x}} \tag{11}$$

$$\text{tangent } sigmoid(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}} \tag{12}$$

The values of weight functions in the input layer, hidden layers, and the output layer have been presented in Tables 2 to 4; also in addition, Table 5 shows the biases associated with the transfer functions of each layer.

Table 2
First layer weight functions ($W_{jx\text{-}ky}$).

x	***p*=1**	***p*=2**	***p*=3**	***p*=4**
1	202.0213	43.2631	181.1284	7.0159
2	45.5452	60.262	20.0581	1.9991
3	0.106	-0.4796	-2.1804	2.5569
4	4.0947	-1.5378	-3.9558	2.8492
5	13.8789	-0.2956	3.4186	-6.7226
6	137.6217	-4.363	3.5732	-9.2149

Table 3
Second layer weight functions ($W_{jx\text{-}ky}$).

y	***x* =1**	***x* =2**	***x* =3**	***x* =4**	***x* =5**	***x*=6**
1	24.0978	0.922	-91.3867	25.9599	-6.4133	-4.2283
2	-0.4556	-3.3241	-1.6047	-1.7602	2.0099	-6.4085
3	22.1346	-20.7459	-124.175	132.3635	208.7892	-24.8667
4	-1.8108	-5.6826	-58.231	15.7797	2.5286	-9.0837
5	3.4065	0.0684	82.3987	-25.8016	10.0343	1.177

Table 4
Third layer weight functions ($W_{ky\text{-}ln}$).

N	***y*=1**	***y*=2**	***y*=3**	***y*=4**	***y*=5**
1	-17.7458	-13.6074	-8.1823	-5.6212	-26.5498

Table 5
The biases.

I	b_{ji}	b_{ki}	b_{li}
1	-101.857	34.2327	15.9753
2	-29.3131	-3.4167	
3	1.4751	-9.0583	
4	0.817	48.2031	
5	-2.4349	-56.4983	
6	-24.4038		

3.2 Evaluation of the model

Figures 2 to 4 demonstrate the regression of the experimental value and the predicted/calculated value of surface tension for the training, testing, and total data.

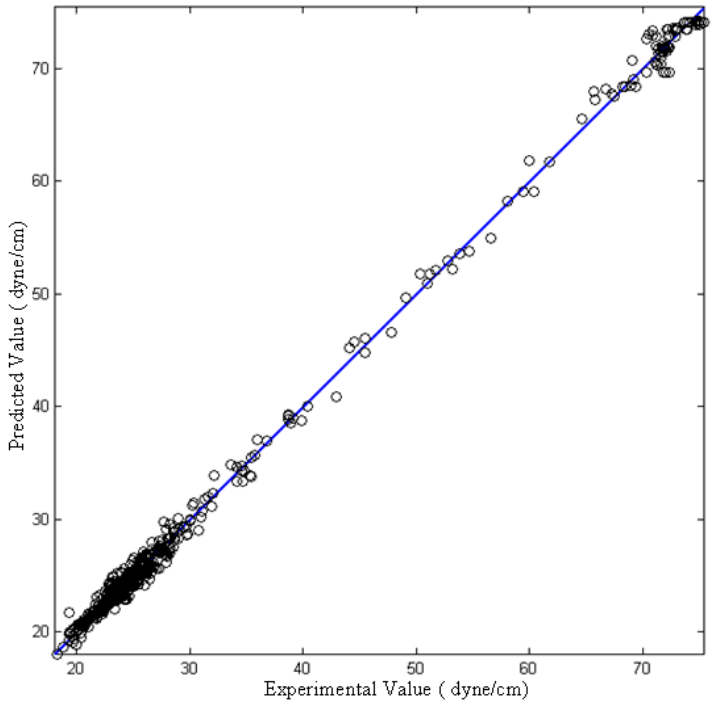

Figure 2
Surface tension calculated by ANN versus the experimental data for the, train data.

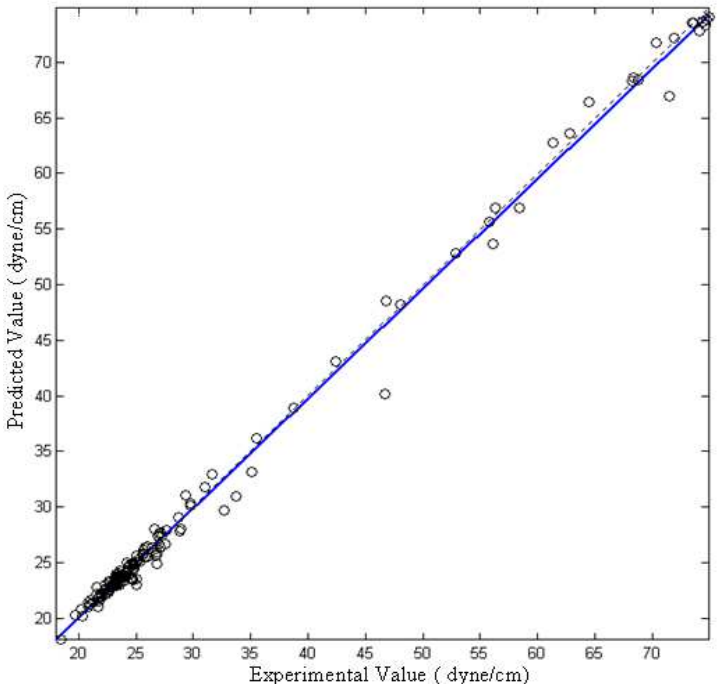

Figure 3
Surface tension predicted by ANN versus the experimental data for the test data.

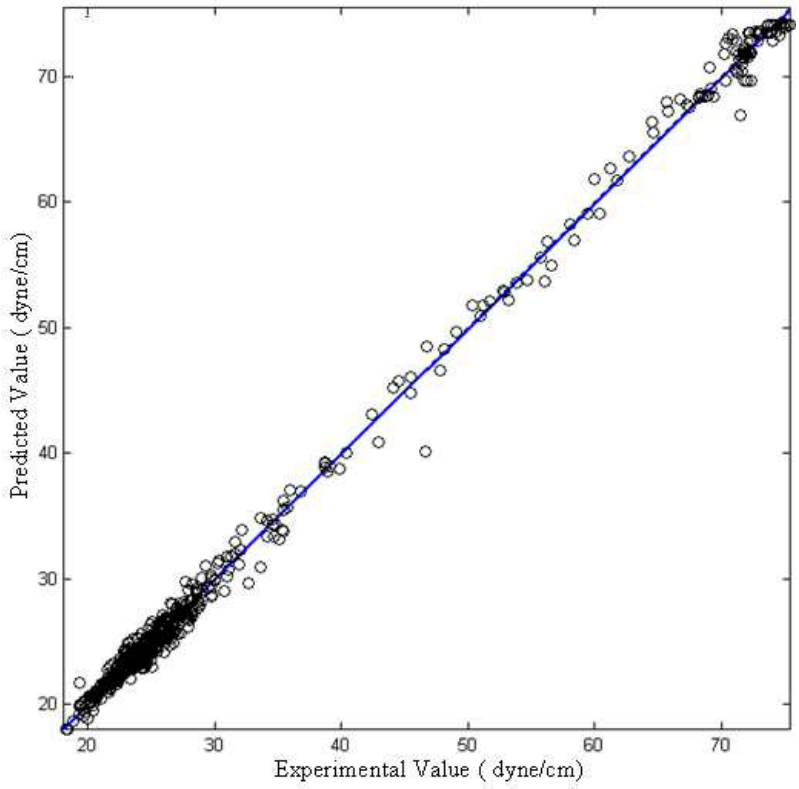

Figure 4
Surface tension predicted/calculated by ANN versus the experimental data for the total data.

The imprecision of the ANN model (in terms of AARD%) for estimating the surface tension of ternary liquid systems for the training, predicted, and total data points was obtained 1.69, 1.86, and 1.72 respectively. The maximum value of AARD% was attained from toluene/benzyl alcohol/ethyl acetate mixture (3.52%), while the minimum one was accomplished for water/ethyl butyrate/methanol (0.93%). The AARD% values of all the studied systems are presented in Table 6.

In order to make a more sensible assessment, the results of the ANN for some systems were compared with previous well-known models, i.e. Flory theory, Brok-Bird equation, and group contribution theory (Brock and Bird, 1955; Pandey et al., 2008). Table 7 presents the comparative results; as it is shown, the accuracy of the ANN model is more than the three studied models; in fact, the differences between the errors are so considerable. This model could be utilized as a new practical method for calculating the surface tension of ternary mixtures, particularly in engineering calculations. It should be noted that Flory theory, group contribution theory, and Brok-Bird equation require at least two or three interactions or adjustable parameters for predicting the surface tension of each ternary mixture, while the ANN model has overcome this disadvantage; in other words, the developed model does not require any adjustable parameters. The aim of this work is developing a general model which could be utilized without requiring detailed theories of thermodynamics. Moreover, the precise calculations and design is an essential necessity in the processes such as separation, distillation, extraction, adsorption, and EOR, which could be provided by the presented model.

Table 6
The obtained AARD% values for the prediction of the surface tension of ternary liquid mixtures.

Compound 1	Compound 2	Compound 3	AARD%
Water	Ethyl Butyrate	Methanol	0.93
Diethyl Carbonate	p-Xylene	Decane	1.32
Sulfuric Acid	Dimethylamine	Water	1.31
Heptane	Toluene	N,N-Dimethylformamide	2.45
Water	Acetone	Toluene	1.37
Water	n-Butyl Acetate	1-Propanol	2.33
n-Hexane	Cyclohexane	Benzene	1.90
Cyclohexane	n-Heptane	Toluene	3.23
n-Pentane	n-Hexane	Benzene	1.43
2,2,4-Trimethyl Pentane	Cyclohexane	Decane	1.44
Hexane	Decane	Hexadecane	1.89
Nitromethane	Benzene	1-Propanol	2.31
2-Propanol	Toluene	Furfural	2.68
Toluene	Benzyl Alcohol	Ethyl Acetate	3.52
Water	Ethyl Propionate	Methanol	1.04
		Total	1.72

Table 7
Comparison of Flory theory, Brok-Bird equation, and group contribution theory with the obtained ANN model.

Ternary mixture			AARD %	
			Flory theory	ANN model
n-Hexane	Cyclohexane	Benzene	4.58	1.90
n-Pentane	n-Hexane	Benzene	6.165762	1.43
Cyclohexane	n-Heptane	Toluene	3.67	3.23
Brok-Bird equation				
n-Hexane	Cyclohexane	Benzene	4.97	1.90
n-Pentane	n-Hexane	Benzene	6.165489	1.43
Cyclohexane	n-Heptane	Toluene	7.55	3.23
Group contribution theory				
n-Pentane	n-Hexane	Benzene	2.05	1.43
Cyclohexane	n-Heptane	Toluene	9.70	3.23

4. Conclusions

Artificial neural network method was successfully applied to predicting the surface tension of ternary mixtures. Following the corresponding-state models, critical properties along with the acentric factor of the mixtures were selected as the ANN input parameters by using the linear mixing rule for calculating mixture properties. The structure of the ANN model is composed of 2 hidden layers with 6

and 5 neurons in the first and second hidden layers respectively. The average absolute relative deviations for the training, the predicted, and the total data points were obtained 1.69, 1.86, and 1.72 respectively. The capability of the ANN model was compared with Flory theory, Brok-Bird equation, and group contribution theory for some systems. The comparative results proved that the deviations of the generated model were lower than the three mentioned models for all the studied systems. The most significant characteristic of the ANN model could be summarized into the following points:

1. The model calculates the surface tension of the mixtures more precisely than the existing methods;
2. The input data are available and the detailed data about the components would not be required.

This model is expected to be very helpful for engineering calculations, as well as software packages. It should be emphasized that the ANN method is a powerful approach to predicting complicated input-output systems.

Nomenclature

AARD%	: Average absolute relative deviations
ANN	: Artificial neural network
ANN-GC	: Artificial neural network-group contribution
EOR	: Enhance oil recovery
GC	: Group contribution
K	: Kelvin
M	: Molecular weight
MMM	: Mohsennia-Modarress-Mansoori
N	: Number of experimental data
P	: Pressure
QSPR	: Quantitative structure property relationship
S	: Specific gravity
SPT	: Scaled particle theory
T	: Temperature
V	: Volume
VTPR	: Volume-translated Peng–Robinson
VTSRK	: Volume-translated Soave Redlich–Kwong
Greek Symbols	
ω	: Acentric factor
Subscripts	
b	: Normal boiling point
c	: Critical
Superscript	
exp	: Experimental
prd	: Predicted

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