International Journal of Engineering

Journal Homepage: www.ije.ir

TECHNICAL NOTE

Predicting the Coefficients of Antoine Equation Using the Artificial Neural Network

A. Khosravi Ghasemi, M. Mohammadpour Mir, S. Nanvakenari, K. Movagharnejad*

Faculty of Chemical Engineering, Babol Noshirvani University of Technology, Babol

PAPER INFO

Paper history:
Received 08 June 2019
Received in revised form 07 July 2019
Accepted 13 Septemeber 2019

Keywords:
Vapor Pressure
Antoine Equation
Modeling
Neural Network
Transfer Functions

ABSTRACT

Neural network is one of the new soft computing methods commonly used for prediction of the thermodynamic properties of pure fluids and mixtures. In this study, we have used this soft computing method to predict the coefficients of the Antoine vapor pressure equation. Three transfer functions of tan-sigmoid (tansig), log-sigmoid (logsig), and linear were used to evaluate the performance of different transfer functions to redict the coefficients of the Antoine vapor pressure equation. The critical pressure, critical temperature, critical volume, molecular weight, and acentric factor were considered as the input variables and the Antoine equation coefficients showed by the symbols A, B, and C were considered as the output variables. The results of this study indicated that the linear transfer function had a better performance than other transfer functions and the topology of 5-6-3 with Levenberg–Marquardt learning algorithm and linear transfer function had the best performance for prediction of these coefficients.

doi: *10.5829/ije.2019.32.10a.03*

1. INTRODUCTION

The thermodynamic properties of fluids, such as vapor pressure and density, etc., are significant parameters in different industries, like petrochemical, pharmaceutical, and chemical processes [1, 2]. Vapor pressure is considered as an important thermodynamic property in many processes of chemical engineering including chemical equilibrium, distillation, evaporation, etc. [3]. Many vapor pressure equations have been developed including Clausius–Clapeyron, Antoine, and Wagner, that each of them includes coefficients which are different for each substance. The physical and chemical properties of the materials or the parameters which lead to achieve these properties are not always available in various thermodynamic modes. Thus, use of methods through which these properties could be achieved is of great importance. Today, smart methods are among the new techniques used in modeling and estimating the properties. In fact, these methods use the hidden knowledge in experimental data to discover the intrinsic relationships between the data to be generalized for other situations. Artificial neural networks are one of these methods. Such networks are inspired by the human brain. In these networks, the data information is stored in the form of network weights after the training process [4]. Each input into the network is multiplied by a synaptic weight and added to a bias and different algorithms are used for network training [5]. Several kinds of researches have been conducted on the estimation of thermodynamic properties using neural networks. Lashkarbolooki et al. [6] predicted the bubble and dew points pressures of binary systems by artificial neural network. They could do it with average absolute relative deviation (AARD) % of 2.66 and corelation coefficient (R^2) of 0.9950. In another study, Moosavi et al. [7] estimated the density of alkanes at high temperature and pressure. They used a combined method includeing an artificial neural network (ANN) with group contribution method (GCM) inputs. The work showed that this method could estimate the density of hydrocarbons with good accuracy. In addition, Moghadassi et al. [8] presented a model by a neural network that could estimate the sulfur dioxide density. The best network arrangement for this case was the Levenberg-Marquardt training algorithm with 15-10-1 topology and had good performance. In the present study, the multilayer perceptron (MLP) neural network with the transfer

*Corresponding Author Email: *k-movaghar@nit.ac.ir* (K. Movagharnejad)

Please cite this article as: A. Khosravi Ghasemi, M. Mohammadpour Mir, S. Nanvakenari, K. Movagharnejad, Predicting the Coefficients of Antoine Equation Using the Artificial Neural Network, International Journal of Engineering (IJE), IJE TRANSACTIONS A: Basics Vol. 32, No. 10, (October 2019) 1353-1357

functions of tangent sigmoid (Tansig), logaritmic sigmoid (Logsig), and linear is used to predict the coefficients A, B, and C of Antoine equation. In general, the capability of different transfer functions in estimating the coefficients of the Antoine equation is investigated.

2. MODELING

2. 1. Antoine Equation Antoine equation determines the vapor pressure on the basis of absolute temperature. Antoine performed a simple modification on Clausius–Clapeyron equation in 1888 and proposed it for a wide range of temperatures. Equation (1) represents the Antoine equation [9]:

$$log_{10}^{p} = A - \frac{B}{C+T} \quad (1)$$

where T represents the absolute temperature in Kelvin, P represents the vapor pressure in bar, and A, B, C represent the coefficients of Antoine equation.

2. 2. Neural Network Design In this study, the Antoine equation coefficients were predicted by a multi-layer perceptron neural network. This network contains three layers, known as the input, hidden, and output layers. The input layer consists of five neurons each of which is related to an input variable. In this study, the critical pressure, critical temperature, critical volume, molecular weight, and acentric factor were the input variables. The output layer included three neurons that were equal to the number of output variables, including the coefficients A, B, and C in the Antoine equation. The number of hidden layer neurons varied from 3 to 10 to select a network with the minimum error and maximum correlation coefficient as the best topology by trial and error method. In this work, 211 experimental data were collected from various studies [10, 11]. 70% of data were considered for training , 15% for validation and 15% for testing. In this study, the Levenberg–Marquardt algorithm was used. This algorithm has faster speed and higher computational volume compared to other algorithms. In general, this algorithm has acceptable performance for prediction or estimation problems. In order to evaluate different transfer functions in the performance of the neural network, three types of transfer functions such as Tansig, Logsig, and linear were used in the hidden layer of a neural network. In addition, the linear function was used in the output layer. Equations (2), (3), and (4) indicate the Tansig, Logsig, and linear functions, respectively [12].

$$\mathrm{F(x)} = 2/((1+\exp(-2\mathrm{x})) - 1) \quad (2)$$

$$\mathrm{F(x)} = 1/(1+\exp(-\mathrm{x})) \quad (3)$$

$$\mathrm{F(x)} = x \quad (4)$$

In order to evaluate the neural network performance, two parameters of absolute relative deviation (ARD) and correlation coefficient (R^2) were used to achieve the best model for estimating Antoine equation coefficients. The ARD and R^2 were obtained from Equations (5) and (6), respectively.

$$\%ARD = \frac{1}{N}\sum_{i=1}^{N} 100 \left|\frac{Xexp - Xcal}{Xexp}\right| \quad (5)$$

$$\mathrm{R}^2 = \frac{\sum_{I=1}^{N}(Xexp - X\ avg)^2 - \sum_{I=1}^{N}(Xexp - X\ cal)^2}{\sum_{I=1}^{N}(Xexp - Xavg)^2} \quad (6)$$

where N represents the number of experimental data, X_{exp} represents the experimental coefficient, X_{cal} denotes the calculated coefficient, and X_{avg} represents the mean of the experimental coefficient [6, 13]. In order to investigate the network performance in estimating each coefficient of the Antoine equation, the ARD was calculated separately for each coefficient.

3. RESULTS AND DISCUSSION

The results of the prediction of Antoine equation coefficients by the MLP neural network under the three transfer functions of Tansig, Logsig, and linear are given in Table 1.

Based on Table 1, the topology 5-6-3 had the best performance in comparison to other topologies among the neural network with the Tansig transfer function. In the higher number of neurons, the neural network performance with Tansig drops, so that its error will increase to estimate the coefficients A, and B. In addition, it can be found that the network with Logsig transfer function in the topology 5-3-3 had a good performance and low error while it had high error in other modes. However, the network with linear transfer function in the topology 5-6-3 had acceptable performance in all modes and its error for all three coefficients was very low compared to other transfer functions. In general, all the three transfer functions had a good performance in estimating Antoine equation coefficients while the neural network with the topology 5-6-3 and linear transfer function had the best performance (low error and high correlation coefficient) among other topologies and various transfer functions. Figure 1 indicates the output values by the neural network and the actual output for training, test, validation, and all data for the best neural network arrangement (topology 5-6-3 and linear transfer function) [14].

Based on Figure 1, the correlation coefficient for the training, validation, and test data was high while the network error was low. According to this figure, the output and target data for training, validation, and testing (all data) coincided on the line of Y=X approximately that showed the modeling is done well. In general, it can be said that the designed network could perform modeling and predict the coefficients A, B and C properly.

TABLE 1. The results of the prediction of Antoine equation coefficients

Topology	Correlation coefficient	Validation correlation coefficient	Transfer function	ARD % (A)	ARD % (B)	ARD % (C)
5-3-3	0.99954	0.99932	Tansig	0.5	0.0097	0.2304
	0.99950	0.99944	Logsig	0.15	0.1433	0.0549
	0.99952	0.99956	pureline	0.04	0.2111	0.0513
5-4-3	0.99960	0.99936	Tansig	2.46	0.0833	0.1109
	0.99946	0.99920	Logsig	1.3	0.3304	0.0028
	0.99952	0.99926	pureline	0.0562	0.0832	0.0094
5-5-3	0.99972	0.99970	Tansig	0	0.1	0.11
	0.99960	0.99954	Logsig	1.38	0.24485	0.067
	0.99970	0.99958	pureline	0	0.0734	0.0146
5-6-3	0.99970	0.99984	Tansig	0.06	0.0834	0.0353
	0.99960	0.99966	Logsig	1.3	0.2234	0.0355
	0.99968	0.99946	pureline	0.02	0.0199	0.0034
5-7-3	0.99986	0.99958	Tansig	1.71	0.2421	0.0951
	0.99960	0.99966	Logsig	1.18	0.1137	0.0262
	0.99962	0.99946	pureline	0	0.0269	0.0711
5-8-3	0.99972	0.99974	Tansig	1.18	0.1137	0.0262
	0.99962	0.99952	Logsig	3.65	0.3832	0.0305
	0.99952	0.99944	pureline	0.02	0.0710	0.002
5-9-3	0.99974	0.99958	Tansig	2.55	0.0613	0.0813
	0.99962	0.99954	Logsig	0.1	0.1207	0.094
	0.99952	0.99954	pureline	0.05	0.3056	0.1232
5-10-3	0.99964	0.99970	Tansig	1.15	0.1326	0.0372
	0.99952	0.99918	Logsig	1.11	0.2127	0.1054
	0.99952	0.99956	pureline	0.02	0.0949	0.0089

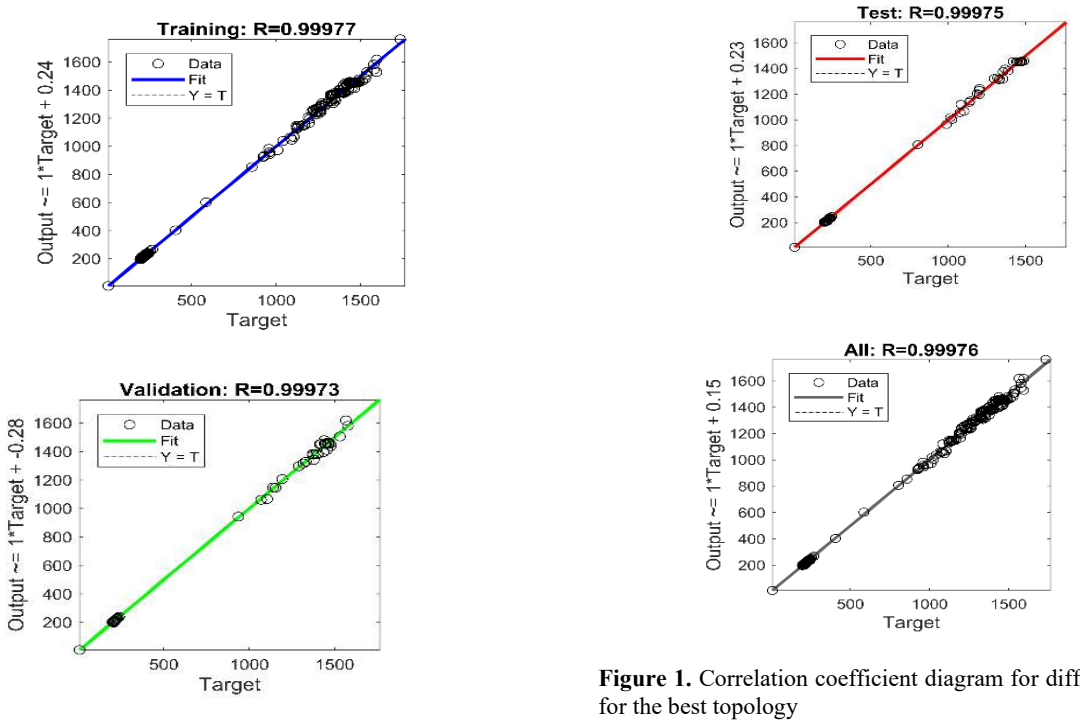

Figure 1. Correlation coefficient diagram for different data for the best topology

Ultimately, we compared our results in this work with another method as presented in Table 2. The results revealed that the AARD of ANN model (this work) is better than that of GCM [15].

TABLE 2. Comparison between this work (ANN) and GCM for Antoine coefficient prediction of selected system.

Compounds	This work (ANN)			Tochigi et al. (GCM) [16]		
	ARD (A) %	ARD (B) %	ARD (C)%	ARD (A) %	ARD (B) %	ARD (C)%
butane	0.293	0.727	0.418	4.698	8.573	0.364
1-butene	0.146	0.144	0.166	4.824	7.904	0.541
pentane	0.726	1.768	0.038	0.581	0.894	0.475
1-hexene	0.291	0.588	0.668	1.018	0.358	1.748
hexane	0.291	1.032	0.958	0	1.199	1.387
1-heptene	0.579	1.678	0.620	1.014	2.473	1.268
heptane	0.290	1.535	1.209	1.741	3.192	0.480
1-octene	0.721	2.569	0.338	2.164	4.269	0.874
octane	0.289	1.907	1.141	2.604	4.187	0.339
4-methylheptane	0.434	1.129	0.526	1.304	2.490	0.503
2,2,3-trimethylbutane	0.736	2.495	1.796	1.472	1.269	2.234
2,3-dimethylhexane	0	0.084	0.102	0.582	1.489	0.588
2-methylhexane	0.291	0.786	0.523	0	0.868	1.161
1,2-pentadiene	0.867	3.438	2.119	3.612	7.021	1.332
1-pentyne	1.434	4.175	2.302	1.004	1.902	0.127
avg	0.492	1.604	0.862	1.775	3.206	0.895

4. CONCLUSION

Based on the conducted studies, the MLP neural network with the transfer functions of Tansig, Logsig, and linear had acceptable performance. In Tansig and Logsig functions, the error increased with the increasing number of neurons while the neural network with linear functions was often better than other transfer functions. In general, the topology 5-6-3 with linear transfer function had the best performance among the other modes and can be used for predicting the constant coefficients of the Antoine equation.

5. ACKNOWLEDGEMENT

The authors acknowledge the funding support of Babol Noshiravani University of Technology through Grant No. BNUT/370675/98.

6. REFERENCES

1. Rohani, A.A., Pazuki, G., Najafabadi, H.A., Seyfi, S. and Vossoughi, M., "Comparison between the artificial neural network system and saft equation in obtaining vapor pressure and liquid density of pure alcohols", ***Expert Systems with Applications***, Vol. 38, No. 3, (2011), 1738-1747.
2. Movagharnejad, K. and Saffar, F., "Predicting the coefficients of the daubert and danner correlation using a neural network model", ***Iranian Journal of Chemical Engineering***, Vol. 15, No. 2, (2018), 79.
3. Sanjari, E., "A new simple method for accurate calculation of saturated vapor pressure", ***Thermochimica Acta***, Vol. 560, (2013), 12-16.
4. Maleki, N., Kashanian, S., Maleki, E. and Nazari, M., "A novel enzyme based biosensor for catechol detection in water samples using artificial neural network", ***Biochemical Engineering Journal***, Vol. 128, (2017), 1-11.
5. Akin, D. and Akba, B., "A neural network (nn) model to predict intersection crashes based upon driver, vehicle and roadway surface characteristics", ***Scientific Research and Essays***, Vol. 5, No. 19, (2010), 2837-2847.
6. Lashkarbolooki, M., Shafipour, Z.S., Hezave, A.Z. and Farmani, H., "Use of artificial neural networks for prediction of phase equilibria in the binary system containing carbon dioxide", ***The Journal of Supercritical Fluids***, Vol. 75, (2013), 144-151.
7. Moosavi, M. and Soltani, N., "Prediction of hydrocarbon densities using an artificial neural network–group contribution method up to high temperatures and pressures", ***Thermochimica Acta***, Vol. 556, (2013), 89-96.
8. Moghadassi, A., Nikkholgh, M., Hosseini, S. and Parvizian, F., "Estimation of vapor pressures, compressed liquid, and supercritical densities for sulfur dioxide using artificial neural networks", ***International Journal of Industrial Chemistry***, Vol. 4, No. 1, (2013), 14.
9. Yaws, C.L., "The yaws handbook of vapor pressure: Antoine coefficients, Gulf Professional Publishing, (2015).

10. Yaws, C. and Yang, H., "To estimate vapor pressure easily", ***Hydrocarbon Processing;***(USA), Vol. 68, No. 10, (1989), 65–68.
11. Yaws, C.L. and Narasimhan, P.K., Critical properties and acentric factor—organic compounds, in Thermophysical properties of chemicals and hydrocarbons. 2009, Elsevier.1-95.
12. Taki, M., Rohani, A., Soheili-Fard, F. and Abdeshahi, A., "Assessment of energy consumption and modeling of output energy for wheat production by neural network (mlp and rbf) and gaussian process regression (GPR) models", ***Journal of Cleaner Production***, Vol. 172, (2018), 3028-3041.
13. Azadbakht, M., Aghili, H., Ziaratban, A. and Torshizi, M.V., "Application of artificial neural network method to exergy and energy analyses of fluidized bed dryer for potato cubes", ***Energy***, Vol. 120, (2017), 947-958.
14. Najafi-Marghmaleki, A., Khosravi-Nikou, M.R. and Barati-Harooni, A., "A new model for prediction of binary mixture of ionic liquids+ water density using artificial neural network", ***Journal of Molecular Liquids***, Vol. 220, (2016), 232-237.
15. Tochigi, K., Yamagishi, M., Ando, S., Matsuda, H. and Kurihara, K., "Prediction of antoine constants using a group contribution method", ***Fluid Phase Equilibria***, Vol. 297, No. 2, (2010), 200-204.

The Prediction of Vapor Pressure Coefficients in Antoine Equation Using Artificial Neural Network

TECHNICAL NOTE

A. Khosravi Ghasemi, M. Mohammadpour Mir, S. Nanvakenari, K. Movagharnejad

Faculty of Chemical Engineering, Babol Noshirvani University of Technology, Babol

P A P E R I N F O

Paper history:
Received 08 June 2019
Received in revised form 07 July 2019
Accepted 13 Septemeber 2019

Keywords:
Vapor Pressure
Antoine Equation
Modeling
Neural Network
Transfer Functions

چکیده

یکی از روش‌های نوین جهت پیش‌بینی خواص ترمودینامیکی شبکه عصبی بوده است. در این تحقیق به منظور بررسی عملکرد توابع انتقال مختلف در پیش‌بینی ضرایب آنتوان از ۳ تابع انتقال تانژانت سیگموئید، سیگموئید لگاریتمی و خطی استفاده شد. در این بررسی فشار بحرانی، دمای‌بحرانی، حجم بحرانی، جرم مولکولی و ضریب بی مرکزی به عنوان متغیر ورودی و ضرایب معادله‌ی آنتوان (A, B, C) نیز متغیر خروجی در نظر گرفته شد. نتایج حاصل از این بررسی بدین گونه بوده که تابع انتقال خطی عملکرد بهتری نسبت به سایر توابع انتقال داشته و توپولوژی ۳-۶-۵ با الگوریتم آموزش لونبرگ مارکوارت و تابع انتقال خطی بهترین عملکرد را داشته است.

***doi**: 10.5829/ije.2019.32.10a.03*