# Prediction of phase equilibria in binary systems containing acetone using artificial neural network

Ali Farzi<sup>\*1</sup>, Ali Tarjoman Nejad<sup>2</sup>

**Abstract** — In this paper, phase equilibrium of eleven binary systems containing acetone is estimated using artificial neural networks (ANN). VLE data were taken from literature for wide ranges of temperature (298.15-391.25K) and pressure (2.640 to 101.33kPa). Based on obtained results, the best structure for ANN is feed-forward network with sigmoid and linear activation functions for hidden and output layers, respectively. The network consists of seven inputs for temperature, pressure, acentric factor, critical temperature and critical pressure of the system, 19 neurons in hidden layer and two neurons in output layer corresponding to vapor and liquid compositions of acetone in binary mixture. The weights were optimized to minimize error between calculated and experimental VLE data using Levenberg-Marquardt back propagation training algorithm. Results show that optimum network architecture is able to predict equilibrium data of binary systems containing acetone with an acceptable level of accuracy AAD % of 0.815, and R<sup>2</sup> of 0.9979.

Index Terms: Phase equilibria, Artificial neural networks, Back propagation, Feed-forward ANN, Acetone

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#### **1** INTRODUCTION

**TAPOR-liquid** equilibrium data play important role for modeling, design and control of chemical processing systems. Usually equations of state are used for estimation of vapor-liquid equilibria. Using EOS for estimation of VLE makes it unsuitable for real time control because of many adjustable parameters used in EOS. Today's, artificial neural networks have gained wide applications for estimation of properties of components such as viscosity [1-3], heat capacity [4-6], density [7-9], thermal conductivity [10-12] and vapor pressure [13]. Many studies have been done in the field of prediction of phase equilibria using artificial neural networks. Sharma, et al. [14] investigated potential application of artificial neural networks in thermodynamics. They predicted vapor-liquid equilibrium for ethane/methane and ammonia/water systems with error level of ±1%. Iliuta, et al. [15] investigated vapor-liquid equilibria in electrolyte solutions. They predicted vapor-liquid equilibrium with AAD% of 2.5 for all experimental data.

Urata, et al. [16] investigated systems containing hydrofluoroethers (HFEs). They calculated activity coefficients using ANNs with reasonable accuracy. Mohanty [17, 18] predicted phase equilibrium for systems containing carbon dioxide. Systems investigated by Mohanty include carbon dioxide, ethyl caproate, ethyl caprilate, and ethyl caprate. The average absolute deviation of all systems for estimation of liquid phase mole fraction was less than 3% and for vapor phase mole fraction less than 0.02%. Govindarajan and Sabarathinam [19] investigated azeotropic systems. Also Ghanadzadeh and Ahmadifar [20] predicted VLE data of binary systems including tert-butanol + 2-ethyl-1-hexanol and n-butanol + 2-ethyl-1-hexanol. They calculated boiling temperature with AAD% of 3.3%. Lashkarbolooki, et al. [21] used ANN model for estimation of equilibrium in systems containing carbon dioxide. Their investigated systems include  $CO_2$  + 1-hexene,  $CO_2$  + n-Hexane and  $CO_2$  + n-butane. They predicted vapor-liquid equilibrium with an acceptable level of accuracy of ARD % of 2.66 and R<sup>2</sup> of 0.9950 within their experimental uncertainty.

In this paper, phase equilibria for eleven binary systems containing acetone are investigated.

# 2 THEORY

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#### 2.1 Artificial neural networks

The idea of artificial neural networks (ANNs) originates from human neural network. ANNs include sets of connected neurons. They are usually comprised of one input layer, one or more hidden layers and an output layer [7]. Output of each neuron before applying activation function is calculated from outputs of previous layers based on (1):

$$s_{j}^{h} = \sum_{i=1}^{n} w_{ij}^{h} + b_{j}^{h}$$
(1)

where  $s_j^h$ ,  $w_{ij}^h$ , and  $b_j^h$  are output of *j*th neuron before applying activation function, weights connecting *i*th neuron (from previous layer) to *j*th neuron in current layer, and bias of *j*th neuron, respectively. Output of each neuron is calculated by an activation function as (2).

$$y_{j}^{h} = F\left(s_{j}^{h}\right) \tag{2}$$

where  $y_j^h$  is output of *j*th neuron and *F* is activation function. Common activation functions are linear (purelin), logarithmic sigmoid (logsig), and hyperbolic tangent sigmoid (tansig) which are defined in equations (3) to (5), respectively:

$$y_j = s_j \tag{3}$$

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$$y_{j} = \frac{1}{1 + e^{-s_{j}}}$$
(4)

$$y_{j} = \frac{e^{s_{j}} - e^{-s_{j}}}{e^{s_{j}} + e^{-s_{j}}}$$
(5)

Generally, input layer uses required data to feed into the network and create the inputs of ANN. The outputs as dependent variables will be generated using output layer, and a hidden layer provides some flexibility [21].

It should be considered that, one of critical parameters is the number of neurons in the hidden layer because if the number of neurons is low then the network maybe unable to reach to the desired error, while a large number of neurons may cause over fitting [22]. Since there is not a specific method to determine the number of neurons of hidden layers, optimum number of neurons usually is determined by adding neurons during the training process, i.e. in a trial and error manner [7].

# **3** DISCUSSION

#### 3.1 Experimental data

Compiling the database to train the network is the first step for neural network modeling. Experimental VLE data for eleven binary systems containing acetone within temperature range of 298.15-391.25K and pressure range of 2.640-101.33kPa are used for training, validating and testing AAN model which comprised of 304 experimental data points. The temperature and pressure range for phase equilibria are reported by the authors summarized in Table 1.

TABLE 1

EXPERIMENTAL DATA AND RANGE OF PARAMETERS USED IN THIS RESEARCH

SystemTemperature (K)Pressure (kPa)Ref.1-Butanol $298.15$ $9.733-25.331$ [23] $331.25 - 388.15$ $99.46$ [24]2-Propanol $298.15$ $5.906 - 30.198$ [25] $328.15$ $34.393-94.308$ [26] $329.93 - 352.93$ $101.33$ [26]Acetic acid $329.25 - 391.25$ $101.33$ [27] $333.85 - 385.25$ $101.33$ [28] $303.15$ $2.640 - 36.530$ [29] $308.15 - 328.15$ $5.346 - 90.081$ [30]Acetonitrile $318.15$ $30.38 - 64.181$ [31] $30.75 - 352.95$ $101.19$ [32]Benzene $318.15$ $33.428 - 67.189$ [33]Ethanol $329.25 - 351.45$ $101.33$ [34] $330.15 - 348.45$ $101.33$ [34] $329.75 - 348.45$ $101.33$ [35] $328.36 - 348.05$ $96.93$ [36] $312.45 - 332.55$ $53.33$ [37]Vinvl acetate $298.15 - 323.15$ $16.731 - 81.093$ [30]				
331.25 - 388.15       99.46       [24]         2-Propanol       298.15       5.906 - 30.198       [25]         328.15       34.393-94.308       [26]         329.93 - 352.93       101.33       [26]         Acetic acid       329.25 - 391.25       101.33       [27]         333.85 - 385.25       101.33       [28]         303.15       2.640 - 36.530       [29]         308.15 - 328.15       5.346 - 90.081       [30]         Acetonitrile       318.15       30.038 - 64.181       [31]         30.75 - 352.95       101.19       [32]         Benzene       318.15       33.428 - 67.189       [33]         Ethanol       329.25 - 351.45       101.33       [34]         330.15 - 348.55       101.33       [34]         329.75 - 348.45       101.33       [35]         328.36 - 348.05       96.93       [36]         312.45 - 332.55       53.33       [37]	System	Temperature (K)	Pressure (kPa)	Ref.
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1-Butanol	298.15	9.733-25.331	[23]
328.15       34.393-94.308       [26]         329.93 - 352.93       101.33       [26]         Acetic acid       329.25 - 391.25       101.33       [27]         333.85 - 385.25       101.33       [28]         303.15       2.640 - 36.530       [29]         308.15 - 328.15       5.346 - 90.081       [30]         Acetonitrile       318.15       30.038 - 64.181       [31]         300.75 - 352.95       101.19       [32]         Benzene       318.15       33.428 - 67.189       [33]         Ethanol       329.25 - 351.45       101.33       [34]         303.15 - 348.55       101.33       [34]         329.75 - 348.45       101.33       [35]         328.36 - 348.05       96.93       [36]         312.45 - 332.55       53.33       [37]		331.25 - 388.15	99.46	[24]
329.93 - 352.93         101.33         [26]           Acetic acid         329.25 - 391.25         101.33         [27]           333.85 - 385.25         101.33         [28]           303.15         2.640 - 36.530         [29]           308.15 - 328.15         5.346 - 90.081         [30]           Acetonitrile         318.15         30.038 - 64.181         [31]           300.75 - 352.95         101.19         [32]           Benzene         318.15         33.428 - 67.189         [33]           Ethanol         329.25 - 351.45         101.33         [34]           330.15 - 348.55         101.33         [34]           232.975 - 348.45         101.33         [35]           328.36 - 348.05         96.93         [36]           312.45 - 332.55         53.33         [37]	2-Propanol	298.15	5.906 - 30.198	[25]
Acetic acid         329.25 - 391.25         101.33         [27]           333.85 - 385.25         101.33         [28]           303.15         2.640 - 36.530         [29]           308.15 - 328.15         5.346 - 90.081         [30]           Acetonitrile         318.15         30.038 - 64.181         [31]           300.75 - 352.95         101.19         [32]           Benzene         318.15         33.428 - 67.189         [33]           Ethanol         329.25 - 351.45         101.33         [34]           300.15 - 348.55         101.33         [34]           289.75 - 348.45         101.33         [35]           328.36 - 348.05         96.93         [36]           312.45 - 332.55         53.33         [37]		328.15	34.393-94.308	[26]
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Benzene         318.15         33.428 - 67.189         [33]           Ethanol         329.25 - 351.45         101.33         [34]           330.15 - 348.55         101.33         [34]           Ethyl acetate         329.75 - 348.45         101.33         [35]           328.36 - 348.05         96.93         [36]         312.45 - 332.55         53.33         [37]	Acetonitrile	318.15	30.038 - 64.181	[31]
Ethanol         329.25 - 351.45         101.33         [34]           330.15 - 348.55         101.33         [34]           Ethyl acetate         329.75 - 348.45         101.33         [35]           328.36 - 348.05         96.93         [36]         312.45 - 332.55         53.33         [37]		330.75 - 352.95	101.19	[32]
330.15 - 348.55         101.33         [34]           Ethyl acetate         329.75 - 348.45         101.33         [35]           328.36 - 348.05         96.93         [36]           312.45 - 332.55         53.33         [37]	Benzene	318.15	33.428 - 67.189	[33]
Ethyl acetate         329.75 - 348.45         101.33         [35]           328.36 - 348.05         96.93         [36]           312.45 - 332.55         53.33         [37]	Ethanol	329.25 - 351.45	101.33	[34]
328.36 - 348.05         96.93         [36]           312.45 - 332.55         53.33         [37]		330.15 - 348.55	101.33	[34]
312.45 - 332.55 53.33 [37]	Ethyl acetate	329.75 - 348.45	101.33	[35]
	-	328.36 - 348.05	96.93	[36]
Vinvl acetate 298 15 - 323 15 16 731 - 81 093 [30]		312.45 - 332.55	53.33	[37]
(int) accuace = = = = = = = = = = = = = = = =	Vinyl acetate	298.15 - 323.15	16.731-81.093	[30]
P-Xylene 313.15 2.648 - 56.603 [38]	P-Xylene	313.15	2.648 - 56.603	[38]
313.15 9.9 - 53.5 [39]		313.15	9.9 - 53.5	[39]
353.15 33.6 - 205.4 [39]		353.15	33.6 - 205.4	[39]
Croton aldehyde 298.15 - 328.15 6.839 - 93.441 [30]	Croton aldehyde	298.15 - 328.15	6.839 - 93.441	[30]
Acetone oxime 329.4 - 342.4 101.3 [40]	Acetone oxime	329.4 - 342.4	101.3	[40]
methyl ether	methyl ether			

In this paper, mole fraction of acetone in liquid and vapor phase is estimated as a function of critical temperature, critical pressure, acentric factor, temperature, and pressure:

$$(x, y) = f(T_c, P_c, \omega, T, P)$$

Physical properties of the components are shown in Table 2.

PHYSICAL PROPERTIES OF STUDIED COMPONENTS	[41]	1
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Component	Molecular weight			Critical pressure	Acentric factor
		point (K)	(K)	(kPa)	
1-Butanol	74.123	390.898	563.098	4420	0.5929
2-Propanol	88.1492	392.148	552	3870	0.6746
Ethanol	46.0699	351.398	513.9	6147	0.6443
Acetic acid	60.0517	391.1	592.7	5770	0.4469
Acetonitrile	41.053	354.799	545.5	4820	0.3269
Ethyl acetate	146.143	463.648	652	3080	0.5595
Vinyl acetate	86.091	346	525	4349	0.34
Benzene	78.11	353.239	562.098	4924	0.215
p-Xylene	106.166	411.51	616.26	3510	0.3258
Croton aldehyde	184.322	523.15	685	1860	0.7538
AOME	75.1106	431.148	630	5220	0.5854

#### 3.2 Error analysis of ANNs

In order to evaluate the accuracy and efficiency of proposed ANN model for prediction of VLE data at different temperatures and pressures, some statistical parameters including average absolute deviation percent (AAD %), average deviation percent (Bias), root mean square error (RMS) and correlation coefficient (R<sup>2</sup>) were utilized which are defined as follows [7]:

$$R^{2} = \frac{\sum_{i=1}^{N} \left(A_{i}^{exp} - \overline{A}\right)^{2} - \sum_{i=1}^{N} \left(A_{i}^{exp} - A_{i}^{cal}\right)^{2}}{\sum_{i=1}^{N} \left(A_{i}^{exp} - \overline{A}\right)^{2}}$$
(7)

where *N* is the number of VLE data points,  $A_i^{exp}$  is the *i*th experimental value,  $A_i^{cal}$  is the *i*th value predicted by ANN model, and  $\overline{A}$  is the average value of experimental VLE data.

#### 3.3 Neural network model

Feed forward neural network is selected as ANN model as all systems are stationary. The schematic of ANN used to predict phase equilibria of binary systems containing acetone is shown in Fig. 1.

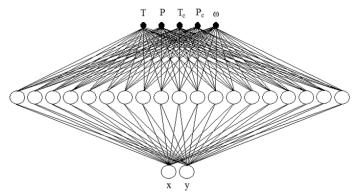


Fig. 1. Schematic of the neural network model used for phase equilibria

In this research 70% of experimental data were used for training, 20% for validating and 10% for testing.

(6)

Usually researchers state that a neural network with only one hidden layer is capable of estimating almost any type of nonlinear mapping [21]. Therefore, in this paper, an ANN with only one hidden layer is selected. Different combinations of activation functions were tested to select the best activation functions for hidden and output layers. The optimum number of neurons in hidden layer was determined based on the minimum AAD% and R<sup>2</sup>

## 3.4 Results

Table 3 shows values of AAD% and R<sup>2</sup> of different activation functions with optimal number of neurons for each case study. According to Table 3, ANN with logsig-purelin activation functions with 19 neurons in hidden layer has the least error.

 TABLE 3

 AAD% AND R<sup>2</sup> OF DIFFERENT ACTIVATION FUNCTIONS WITH OPTIMAL

 NUMBER OF NEURONS IN EACH CASE

Activation function		Number of neurons				
Hidden Output			AA	.D%	R	2
layer	layer		Train	Test	Train	Test
Logsig	Purelin	19	0.7176	0.8581	0.9984	0.9981
Logsig	Logsig	20	1.4393	1.6264	0.9912	0.9892
Logsig	Tansig	18	1.0049	1.2491	0.9971	0.9959
Tansig	Logsig	17	1.1451	1.3299	0.9924	0.9913
Tansig	Tansig	19	0.9575	1.1625	0.9975	0.9965

Table 4 shows values of AAD% and R<sup>2</sup> of different number of neurons in hidden layer with sigmoid-purelin activation functions. Results show that the trained neural network can estimate phase equilibrium data, precisely.

ТА	BLE	4

AAD% and  $R^2$  obtained with different number of neurons in hidden layer and sigmoid-linear activation function

							1	-1.4420	
		AAD%	<b>R</b> <sup>2</sup>			AAD%	R <sup>2</sup>	2	-1.4321
3	train	7.083	0.8791	14	train	0.8524	0.9977	3	1.9846
3	test	7.559	0.863	14	test	1.213	0.9955		
4	train	3.791	0.9667	15	train	0.851	0.9981	4	-2.7383
т	test	4.886	0.9453	15	test	1.294	0.9955	5	-3.5909
5	train	3.413	0.9764	16	train	0.8392	0.9977	6	-2.7665
5	test	4.232	0.9542	10	test	1.035	0.991		
6	train	2.921	0.9811	17	train	0.8052	0.9981	7	0.3179
0	test	3.572	0.9659	17	test	0.949	0.9953	8	1.1780
7	train	2.349	0.9894	18	train	0.736	0.9981	9	0.2329
1	test	3.088	0.9772	10	test	0.892	0.9957	10	-4.1214
8	train	1.886	0.9922	19	train	0.7176	0.9984		
0	test	2.706	0.9853	17	test	0.8581	0.9981	11	0.0138
9	train	1.857	0.9924	20	train	0.7122	0.9985	12	1.2598
,	test	2.24	0.9891	20	test	0.8715	0.9966	13	0.6373
10	train	1.426	0.9955	21	train	0.7106	0.9985		
10	test	1.9604	0.9893	21	test	0.897	0.9963	14	-3.0632
11	train	1.314	0.9961	22	train	0.7113	0.9986	15	-3.2319
11	test	1.931	0.9879	22	test	0.9197	0.996	16	1.3601
12	train	1.096	0.997	23	train	0.7083	0.9987		0.0000
12	test	1.7533	0.9884	25	test	0.9614	0.9956	17	2.8323
13	train	0.9312	0.9974	24	train	0.7012	0.9986	18	-1.4980
10	test	1.477	0.9964	27	test	0.1083	0.9936	19	-4.1945

Fig. 2 illustrates comparison between predicted and experimental data. The perfect fit is indicated by the solid line. Results in Fig. 2 show a good correlative capability of ANN model.

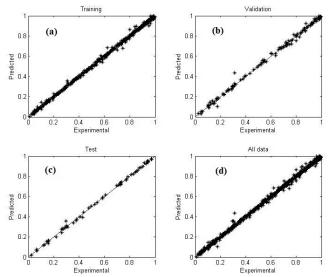


Fig. 2. Comparison between predicted and experimental data for (a) training, (b) validation, (c) test, and (d) total data set

The weight and bias values of the optimal architecture are shown in Table 5. Several calculations have been performed to examine the capability of ANN. Results of predicting vapor liquid equilibria based on available data points of each system are summarized in Table 6.

 TABLE 5

 The weight and bias values of the optimal architecture

		Tc	Pc	w	Т	Р	Bias
=	1	-1.4420	-0.0892	1.9562	0.4218	1.18038	2.1536
-	2	-1.4321	-2.7192	3.4760	0.4321	1.10668	2.8404
	3	1.9846	-3.7186	3.1848	3.5962	-0.2398	-4.9793
	4	-2.7383	1.4259	2.3208	-2.4830	3.9994	4.3073
	5	-3.5909	-2.7672	-4.5301	3.7526	-2.1980	3.7959
	6	-2.7665	-3.2084	5.2964	-4.3322	2.0525	0.3778
	7	0.3179	0.4387	0.0233	2.0595	-3.4416	-1.8448
	8	1.1780	-2.1007	-0.2451	3.5252	3.3067	2.9484
	9	0.2329	-3.0839	1.4379	-3.0267	3.3013	1.4887
	10	-4.1214	1.9825	0.7078	1.5427	2.5526	0.3177
	11	0.0138	-0.4667	-0.7542	1.1157	2.9490	-0.0156
	12	1.2598	-5.4285	-0.8154	-1.5749	-3.1135	-0.1067
	13	0.6373	-1.1250	2.1946	1.2423	0.6809	-2.1425
	14	-3.0632	1.6792	2.1460	1.3543	0.5092	-0.9694
	15	-3.2319	-2.2977	2.0497	-2.5934	-0.7047	-2.9267
	16	1.3601	3.9714	5.7476	-2.1223	-1.9046	-5.7501
	17	2.8323	-1.9016	1.9343	-2.7668	1.7352	1.3446
	18	-1.4980	-0.0338	-0.9824	-7.3949	2.3041	-7.2597
_	19	-4.1945	-2.3838	1.2778	0.5747	-1.7096	-3.6355

Neuron	1	2	3	4	5	6	7	8	9	10
Layer	-1.7878	31.1185	-0.7783	3.2476	0.7388	-0.4506	5.1168	1.1308	-0.3763	2.7447
Weights	<b>s</b> -1.2502	1.05108	5.0894	2.6642	2.0833	0.0867	1.8141	0.3925	-0.9799	1.8490
Neuron	11	12	13	14	15	16	17	18	19	Bias
Neuron Layer		12 31.5444							17	

#### TABLE 6

DEVIATIONS OF PREDICTION OF VAPOR-LIQUID EQUILIBRIA BASED ON NEURAL NETWORK MODEL DEVELOPED BY EXPERIMENTAL DATA POINTS OF EACH SYSTEM

System	AAD%	Bias%	RMS	R <sup>2</sup>
1-Butanol	0.7888	0.8446	0.1140	0.9989
2-Propanol	0.7989	-1.0310	0.0894	0.9973
Ethanol	0.3847	-0.1444	0.0143	0.9995
Acetic acid	1.1730	-0.3501	0.0874	0.9970
Acetonitrile	0.7290	-1.1412	0.1157	0.9982
Ethyl acetate	0.5533	-0.3631	0.0339	0.9993
Vinyl acetate	0.6206	0.2226	0.0255	0.9992
Benzene	0.2108	0.0375	0.0097	0.9999
P-Xylene	1.1869	-0.0750	0.0584	0.9962
Croton aldehyde	0.7072	-0.2637	0.0622	0.9965
AOME	1.5374	0.3210	0.0346	0.9937
Overall	0.8154	-0.2139	0.0653	0.9979

Comparison between experimental data and predicted values of neural network for each of the binary systems are shown in Figs (3) and (4).

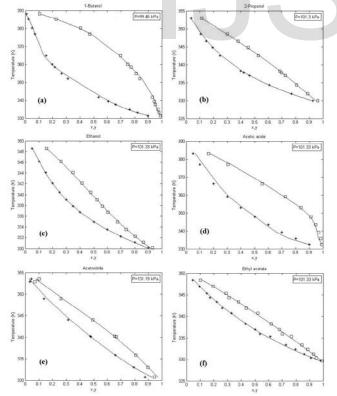


Fig. 3. Comparison between predicted (-) and experimental data, (a) 1-Butanol, (b) 2-Propanol, (c) Ethanol, (d) Acetic acid, (e) Acetonitrile, and (f) Ethyl acetate

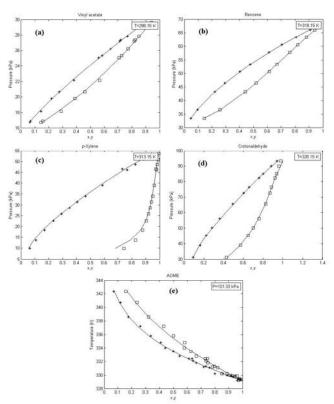


Fig. 4. Comparison between predicted (-) and experimental data, (a) Vinyl acetate, (b) Benzene, (c) p-xylene, (d) Croton aldehyde, and (e) AOME

## 4 CONCLUSIONS

In this paper, artificial neural network models have been developed for eleven binary systems containing acetone to estimate vapor-liquid equilibria within temperature range of 298.15-391.25 K and pressure range of 2.640-101.33 kPa. Out of 304 experimental data points, 70% were used for training of neural network, 20% for validating and 10% for testing. Based on the obtained results, the best structure is feed-forward network, logsig activation function for hidden layer and purelin activation function for output layer. Levenberg-Marquardt back propagation training algorithm was used for network training. Multilayer perceptron model consists of seven inputs, 19 neurons in hidden layer and two neurons in output layer. The weights are optimized to minimize the error between calculated and experimental VLE data. The absolute average error for estimating the VLE was found to be quite low. Obtained results show that the optimum neural network architecture is able to predict equilibrium data of binary systems containing acetone with an acceptable level of accuracy of AAD% of 0.815, R<sup>2</sup> of 0.9979 and RMS of 0.0653.

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