Multilayer Perceptron Neural Network Based Models for the Prediction of Vapor-Liquid Equilibrium

Vishakha Lakshete, Veena Patil-Shinde

Abstract: Vapor-Liquid Equilibrium (VLE) data are important for the design, analysis, control, and modeling of process equipment such as distillation columns, absorbers, and reactors in the chemical industries. In the present study, widely employed feed-forward neural network i.e. multi-layer perceptron (MLP) has been used to develop MLPNN-based models. The MLPNN possesses an ability of learning and generalizing the nonlinear relationships that exist between the input(s), and related output(s) data set. The MLPNN-based VLE models have been developed for prediction of vapor phase composition of ternary system (benzene + cyclohexane + anisole) by using experimental data. The inputs for model development contain physical property of the pure components (acentric factor) and thermodynamic parameters (equilibrium temperature, liquid phase composition). The proposed MLPNN-based model is trained by using an error-back propagation (EBP) algorithm. Total number of experimental data points were extracted from literature is 117 in which 75% i.e. 88 data points were used as training set for developing the MLPNN models and the 25% i.e. 29 data points were used as test set for assessing generalization ability of the developed MLPNN models. It has been observed that data predicted by MLPNN-based models possesses good prediction accuracy and generalization ability of proposed models.

Keyword: Vapor-liquid equilibrium, Artificial neural network, Data prediction, Thermodynamic models.

I. INTRODUCTION

Vapor-liquid equilibrium data is necessary for design, analysis, control, and development of various chemical processes [1],[2]. Vapor-liquid equilibrium is an intrinsic factor for the designing and modeling of separation processes like distillation, extraction, absorption and adsorption [3]. VLE is a condition where liquid and its vapor state are in equilibrium with each other. In other words, a state where the rate of evaporation of liquid mixture equals the rate of condensation of vapor mixture on a molecular level [4]. Accurate measurements of VLE through experimentation for ternary or higher order systems are time-consuming, tedious, and expensive. It isn’t ever possible to conduct VLE experiments in entire ranges of pressures and temperatures practically. Consequently, conventional thermodynamic models are used to estimate vapor-liquid equilibrium.

Although, conventional thermodynamic models like equation of state (EoS) and the activity-coefficient models are used to estimate VLE data, these models need complete information of physicochemical facts essential for process [5]. The prediction of the VLE data by using thermodynamic models is tricky because it contains the number of parameter like binary adjustable parameter. Estimation of these parameters in order to get the best set by iterative methods is often tedious and the timewasting exercise [6].

Data-driven is second method (i.e. empirical) for VLE modeling in which detailed knowledge of physico-chemical phenomena is not required. Nonlinear or linear regression methods are used in formulating the models. Although, linear regression method is applicable for the systems containing linear VLE behavior (ideal systems), most of the systems exhibit nonlinear VLE behavior which depends on operating parameters. This, selection of an accurate data-fitting function (nonlinear) is difficult. So to overcome above mentioned difficulties for conventional thermodynamic models and use of regression methods for VLE modeling, there is need of alternative nonlinear modeling technique.

The nonlinear modeling technique termed artificial neural networks (ANNs) which is artificial intelligence (AI) based [7] is used as an alternative to the conventional thermodynamic models and regression based modeling. This methodology has been used in the arena of thermodynamics for the vapor-liquid equilibrium prediction [8]. In addition, artificial neural networks (ANNs) technique has been used by many researchers for modeling in various areas of science. The ANN technique has been used, for instance, in prediction of the high pressure VLE of the six binary systems [9], prediction of CO₂ mole fraction in vapor and liquid phase for binary system [10], predictions of bubble point pressure and vapor phase composition of the binary systems [11], prediction of VLE data by using radial basis function network [12]. Prediction of the VLE data for the binary systems containing propane [13], API gravity of crude oil predictions [14], gasification performance prediction by use of AI-based techniques [15], [16].
In the present study, feed-forward artificial neural network namely, multi-layer perceptron (MLP) has been utilized for developing the models to predict mole fraction of benzene \((y_1)\) and cyclohexane \((y_2)\) in vapor phase for ternary system (benzene + cyclohexane + anisole).

**Table-I: Inputs and outputs of the two MLPNN-based models.**

<table>
<thead>
<tr>
<th>Model</th>
<th>No of inputs</th>
<th>Inputs of model</th>
<th>Output of model</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>6</td>
<td>Mole fractions of benzene ((x_1)), and cyclohexane ((x_2)) in the liquid phase; temperature ((T));acentric factors of benzene ((w_1)), cyclohexane ((w_2)) and anisole ((w_3))</td>
<td>Mole fraction of benzene in the vapor phase ((y_1))</td>
</tr>
<tr>
<td>II</td>
<td>6</td>
<td>Mole fractions of benzene ((x_1)), and cyclohexane ((x_2)) in the liquid phase; temperature ((T));acentric factors of benzene ((w_1)), cyclohexane ((w_2)) and anisole ((w_3))</td>
<td>Mole fraction of cyclohexane in the vapor phase ((y_2))</td>
</tr>
</tbody>
</table>

An entire literature invention shows that, this is the first exemplar where in MLPNN-based models are developed for VLE prediction for the avowed ternary system. Experimental VLE data reported in literature [17] is used to develop the proposed MLPNN-based models, the input space and outputs to be predicted are given in the Table-I. Predicted values were compared with its corresponding experimental values which give good prediction accuracy and the generalization ability for the developed model.

This paper is organized as follows. The next section briefs about numerous thermodynamic models used for the VLE predictions. A review of artificial neural networks and multi-layer perceptron is given in next section. In Section 4 details of data used for the MLPNN modeling is given. The “Results and discussion” section provides details about the MLPNN-based models for the prediction of vapor phase composition of benzene \((y_1)\) and cyclohexane \((y_2)\). Lastly conclusions regarding the study are provided.

II. CONVENTIONAL THERMODYNAMIC MODELS

A. Equation of state models

Vapor-liquid equilibrium data are usually estimated using thermodynamic models which are based on criterion of the phase equilibrium i.e. chemical potentials of each of the components in each of the phases are equal. A conventional method used to predict the VLE is the equation of state (EoS). EoS is a competent tool for computing phase equilibrium and thermodynamic properties of fluids of the systems in mixture or pure form. Equation of state are broadly used in various practical and theoretical studies such as the petroleum industry, reservoir fluids, chemical process design, etc., further these can be applied to systems containing hydrocarbons, but it is difficult for systems that contain polar compounds. The first equation which is used for prediction of vapor-liquid equilibrium was Van der Waals equation of state [18]. Next, Redlich-Kwong equation of state [19] obtained by improving Van der Waals EoS by adjusting Van der Waals attractive pressure term that improves prediction of vapor phase physical properties. Soave [20] proposed important modifications in Redlich-Kwong equation for betterment in accuracy of the prediction of equilibrium ratios and liquid density. The Peng-Robinson EoS [21] was developed for handling of vapor and liquid properties near-equilibrium conditions and it is good for betterment in accuracy of the prediction of the vapor pressure, equilibrium ratios and liquid densities [22]. Since design, operation, control, and modeling of various chemical processes are based on thermodynamic models and VLE predictions, it is important that equations of state models are easy to use and needs minimum number of the inputs, which is able to give exact predictions.

B. Activity Coefficient models

There are various methods available for prediction of VLE such as, analytical solution of groups method (ASOG) [23], universal functional-group activity coefficients (UNIFAC) method, Van Laar, Wilson, two constant margules, universal quasi-chemical (UNIQUAC) equation, non-random two-liquid (NRTL) [24]. All above mentioned thermodynamic VLE models are applied for moderately non-ideal systems. For non-polar solvents such as hydrocarbons, alcohols, ketones UNIQUAC, Wilson and NRTL models gives good predictions. UNIFAC method is used in the design calculations of distillation columns [25].

III. ARTIFICIAL INTELLIGENCE (AI) BASED MODELING TECHNIQUES

Artificial Intelligence (AI) is a branch of computational science, intended for development of computers to employ in human like thought processes such as learning, reasoning, and self-correction. AI is basically associated with development of techniques and algorithms, which permit computers to “learn” and utilize this knowledge to solve problems such as function approximation and classification. AI-based modeling technique, viz. genetic programming (GP) and artificial neural networks (ANNs) [26]; machine learning (ML) based modeling technique such as support vector regression (SVR) [27] are frequently used as an substitutes to modeling which is regression based. They have various applications in arena of thermodynamics. A widely used AI-based modeling technique named artificial neural network is described briefly in next section.

A. Artificial Neural Networks

Artificial neural networks originate from study of methods for information processing in the biological nervous system, especially the human brain. ANNs are composed of highly interconnected systems of simple processing elements (artificial nodes).
They can learn complex nonlinear interrelationships existing between inputs and resultant output(s). An artificial neural network may be classified according to direction of information flow in it. Three types of connectivity patterns exist i.e. feed-forward, feed-back and recurrent. Once the model is trained with ANN architecture, then the developed model is ready to predict the outputs for new set of input data, which is not utilized.

<table>
<thead>
<tr>
<th>System</th>
<th>Temperature (T) (K)</th>
<th>Pressure (P) (kPa)</th>
<th>Mole fraction of benzene in the liquid phase (x_1)</th>
<th>Mole fraction of cyclohexane in the liquid phase (x_2)</th>
<th>Mole fraction of benzene in the vapor phase (y_1)</th>
<th>Mole fraction of cyclohexane in the vapor phase (y_2)</th>
<th>N_{dp}</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene (1)</td>
<td>351.03-421.09</td>
<td>101.32</td>
<td>0.019-0.980</td>
<td>0.008-0.959</td>
<td>0.023-0.990</td>
<td>0.010-0.974</td>
<td>117</td>
<td>[17]</td>
</tr>
<tr>
<td>Cyclohexane (2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Anisole (3)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

N_{dp} is number of data patterns

To train the model [28], ANN has particular applications like, pattern recognition, data processing, and the nonlinear control through the learning process [29]. Feed-forward neural network (FFNN) namely, multi-layer perceptron (MLP) and radial basis function network (RBFN) are most widely used to build a model.

B. Multi-layer Perceptron Neural Network

A multi-layer perceptron neural network (MLPNN) has a feed-forward structure i.e. flow of information is only in forward (one) direction, it approximates nonlinear relationships that exist between the input, and output data sets [30]. The MLPNN architecture with one hidden layer is depicted in Fig. 1. It comprises three layers of processing nodes. The first layer, called an input layer in which inputs to the network are defined. The last layer, called the output layer, returns output values of corresponding to the specified inputs. All layers in between input and output layer are called hidden layer. These layers houses N, M and S number of processing nodes, respectively. A number of nodes (n) in input layer equal to the number of inputs to the MLP neural network, whereas number of nodes (s) in output layer equals to the number of outputs in the system being modeled. The number of hidden layers and the number of nodes in hidden layer are selected heuristically based on good prediction accuracy and the generalization capability of MLPNN-based model. Each node of MLPNN is linked to all other nodes in succeeding layer through connection weights i.e. between input and hidden layers and between hidden and output layers. In the MLPNN, an input and hidden layer has a bias node with fixed output of +1.

Fig. 1 shows MLPNN with a one hidden layer. Each input node in input layer passes information to each hidden node in hidden layer and hidden nodes pass the net activation through the appropriate nonlinear transfer function like logistic sigmoid to enumerate their outputs [27]. When input vector X_p is applied to input layer, each hidden layer neuron first computes the activation according to the weighted-sum of its inputs using the following equation,

\[
net_{pm}^h = (w_{pm}^h)x_p + b_m^h = \sum_{i=1}^{n} w_{mi}^h x_{pi} + b_m^h = \sum_{i=1}^{n} w_{mi}^h x_{pi} + b_m^h = \sum_{i=1}^{n} \sum_{j=1}^{m} w_{mj}^{h,i} x_{pj} + b_m^h; \quad m = 1, \ldots, M
\]

where, \(net_{pm}^h\) represent activation of m\(^{th}\) hidden layer neuron. The vector \(w_{m}^h\) denotes the weights of the connections linking the input layer nodes to m\(^{th}\) hidden node, and \(b_m^h\) represents strength of the link between the bias and m\(^{th}\) hidden node. The output of m\(^{th}\) hidden node, \(y_p^m\), when p\(^{th}\) input is applied to network and is evaluated using a nonlinear transfer function. The outputs of the processing nodes in first hidden layer form inputs to the nodes in the subsequent layer; this layer could be another hidden layer, or output layer. Outputs of these nodes are computed similarly as shown in Eq (2). It may, however, be noted that output layer neurons can use either linear or a nonlinear transfer function to compute their outputs. The output layer units, indexed as \(S\), determine their activation as the weighted-sum of the hidden layer outputs \(y_p^j\) (\(j = 0,1,2,\ldots,S\)) as,

\[
y_j = \sum_{m=1}^{M} w_{mj}^o y_p^m + b_j^o; \quad j = 0,1,2,\ldots,S
\]
Multilayer Perceptron Neural Network Based Models for the Prediction of Vapor-Liquid Equilibrium

\[ \text{net}_{p}^{h} = (w_{i}^{h})^T y_{i}^{h} + b_{p}^{h} = \sum_{j=0}^{N} w_{ij}^{h} y_{j}^{h} + b_{p}^{h}; \quad s = 1, \ldots, S \nonumber \]

Where, \( w_{ij}^{h} \) and \( y_{j}^{h} \) represent the weights and the outputs of hidden layer, \( b_{p}^{h} \) is bias, \( N \) is total number of hidden units, \( S \) denotes the number of data patterns in the sample set; \( i \) is the index of input patterns; \( j \) is the index of hidden units. 

\[ f(x) = \frac{1}{1+e^{-x}} \quad (3) \]

Different types of transfer functions have been used, such as step threshold, linear, ramp threshold, logistic sigmoid, hyperbolic tangent, and Gaussian [28]. In the present study, the forward pass, outputs are yielded by comparing computed and desired output to determine error incurred by network in estimating the target outputs. A single training iteration is done when weight-updation process is carried out for all data points in the set of data. MLPNN training is continued till performance is achieved. Commonly, “root mean squared error” (RMSE) is used as error function in the MLPNN training and it is calculated as,

\[ \text{RMSE} = \sqrt{\frac{1}{N_{dp}} \sum_{i=1}^{N_{dp}} (y_{i} - \tilde{y}_{i})^2} \quad (5) \]

Where \( N_{dp} \) denotes number of data points in the sample set; \( i \) is pattern index; \( y_{i} \) is the \( i \)th experimental value; \( \tilde{y}_{i} \) is the corresponding MLPNN-predicted output. The detailed method to obtain a best MLP neural network model is provided in [29].

Table-III: Mean and standard deviation magnitudes of two MLPNN-based models

<table>
<thead>
<tr>
<th>Model</th>
<th>Inputs</th>
<th>Outputs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>Standard deviation</td>
<td>Mean</td>
</tr>
<tr>
<td>I</td>
<td>( \bar{X}<em>{1} = 354.12 ) (K); ( \bar{X}</em>{2} = 0.401 );</td>
<td>( \overline{Y}_{1} = 0.476 );</td>
</tr>
<tr>
<td>II</td>
<td>( \bar{X}<em>{3} = 0.408 ); ( \bar{X}</em>{4} = 0.209 ); ( \bar{X}<em>{5} = 0.212 ); ( \bar{X}</em>{6} = 0.353 );</td>
<td>( \overline{Y}_{2} = 0.491 );</td>
</tr>
</tbody>
</table>

Linear function,

\[ f(x) = ax \quad (4) \]

A training of the MLPNN is needed and this is implemented by a widely used technique error-back propagation (EBP) algorithm [31] which is based on a nonlinear version of the Windrow-Hoff rule, known as generalized delta rule (GDR). Error-back propagation is widely used algorithm for supervised training of multi-layer perceptron neural network. It comprises of two types of passes through the network layers (i) forward (ii) reverse. In the forward pass, outputs are evaluated by using the input pattern which is applied to non-processing units of input layer. In the reverse pass, the network’s weights are updated. The weight-updation is done by comparing computed and desired output to determine error incurred by network in estimating the target outputs. A single training iteration is done when weight-updation process is carried out for all data points in the set of data. MLPNN training is continued till performance is achieved. Commonly, “root mean squared error” (RMSE) is used as error function in the MLPNN training and it is calculated as,

\[ \text{RMSE} = \sqrt{\frac{1}{N_{dp}} \sum_{i=1}^{N_{dp}} (y_{i} - \tilde{y}_{i})^2} \quad (5) \]

Where \( N_{dp} \) denotes number of data points in the sample set; \( i \) is pattern index; \( y_{i} \) is the \( i \)th experimental value; \( \tilde{y}_{i} \) is the corresponding MLPNN-predicted output. The detailed method to obtain a best MLP neural network model is provided in [29], [30].

IV. DATA

In the present study, an experimental VLE data reported in literature were used to develop MLPNN-based VLE models [17]. Source and ranges of data such as pressure, temperature, liquid and vapor phase composition are listed in Table II. The experimental data is normalized by using Z-transformation method. Experimental data set was divided randomly in the ratio 75:25 as training and the test set, respectively. Where transfer functions named logistic sigmoid and the linear are used to compute output of hidden and the output layer, respectively and are given below:

Logistic sigmoid function,

\[ f(x) = \frac{1}{1+e^{-x}} \quad (3) \]

75% of data were used as training set i.e. for developing the MLPNN-based models and 25% of data were used as test set i.e. for testing the generalization ability of developed models. The method to obtain normalized variables is given below:

\[ \sigma_{j}^{n} = \frac{x_{j} - \bar{x}_{j}}{\sigma_{y_{j}}} ; \quad j = 1, 2, \ldots, N_{dp} \quad (6) \]

Where, \( N_{dp} \) denotes the number of data patterns in experimental data set; \( x_{j} \) (n=1, 2, ..., N; N=6) denotes the normal score (standardized variable) concerning to values of six inputs given in Table-I. \( \bar{x}_{j} \) denotes the \( j \)th value of \( n \)th un-normalized predictor (i.e. input) variable, \( x_{j} \); \( \bar{x}_{j} \) represents the mean of the \( x_{j} \) and \( \sigma_{y_{j}} \) refers to standard deviation of the \( x_{j} \). Outputs of the models were normalized by same method as model inputs and it is given as follows:

\[ \sigma_{j}^{q} = \frac{y_{j} - \bar{y}_{j}}{\sigma_{y_{j}}} \quad j = 1, 2, \ldots, N_{dp} \quad (7) \]

Where, \( y_{j} \) (q=1,...,Q; Q=2) denotes normal score (standardized variable) concerning to values of two outputs given in Table-I. \( \bar{y}_{q} \) denotes the \( q \)th value of \( q \)th un-normalized output variable, \( y_{q} \); \( \bar{y}_{q} \) refers mean of \( y_{q} \) and \( \sigma_{y_{q}} \) refers standard deviation of \( y_{q} \). The inputs for MLPNN-based model-I and II are same but outputs are different. The mean and the standard deviation values used in the Eqs. (6) and (7) are given in Table-III, where \( \bar{x}_{1}, \bar{x}_{2}, \bar{x}_{3}, \bar{x}_{4}, \bar{x}_{5}, \bar{x}_{6} \) and \( \sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4}, \sigma_{5}, \sigma_{6} \) respectively, represents the mean and standard deviation values of temperature (T), mole fraction of benzene (\( x_{1} \)) and cyclohexane (\( x_{2} \)) in the liquid phase and the acentric factors of benzene (\( w_{1} \)), cyclohexane (\( w_{2} \)), and anisole (w3).
V. RESULT AND DISCUSSION

A. MLPNN-based vapor-liquid equilibrium modeling

“RapidMiner studio” software was used in developing MLPNN-based models [32]. It has number of operators such as ‘normalize’ for preprocessing input-output data; ‘retrieve’ to access stored input-output data into repository and loads them into the process panel. Next is ‘neural net’, in which training is done by EBP algorithm; ‘apply model ’, this operator pertains a model on given example set; ‘performance (regression)’, this operator is used to estimate statistical measures such as correlation coefficient (CC) and root mean squared error (RMSE) for assessing good prediction accuracy and generalization ability of the MLPNN-based models. These were calculated for both data sets i.e. training and test by using experimental and corresponding model predicted values.

The MLPNN-based optimal model was selected based on their magnitudes i.e. high CC and lower RMSE for both sets i.e. training and test sets.

The aim of present study is to develop two MLPNN-based model-I and II, for the prediction of the mole fraction of benzene ($y_1$) and cyclohexane ($y_2$) in vapor phase, respectively. Total of 117 isobaric VLE experimental data points of ternary mixture (benzene-cyclohexane-anisole) sourced from the literature [17] have been used in this study. This data consisting of the experimental conditions (liquid phase composition, vapor phase compositions and temperature) and pure component properties (acentric factor) are given in Tables II and IV, respectively. From total of 117 the experimental data points, 88 data points were used as training set and 29 data points as test set for constructing and evaluating generalization ability of the models [33].

Table-IV: Pure component properties used in the study.

<table>
<thead>
<tr>
<th>Component</th>
<th>Acentric Factor ($\omega$)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>$w_1$ = 0.209</td>
<td>[34]</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>$w_2$ = 0.212</td>
<td>[34]</td>
</tr>
<tr>
<td>Anisole</td>
<td>$w_3$ = 0.353</td>
<td>[34]</td>
</tr>
</tbody>
</table>

B. MLPNN-based model-I for prediction of mole fraction of benzene in vapor phase ($y_1$)

MLPNN-based model-I contains six inputs nodes (N=6), namely, mole fraction of benzene ($x_1$), and cyclohexane ($x_2$) in the liquid phase, acentric factors of benzene ($w_1$), cyclohexane ($w_2$), and anisole ($w_3$), and temperature (T). Single output node represent mole fraction of benzene ($y_1$) in vapor phase. To construct an optimal MLPNN model-I, structural parameters are number of hidden layer=one; number of nodes in each hidden layer=six and EBP algorithm-specific parameters such as learning rate ($\eta$) = 0.5; momentum (\(\mu\)) = 0.05 need to be rigorously studied. The details about the optimal MLPNN-based model-I are given in the Table V. Fig.2, shows schematic representation of MLPNN-based model-I for prediction of mole fraction of benzene in vapor phase ($y_1$). The predictions given by MLPNN-based model-I yielded high CC and lower RMSE values and they are given in Table VI for both sets i.e. training and test. It shows that the MLPNN-based model-I has an excellent prediction accuracy and generalization ability of mole fraction of benzene in vapor phase. Comparison of experimental and predicted mole fractions of benzene in the vapor phase ($y_1$) of MLPNN-based model-I is shown in Fig.3. A close agreement between the experimental and model predicted $y_1$ values relating to training and test set data shows of indicates a good prediction and the generalization performance by MLPNN-based model-I.

Fig.2. Schematic of MLPNN-based model-I for prediction of vapor phase composition of benzene ($y_1$)

Fig.3. Comparison of experimental and predicted mole fractions of benzene in the vapor phase ($y_1$) of MLPNN-based model-I
C. MLPNN-based model-II for prediction of mole fraction of cyclohexane in vapor phase (y2)

The MLPNN-based model-II consist of same input space as used in developing the MLPNN-based model-I. However, model output designates mole fraction of cyclohexane in the vapor phase (y2). An optimal MLPNN-based model-II was obtained by using structural and EBP algorithm parameters such as one hidden layer, seven nodes in hidden layer, learning rate = 0.5 and momentum = 0.05. The details about the optimal MLPNN-based model-II are given in the Table V. The predictions given by MLPNN-based model-II yielded high CC and lower RMSE values and they are given in the Table VI for both sets i.e. training and test. It shows that the MLPNN-based model-II has good prediction accuracy and generalization ability of mole fraction of cyclohexane in vapor phase. Comparison of experimental and predicted mole fractions of cyclohexane in the vapor phase (y2) of MLPNN-based model-II is shown in Fig.4. A close match between the experimental and model predicted y2 values relating to the training and test data set indicates good prediction and the generalization performance by MLPNN-based model-II.

Table-V: Details of the optimal MLPNN-based models.

<table>
<thead>
<tr>
<th>Model No.</th>
<th>Input Layer</th>
<th>Hidden Layer</th>
<th>Output layer</th>
<th>Momentum</th>
<th>Learning rate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>No. of nodes</td>
<td>No. of hidden nodes</td>
<td>No. of nodes</td>
<td>Transfer Function</td>
<td>Output variable</td>
</tr>
<tr>
<td>I</td>
<td>6</td>
<td>1</td>
<td>6</td>
<td>Logistic sigmoid</td>
<td>y1</td>
</tr>
<tr>
<td>II</td>
<td>6</td>
<td>1</td>
<td>7</td>
<td>Logistic sigmoid</td>
<td>y2</td>
</tr>
</tbody>
</table>

![Fig.4. Comparison of experimental and predicted mole fractions of cyclohexane in the vapor phase (y2) of MLPNN-based model-II](image)

### VI. CONCLUSION

In the present work, a two MLPNN models were developed for the ternary system, benzene-cyclohexane-anisole for the prediction of mole fraction of benzene (y1) and cyclohexane (y2) in vapor phase using an experimental data reported in the literature. The input space in these models include mole fraction of benzene (x1) and cyclohexane (x2) in liquid phase, temperature (T), and the acentric factors of benzene (w1), cyclohexane (w2) and anisole (w3). An EBP algorithm was utilized to train models. The developed MLPNN-based models for prediction of vapor phase composition have good output prediction accuracy and the generalization ability as shown by high correlation coefficient and low root mean squared error magnitudes for training and test data sets. The result shows good match between model predicted values and its corresponding experimental counterparts. So, artificial neural networks such as MLPNN can be a successful tool to represents complex nonlinear systems effectively as a prediction of VLE data, if developed efficiently. The MLPNN-based VLE modeling methodology exemplified here may be used in developing the industrially important models for binary and higher order systems.

### REFERENCES


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