MODELING COMBINED ISOBARIC VLE OF FOUR TERNARY MIXTURES USING ARTIFICIAL NEURAL NETWORKS

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ABSTRACT- Vapour-Liquid Equilibria is a multidisciplinary theme having diversified areas of application including designing of several chemical process equipments. There are theoretical and thermodynamic models reported in the literature, however the accuracy gets lowered because of multivariable non-linear behavior of the system making it complex. The objective of the present work is to develop Multilayer Perceptron network for estimation of VLE of four types of ternary mixtures involving combinations of eight components. Vapour-Liquid Equilibria of ternary mixtures reported in the literature have been used in the present work that include, hexane-ethanol-benzene, methanol-ethanol-water, acetone-benzene-cyclohexane, methanol-water-acetic acid. The correlation is to be developed for input parameters, molecular weights of the individual components and equilibrium temperature with the output parameters, equilibrium liquid and vapour phase compositions. There are 127 data points which are divided in two parts, training and test data set containing 117 and 10 points respectively for developing ANN model using elite-ANN©. The range of applicability of the developed models for temperature is from 327.85 to 377.75 K. The ANN model 3 developed has been successful with high accuracy levels of RMSE of 0.1434 & 0.1214 for training and test data sets respectively.

Keywords- VLE, Artificial Neural Network, ternary system, modeling

I. INTRODUCTION
Vapour Liquid Equilibrium data for various binary, ternary & multicomponent mixtures play a vital role in designing process equipments like distillation columns, absorbers, reactors in the chemical industries. Distillation columns are designed based on the boiling point difference of the components in the mixtures being separated. The height of distillation columns is determined by the vapour liquid equilibrium (VLE) data for the mixture. A good understanding of VLE is essential for the analysis, design, and control of distillation columns. Vapour–liquid equilibrium is a condition where a liquid and its vapour are in equilibrium with each other, a state where the rate of evaporation of liquid mixture equals the rate of condensation of vapour mixture on a molecular level such that there is no net change of vapour-liquid composition. Distillation can be effective in separation of chemical components from a mixture only if the compositions of the components in the vapour and liquid phases that are in equilibrium with each other are different. The importance of the theme of the vapour liquid equilibria can be gauged from the fact that there are likely to be hundreds of thousands of binary, ternary, multicomponent mixtures requiring estimation of VLE data. Such a large experimentation is tedious, uneconomical and hence there is need for estimation using models. The correlations involved in generating VLE
data are often non linear and complex in nature and are generally estimated using thermodynamic models based on the phase equilibrium criteria of equality of chemical potential in both phases. Several thermodynamic models such as NRTL, UNIFAC, UNIQUAC and Wilson have been used to estimate VLE. Another approach for VLE estimation is based on equation of state. In some cases empirical and semi empirical equations are employed to predict VLE data. The constants in these equations are obtained from regression of the experimental measurements. Empirical equations do not take in to account the detailed mechanisms of VLE systems. Traditionally thermodynamic models and empirical equations have been serving requirement of the industry. The development of numerical tool such as ANN has paved the way for alternate methods to predict the VLE.

II. LITERATURE SURVEY

Artificial Neural Network

An Artificial Neural Network (ANN) is an interdisciplinary theme that is based upon the working principle of biological nervous system, such as brain processes information. It is composed of networks of interconnected processing elements (neurons) called nodes working unison to solve specific problem[1]. The most common type of feed forward neural network is Multi Layer Perceptron (MLP). It consists of input and output layers, with at least one layer of processing unit in between them. The layers between the input and output layers are termed “hidden” since they do not communicate with the outside world directly. The nodes between the two successive layers are fully connected by means of weights. That is outputs from the input layer are fed to hidden layer units, which in turn, feed their outputs to the next hidden nodes. The hidden node passes the net activation through a nonlinear transformation of a linear function, such as the logistic sigmoidal to compute their outputs. For the training of such a MLP error back propagation algorithm suggested by Rumelhart[2] is popular. This is based on a nonlinear version of the Windro-Hoff rule known as Generalized Delta Rule (GDR). Various applications of ANN are an approach to fault diagnosis in chemical processes [3], fault diagnosis in complex chemical plants [4], incipient fault diagnosis of chemical process [5], leak detection in liquefied gas pipeline [6], for estimation of mass transfer coefficient for fast fluidized bed solids [7], modeling of distillation column [8], detergent formulation [9], modeling of unsteady heat conduction in semi infinite solid [10], prediction of mass transfer coefficient in down flow jet loop reactor [11], modeling of packed column [12], modeling of steam table [13], modeling of Gurney-Lurie and Heisler Charts [14] and similar others were also reported.

III. MATERIALS AND METHODS

Defining VLE at isobaric condition of ternary mixture requires equilibrium temperature to be specified along with composition of the liquid mixture. The objective of the present work is to apply Multilayer Perceptron network for modeling of VLE of four quaternary mixtures involving combinations of eight components. Vapour-Liquid Equilibria of ternary mixtures reported in the literature [21] have been used in the present work that include, hexane-ethanol-benzene, methanol-ethanol-water, acetone-benzene-cyclohexane, methanol-water-acetic acid. The correlation is to be developed for input parameters, molecular weights of the individual components and equilibrium temperature with the output parameters, equilibrium liquid and vapour phase compositions. There are 127 data points which are divided in two parts, training and test data set containing 117 and 10 points respectively for developing ANN model using elite-ANN©[22]. A typical architecture of ANN used in developing the model in the present work is shown in figure 1.

Two different ANN models 1 and 2 have been developed having different topologies. The architecture of the topology of the ANN model 1 & 2 is as given in table 1. All the data set are used for developing models 1 & 2.
The comparison between predicted output values using ANN model 1 and model 2 with actual output values has been carried out for both parameters equilibrium liquid and vapour phase compositions. Based on the prediction accuracy of the models developed, the appropriate model having more accuracy is selected for developing ANN model using train data set as given in Table1.

The comparison of the actual and predicted values obtained using model 1 and 2 have been carried out. Fig 2, 3, 4 & 5 show the graphs plotted between actual and predicted values using ANN model 1 and model 2 for liquid and vapour phase compositions of component 1 & component 2 respectively.
Figure 5: Comparison of actual and predicted values using ANN model 1 and model 2 for vapour phase compositions for component 2

<table>
<thead>
<tr>
<th>Type of Model</th>
<th>Input layer</th>
<th>1st Hidden layer</th>
<th>2nd Hidden layer</th>
<th>3rd Hidden layer</th>
<th>Output layer</th>
<th>Data points</th>
<th>Iterations</th>
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<tr>
<td>ANN Model 1</td>
<td>7</td>
<td>0</td>
<td>5</td>
<td>5</td>
<td>4</td>
<td>Training</td>
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<tr>
<td>ANN Model 2</td>
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<td>10</td>
<td>10</td>
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RMSE training error: 0.1205, RMSE test error: 146521ms

Table 1: ANN topology for model 1 and 2

Figure 6: Graphical view of the iterations versus error for training and test data

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<thead>
<tr>
<th>Type of Model</th>
<th>Input layer</th>
<th>1st Hidden layer</th>
<th>2nd Hidden layer</th>
<th>3nd Hidden layer</th>
<th>Output layer</th>
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</thead>
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<td>10</td>
<td>10</td>
<td>4</td>
<td>Training</td>
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<td>10</td>
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RMSE training error: 0.1434, RMSE test error: 0.1214

Table 2: ANN topology for model 3
Figures 7, 8, 9 & 10 show the comparison of the predicted & actual liquid and vapour phase composition for component 1 & 2 of training data set. Similarly figures 11, 12, 13 & 14 show the comparison of the predicted & actual liquid and vapour phase composition for component 1 & 2 of test data set. As can be seen from these graphs there is close proximity between actual and predicted values.

![Figure 7: Comparison of the predicted & actual liquid phase composition for component 1 of training data set](image)

![Figure 8: Comparison of the predicted & actual liquid phase composition for component 2 of training data set](image)

![Figure 9: Comparison of the predicted & actual vapour phase composition for component 1 of training data set](image)

![Figure 10: Comparison of the predicted & actual vapour phase composition for component 2 of training data set](image)
The objective of the present work was to develop ANN model for estimation of Vapour liquid equilibria having 4 ternary mixtures involving 8 components. Based on the observations, results and discussion, it can be said that, the ANN model 3 developed in the present work has been successful with acceptable accuracy levels. The novel feature of this work is incorporation of 4 ternary mixtures involving 8 components in single model which is not possible in conventional, empirical and thermodynamic models. It is worth mentioning here that ANN model 3 could include the parameters like DDB number in identifying the component. The work is demonstrative and it is felt necessary to extend it for more number of ternary mixtures with large number of components.

IV. CONCLUSION

The objective of the present work was to develop ANN model for estimation of Vapour liquid equilibria having 4 ternary mixtures involving 8 components. Based on the observations, results and discussion, it can be said that, the ANN model 3 developed in the present work has been successful with acceptable accuracy levels. The novel feature of this work is incorporation of 4 ternary mixtures involving 8 components in single model which is not possible in conventional, empirical and thermodynamic models. It is worth mentioning here that ANN model 3 could include the parameters like DDB number in identifying the component. The work is demonstrative and it is felt necessary to extend it for more number of ternary mixtures with large number of components.
Acknowledgement:
Authors are thankful to Director, LIT, Nagpur for the facilities and encouragement provided. Authors also wish to express the sincere gratitude towards the officials of Dortmund Data Bank for giving the permission for the VLE data used in the present work.

Nomenclature:

<table>
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<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tr>
<td>ANN</td>
<td>ARTIFICIAL NEURAL NETWORK</td>
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<tr>
<td>VLE</td>
<td>VAPOUR-LIQUID EQUILIBRIA</td>
</tr>
<tr>
<td>NRTL</td>
<td>NON-RANDOM TWO LIQUID MODEL</td>
</tr>
<tr>
<td>UNIFAC</td>
<td>UNIVERSAL FUNCTIONAL ACTIVITY COEFFICIENT</td>
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<td>UNIQUAC</td>
<td>UNIVERSAL QUASI-CHEMICAL ACTIVITY COEFFICIENT</td>
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<td>DDB</td>
<td>DORTMUND DATA BANK</td>
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V. REFERENCES: