# Modeling Combined VLE of Ten Binary Mixtures using Artificial Neural Networks

S.L.Pandharipane
Associate Professor,
Department of
Chemical Engineering,
LIT, RTMNU,
Nagpur, India.

Anish M. Shah
M.Tech sem IV,
Department of
Chemical Engineering,
LIT, RTMNU,
Nagpur, India.

Ankit Singh
M.Tech sem IV,
Department of
Chemical
Engineering, LIT,
RTMNU,
Nagpur, India.

Sagar G. Ahire
B.Tech Sem VIII
Department of
Chemical
Engineering, LIT,
RTMNU

## ABSTRACT

Vapour-Liquid Equilibria(VLE) is a topic of importance because of its several areas of applications including designing of process equipments. There are theoretical and thermodynamic models reported in the literature for estimation of VLE, however the accuracy is affected because of more than one component involved in the system. The objective of the present work is to utilise Multilayer Perceptron network for modeling of VLE of ten binary mixtures involving combinations of nine components. Vapour-Liquid Equilibria of binary mixtures reported in the literature have been used in the present work that include acetone-ethyl acetate, acetone-methanol, acetone-hexane, water-1,2 ethandiol, ethanol-acetic acid, ethanol-water, methanol-ethanol, benzene-acetic acid and benzene-water. In present work in addition to these parameters molecular weight of components along with DDB number for individual components are also included. The correlation is to be developed for input parameters, molecular weights of the individual components, equilibrium temperature and system pressure with the output parameters equilibrium liquid and vapour phase compositions. There are 222 data points which are divided in two parts, training and test data sets, containing 201 and 21 points respectively, for developing ANN models 1, 2 & 3 using **elite-ANN©**. The accuracy of the ANN model 3 developed is within acceptable limits of RMSE of 0.0894 & 0.1848 for training & test data respectively. The range of applicability of the developed models for temperature and pressure is 312.45 to 448.95 K and 23.371 to 101.33 kPa. Thus there is a lot of scope to explore developing ANN models with systems incorporating binary mixtures of several components.

## General Terms

ARM Based Embedded Systems, Portability.

## Keywords

VLE, Artificial Neural Network, binary system

## 1. INTRODUCTION

Vapour Liquid Equilibrium data for various binary, ternary & multi component 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. Thus the sizes, particularly the height of distillation columns are determined by the vapour liquid equilibrium (VLE) data for the mixtures. A reasonably good understanding of VLE is essential for the analysis, design, and control of distillation columns. Vapour–

liquid equilibrium (VLE) is a condition where a liquid and its vapour are in equilibrium with each other, such that the rate of evaporation equals the rate of condensation on a molecular level & there is no net vapour-liquid interconversion. Distillation can be employed for only if the compositions of 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 system 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, UNIFAQ, UNIQUAC and Wilson have been used to describe VLE. Another approach for phase calculation is based on equation of state. In some cases empirical and semi empirical equations are employed to predict VLE data. The constant 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.

### 1.1 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 a large number of interconnected processing elements called nodes working in a network to solve specific problem. [1]

The most common type of feed forward neural network is Multi Layer Perceptron (MLP). It consists of multilayer structure, with input and output layers & has at least one layer of processing units in between them called "hidden", since it does not communicate with the outside world directly. The nodes between the two successive layers are fully connected by means of constants called weights. The outputs from the input layer are fed to hidden layer units, which in turn, feed their outputs to the next hidden nodes present in the next layer. All the hidden nodes pass their net activation through a nonlinear transformation of a linear function, like the logistic sigmoidal to compute their outputs. For the training of 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],[7], for estimation of mass transfer coefficient for fast fluidized bed solids[8], modeling of distillation column[9], detergent formulation[10], modeling of unsteady heat conduction in semi infinite solid[11], prediction of mass transfer coefficient in downflow jet loop reactor[12] and modeling of packed column[13] and similar other[14, 15, 16] were also reported. [17, 18]

A typical topology of ANN model used in the present work is shown fig 1.
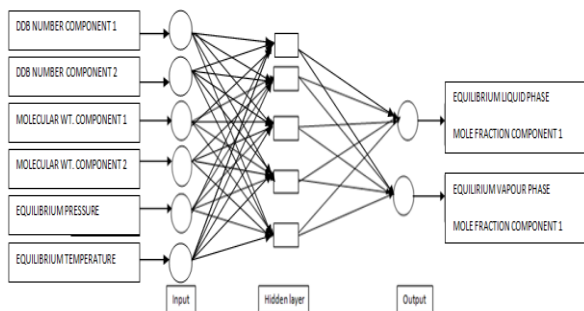


**Figure 1 Architecture of topology of ANN model:**

## 1.2 Methodology

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 obtained[19] 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.

**Table 1. ANN topologies for Model 1 & 2**

| Model | No. of neurons | | | | | Data points | Iterations |
|---|---|---|---|---|---|---|---|
| | Input layer | 1st Hidden layer | 2nd Hidden layer | 3rd Hidden layer | Output layer | Training | |
| | | | | | | 222 | 50000 |
| ANN 1 | 6 | 0 | 5 | 5 | 2 | RMSE 0.11531 | Time 70263 m |
| ANN 2 | 6 | 10 | 10 | 10 | 2 | RMSE 0.0819 | Time 23797 m |

The comparison of the actual and predicted values obtained using model 1 and 2 have been carried out. Fig 2 & 3show the graphs plotted between actual and predicted values using ANN model 1 and model 2 for liquid and vapour phase compositions respectively. Fig 4 shows the iterations versus error during training mode for ANN model 3.
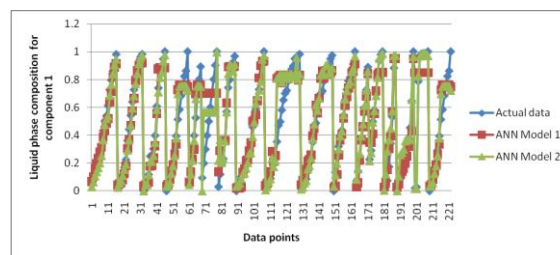


**Figure 2 Comparison of actual and predicted values using ANN model 1 and model 2 for equilibrium liquid phase compositions**
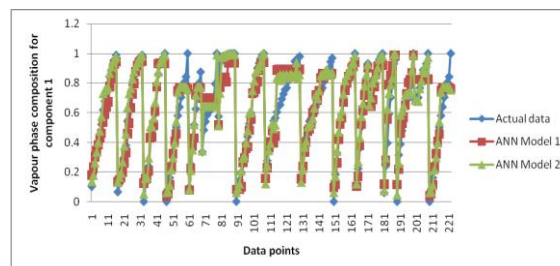


**Figure 3 Comparison of actual and predicted values using ANN model 1and model 2 for equilibrium vapour phase compositions**

As the % error is less for ANN model 2 hence it is selected for further processing & developing the model. The utility of ANN model is in prediction of not only training data set but test data set as well. The test data set is used for validating the model developed consists of the data points which are not used in developing the model. In present work data is thus divided into two parts, training & test data set with 201 & 21 data points respectively. The details of architecture & training for ANN model 3 is as given in table 2.

**Table 2 Topology of ANN model 3**

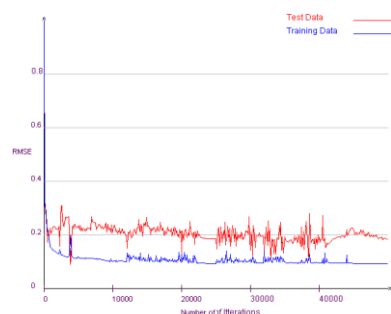| Model | No. of neurons | | | | | Data points | |
|---|---|---|---|---|---|---|---|
| | Input layer | 1st Hidden layer | 2nd Hidden layer | 3rd Hidden layer | Output layer | Training | Testing |
| ANN Model 3 | 6 | 10 | 10 | 10 | 2 | 201 RMSE 0.0894 | 21 RMSE 0.1848 |



**Figure 4 Pictorial views of the iterations versus error for training and test data**

Fig 5 and Fig 6 show the comparison of the predicted & actual liquid and vapour phase composition for training data set. Similarly fig 7 and fig 8 show the comparison of the predicted & actual liquid and vapour phase composition for test data set. As can be seen from these graphs there is close proximity between actual and predicted values.
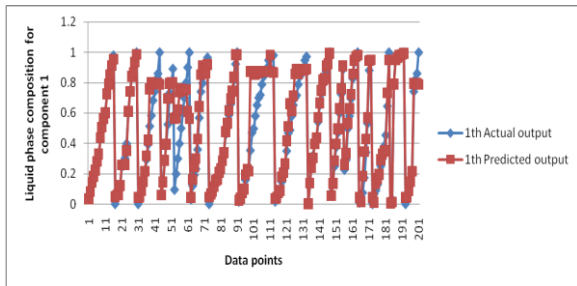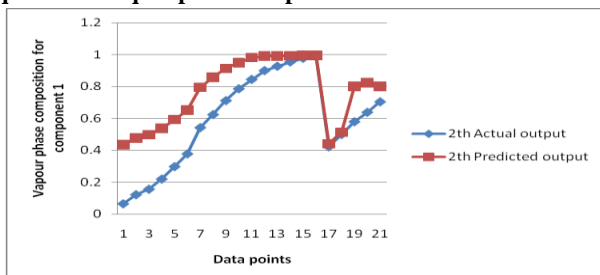


**Figure 5 Comparison of the predicted & actual equilibrium liquid phase composition for training data set**
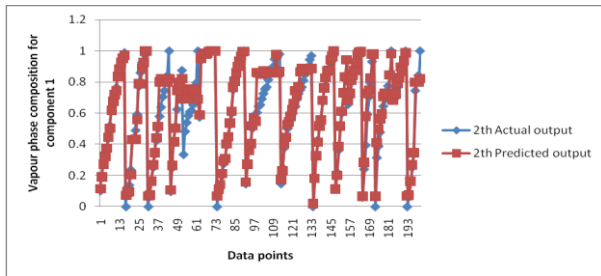


**Figure 6 Comparison of the predicted & actual equilibrium vapour phase composition for training data set**
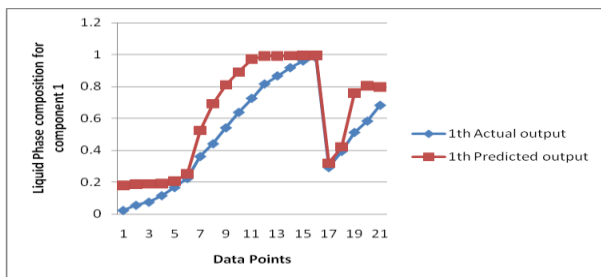


**Figure 7 Comparison of the predicted & actual equilibrium liquid phase composition for test data set**



**Figure 8 Comparison of the predicted & actual equilibrium vapour phase composition for test data set**

Figure 9 shows the relative error 1 and 2 for the parameters equilibrium liquid and vapour phase compositions respectively for all training data points; barring few points the relative error is within acceptable range of $\pm$ 15%. Average relative error for parameter 1 is 13.84% and for parameter 2 is 6.97%.
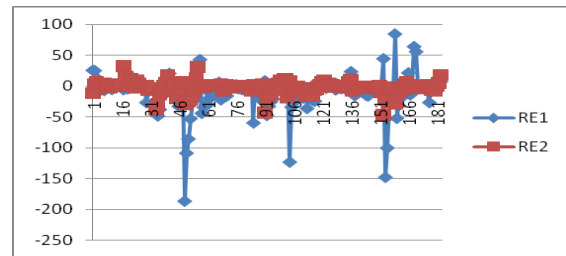


**Figure 9. Comparison of relative errors for parameter 1 and parameter 2 for training data set**

Similarly fig 10 shows the relative error 1 and 2 for the parameters equilibrium liquid and vapour phase compositions respectively for all test data points. As can be seen from the graph, barring few data points the relative error is in the range of $\pm$ 25%. Average relative error for parameter 1 is 23.324% and for parameter 2 is 31.79%.
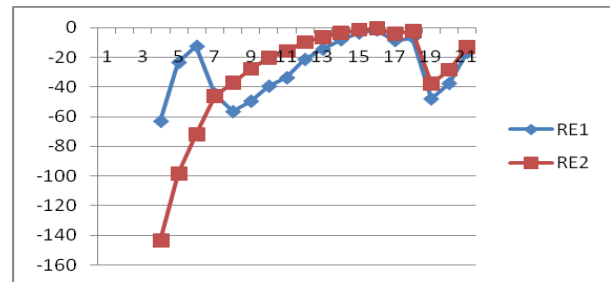


**Figure 10 Comparison of relative errors for parameter 1 and parameter 2 for test data set**

## 2. CONCLUSION

The objective of the present work was to develop ANN model for estimation of vapour liquid equilibria having ten binary mixtures involving nine 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 of RMSE of 0.0894 & 0.1848 for training & test data respectively. The range of applicability of the developed models for temperature and pressure is 312.45 to 448.95 K and 23.371 to 101.33 kPa. The novel feature of this work is incorporation of ten binary mixtures involving nine 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 binary mixtures with large number of components.

## 3. ACKNOWLEDGEMENT

## 4. REFERENCES

[1]. Anderson J.A, An Introduction to Neural Networks (Prentice-Hall of India, Pvt Ltd New Delhi), 1999.

[2]. Rumelhart D E & McClleland Back Propagation Training Algorithm Processing, M.I.T Press, Cambridge Massachusetts, (1986).

[3]. Fan J Y, Nikolau M & White R E, AIChE, 39 (1) (1993) 82.

[4]. Hoskins J C, Kaliyur K M & Himmelblau D M, AIChE, 37(1) (1991) 137.

[5]. Watanabe K, Abe M, Kubota M & Himmelblau D M, AIChE, 35 (11) (1989) 1803.

[6]. Belsito S & Banerjee S AIChE 44 (12), (1998), 2675.

[7]. Pandharipande S L & Badhe Y P, Chem Eng World 38(6) (2003) 70.

[8]. Zamankhan P, Malinen P & Lepomaki H, AIChE, 43(7), (1997) 1684

[9]. Baratti R, Vacca G & Servida A, Hydrocarbon Processing, (1995) 35.

[10]. Pandharipande S L, Agarwal R S, Gogte B B & Badhe Y P, Chem Eng World 38 (5) (2003) 78.

[11]. Pandharipande S L & Badhe Y P, Chem Eng World 38 (8) (2003) 82.

[12]. Pandharipande S L & Badhe Y P IChE, 45(4) (2003) 256.

[13]. Pandharipande S L & Mandavgane S A, Indian J Chem Technol, 11 (6) (2004) (820)

[14]. Pandharipande S L, Bhaise A & Poharkar A, Chem Eng World, 39 (1) (2004) 50.

[15]. Pandharipande S L & Badhe Y P, J Inst Eng, 84 (3) (2004) 65.

[16]. Pandharipande S L & Badhe Y P, **elite-ANN**©, ROC No SW-1471/2004.

[17]. Hajir Karimi and Fakhri Yousefi Chin. J. Chem. Eng., 15(5) 765—771 (2007)

[18]. Maria C lluita, Ion lluita, Faical larachi Chemical Engineering Science Vol 55, Issue 15 2813-2825 (2000)

[19]. Dortmund Data Bank website: http://www.ddbst.com/en/ddbst/index.php.