ARTIFICIAL NEURAL NETWORK MODELS FOR THE PREDICTION OF REFRACTIVE INDEX OF PURE ALCOHOLS

[1]KAMYAR MOVAGHARNEZHAD, [2]FATEME KORD, MEHRASA SARAIE

Faculty of Chemical Engineering, Babol Noshiravani University of Technology
E-mail: [1]movagharnejad@yahoo.com, [2]kordfatemeh@rocketmail.com

Abstract- In this study, the refractive index of 9 pure samples of 1-alcohols were experimentally investigated at (22 °C and 25 °C). These data were used to establish two different neural network models of multi-layer perceptron (MLP) and radial basis function (RBF)for prediction of refractive indexes of pure alcohols. For this purpose the temperature, molecular mass, and functional groups of the compounds were considered as the input parameters and the refractive index was considered as the only output of the two neural networks. 70% of the data are given as the training data, 15% as the validation data and 15% as the test data. The optimized MLP neural network had the mean square error (MSE) of 0.00000483712 for the training data, 0.0000649641 for the validation data, 0.000011277 for test data and the correlation coefficient (R) of 0.99238 with 6 optimal neurons in the hidden layer. Also in the optimized RBF neural network with 15 neurons had the minimum MSE of 0.0000135835.

Keywords - refractive index, Artificial Neural Network, alcohol, optimization, volumetric percentages

I. INTRODUCTION

Refractive index (n_D) is defined by the International Union of pure and Applied Chemistry as the ratio of the speed of light in a vacuum to that in a given medium [1]. The refractive index is considered as a fundamental physical property, especially in optics. It can indicate the purity of a substance or its concentration ina binary liquid mixture. It can also provide useful information about the intermolecular forces between different molecules. This fundamental property is related to other physicochemical properties such as density, surface tension, critical temperature, polarizability and boiling point [2,3].

In 2014, Gharagheizi et al. estimated the refractive index of pure organic compounds using an artificial neural network and group contribution methods. A group contribution method is known to predict the properties of pure components and mixtures using group or atomic properties. In this method, it is not necessary to know thousands of properties of compounds, but it is only needed to include data for a small group. So, the properties of each molecule may be determined by its components. 80% of the data were used for training, 10% for validation and the remaining 10% for testing. The neural network could estimate this set with a percentage Absoloute Average Relative Deviation (AARD%) of 0.83 [4].
In 2014, Sattari et al. continued the studies of Gharagheizi et al. They predicted the refractive index of ionic liquids (Ils) by using group contribution in the neural network. The researchers selected ILs because of their wide applications. Extraction and separation processes, solar panels, fuel cells, polymer and biopolymer processing, gas separation and carbon dioxide capturing are just some examples of these wide applications. The method was developed using refractive index data (λ = 589nm) of ILs extracted from the NIST Standard Reference Database. 80% of the data were used as the training set and 20% as the testing set. Finally, it was concluded that a linear summation of functional groups may provide a simple and reliable linear model. This neural network was used to determine the refractive index of ILs with an AARD% of 0.32% for the training data and 0.45% for the test data [5].
Coutinho and Gardas [2]introduced a group contribution model with ten particle-based ILs and composed of seven different types of anions, but this model could not predict the refractive index of ILs with different cations. Similar findings were found in the work of other researchers.

In 2015, Sattariet al.improved their previous work to predict the refractive index of the previous ILs data set by a new model called the QuantitativeStructure-Property Relationship method (QSPR). This method was presented to consider the cationic and anionic structure of compounds, instead of using the group contribution method. 80% of the data wereused for training and 20% for testing.

The genetic estimation function was used to select the parameters of the QSPR model. This neural network was finally able to estimate the refractive index of ILs with an AARD% of 0.47% for training data and 0.6% for testing data. Comparing the results of these research groups, it can be concluded that the method using the group contribution, yields a better result than the QSPR method [6].

Cano-Gómez [7] et al. measured the refractive index of pure 1-alcohols from methanol to 1-decanol at temperatures from (293 to 353)K. He used a straight line to represent the temperature functionality of the refractive indexes. This work claimed to present a generalized correlation for the refractive index of 1-alcohols as a function of the carbon number and the temperature.

In this study, the refractive index of 9 pure samples of 1-alcohols was measured and investigated.The functionality of these data to the temperature and number of carbon atoms was also studied. These data were also modeled with two different artificial neural networks of Multi-LayerPerceptron and Radial BasisFunction to give reasonable predictions.

II. EXPERIMENTAL DATA

Generally, the refractive index is a function of the temperature and the carbon number for a similar series of organic materials such as alcohols.

The liquid temperature was kept constant at 22°C and 25°C. Alcohol samplesfrom methanol to1-decanol except 1-nanonol were prepared and the refractive indexes of them were measured with a standard apparatus.

Table 1 and 2 represent the refractive index of samples at 22 °C and 25 °C.

sample	Redractive index
methanol	1.3285
ethanol	1.348
1-propanol	1.3842
1-butanol	1.3982
1-pentanol	1.409
1-hexanol	1.4165
1-heptanol	1.4228
1-octanol	1.4271
1-decanol	1.4355

1.
2.

Table 1: the refractive index of 1-alcohols at 22°C

sample	Refractive index
methanol	1.3265
ethanol	1.3466
1-propanol	1.3828
1-butanol	1.3969
1-pentanol	1.4072
1-hexanol	1.4154
1-heptanol	1.4221
1-octanol	1.4262
1-decanol	1.4351

Table 2: the refractive index of 1-alcohols at 25°C

Figure 1 and 2 represent the behavior of Refractive index with increasing number of carbon at 22 and 25 ° C.

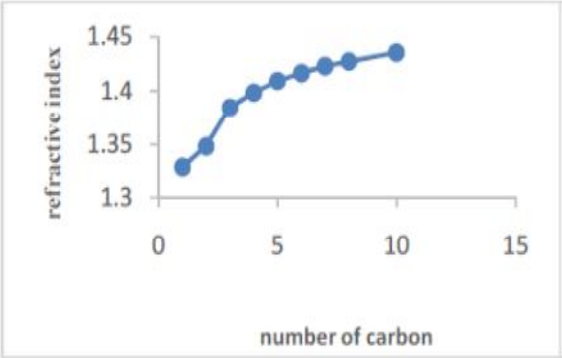


Figure 1: behavior of Refractive index with increasing number of carbon at 22°C

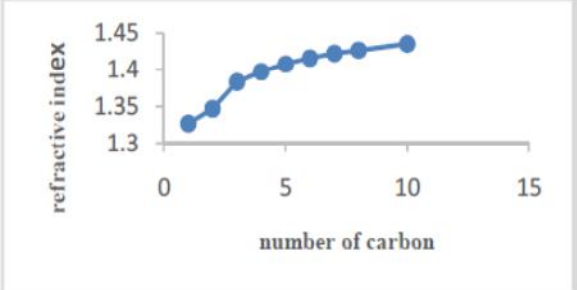


Figure 2: behavior of Refractive index with increasing number of carbon at 25°C

III. MODELING

Although some of the properties of pure substances or liquid mixtures are reported in the scientific literature, the measured data do not meet the needs of the wide industrial applications. In addition, experimental measurements are not always possible, in some cases it may be lengthy or time consuming. To solve this problem, prediction methods have been expanded using little experimental data. One of these prediction methods is the use of artificial neural network.

In this research we used Multilayer Perceptron artificial and Radial Basis Function artificial neural network to predict the refractive index of pure1-alcohols. The neural network includes three layers, named input layer, middle or hidden layer and output layer. The number of neurons in the middle layer has to be optimized during the network design. In this work sigmoid functions have been selected as the transfer functions.So, after reviewing various transfer functions, the hyperbolic tangent sigmoid was selected for the middle layer and the linear transfer function for the output layer. Also, 70% of the data were classified as training data, 15% as validation data and 15% as the test data.We also used the Lewenberg Marquard algorithm as the training function.

At first, we increased the number of neurons to 15 in the MLP neural network to find the optimal number of neurons in the hidden layer. The optimizing criteria was minimizing the Mean Squared Error of the model predictions in comparison to the test data.

The maximum number of neurons in a layer can be calculated from the following equation:

$$n_1 \leq \frac{k(n_i+n_o)-n_o}{n_i+n_o+1} \quad (1)$$

In the above relationship, k is the number of samples, n_i is the number of inputs and n_o is the number of outputs. According to calculations, the maximum number of neurons for the pure data is 15 neurons.

Number of Neurons	Regression of all	MSE of test
1	0.99117	6.75077E-05
2	0.99325	4.28515E-05
3	0.98684	0.000175632
4	0.99644	4.40521E-05
5	0.99159	0.000104929
6	0.99238	4.83712E-06
7	0.9717	0.000399383
8	0.99857	1.33902E-05
9	0.998	0.000024142
10	0.99279	5.55883E-06
11	0.75633	0.000213489
12	0.94734	0.000110213
13	98455	6.46212E-05
14	0.98822	1.55108E-05
15	0.97962	0.00030087

Table 3: MSE of test data vs the no. of neurons for the hidden layer

IV. RESULTS AND DISCUSSION

Table 3present the MSE and the regression values obtained from the MLP neural network for thetest data. According to Table 3, the MLP network with 6 neurons in the hidden layer gives the most accurate results, therefore, the neural network modelmay be presented as follows in the figure 3:

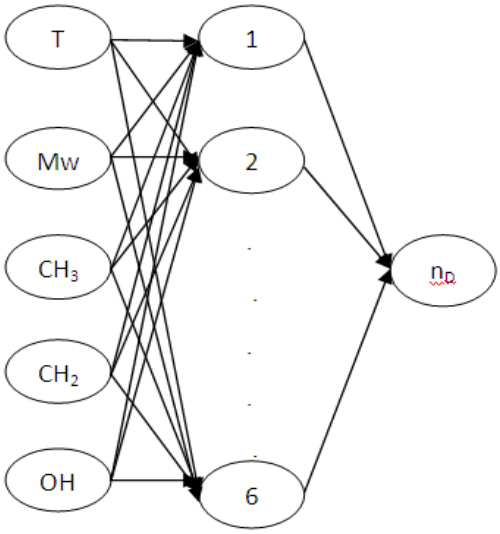


Figure 3: The architecture of the three-layer neural MLP neural network

After determining the number of optimal neurons, the weights and biases of the input and hidden layerswere calculated thatare presented in the Tables4and 5.

Input weight	T	Mw	CH2	bias
neuron 1	1.3515	-1.058	1.8311	-2.5288
neuron 2	2.7914	0.9721	0.5894	-1.2554
neuron 3	-1.9048	1.7157	1.1114	0.7166
neuron 4	1.485	1.1424	-1.7743	0.4668
neuron 5	0.2321	-2.6616	-0.8712	1.1935
neuron 6	-1.6475	1.5005	1.3133	-2.3537

Table 4: Weights and biases of the input layer of the MLP neural network

layer weight	
neuron 1	-0.0196
neuron 2	1.5213
neuron 3	1.0712
neuron 4	-0.4342
neuron 5	0.803
neuron 6	1.0693

Bias = 0.7606

Table 5: Weights and bias of the output layer of MLP neural network

The RBF neural network was also used to predict the refractive index of pure alcohols in this study. Table 6 shows the RBF specification in the neural network.

Goal	e-05
MaxNeuron	15
Spread	1
DisplayAt	1

Table 6: The specificationsof the RBF neural network

The table 6 presents the results of different RBF neural networks used to predict the refractive index.

number of neurons	MSE
neuron 0	0.0012172
neuron 2	0.0010244
neuron 3	0.0009474
neuron 4	0.000878
neuron 5	0.000783
neuron 6	0.0006924
neuron 7	0.0006112
neuron 8	0.0005199
neuron 9	0.0004386
neuron 10	0.0003466
neuron 11	0.0002719
neuron 12	0.0001794
neuron 13	0.0001133
neuron 14	2.195E-05
neuron 15	1.358E-05

Table 6: RBF design for pure samples

Performance = 1.36E-05

CONCLUSION

This article has shown that the rate of refractive index of organic 1-alcohols strongly depends on the temperature and number of carbon atoms. It was also observed that at a constant temperature the refractive index of 1-alcohols increases with increasing the number of carbon atoms (or the molecular weight) and it also decreases with increasing the temperature. It may be concluded that the optimized MLP and RBF neural networks are able to predict the refractive index of pure alcohols with a reasonable accuracy. This procedure may be extended to liquid mixtures especially binary 1-alcohol mixtures to see the probable ability of the method to predict the refractive index of the mixtures.

REFERENCES

[1] M. Deetlefs, K.R. Seddon, M. Shara, Neoteric optical media for refractive index determination of gems and mineral, Royal society od chemistry, 30, 317-326, 2006

[2] R.L. Gardas, J.A.P. Coutinho, Group contribution methods for the prediction of thermophysical and transport properties of ionic liquids, American Institute of Chemical Engineers, 55, 1274-1290, 2009.

[3] F. Gharagheizi, P. Ilani-Kashkouli, A. Karimi, A.H. Mohammadi, D. Ramjugeranth, A chemical structure based model for the estimation of refractive indices of organic compounds, Fluid phase equilibria, 384, 1-13, 2014.

[4] F. Gharagheizi, P. Ilani-Kashkouli, A. Karimi, A.H. Mohammadi, D. Ramjugeranth, Group contribution model for the prediction of refractive indices of ionic liquids, Chemical and engineering data, 59(6), 1930-1943, 2014.

[5] M. Sattari, A. Karimi, D. Ramjugeranth, A group contribution method for estimating the refractive indices of ionic liquids, Jurnal of molecular liquids, 200, 410-415, 2014

[6] M. Sattari, A. Karimi, D. Ramjugeranth, Prediction of refractive index of ionic liquids-A quantitative structure-property relationship based model, Taiwan institute of chemical engineer,52, 1-16, 2015

[7] J. J. Cano-Gómes, G. A. Iglesias-Silva, V. Rico-Ramirez, M. Ramos-Estrada, Kenneth R. Hall, A new correlation for the prediction of refractive index and liquid densities of 1-alcohols, Fluid phase equilibria, 387, 117-120, 2015.

★★★