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Full Length Research Paper

Prediction and optimization of vapor-liquid equilibrium (VLE) data for equimolar ethanol/water mixture using adaptive neuro-fuzzy inference system

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ABSTRACT: This research work explores the calculation of vapor phase fraction (VPF) data for an equimolar mixture of ethanol/water system through applications of Artificial Neuro-Fuzzy Inference System (ANFIS). The calculation of VPF data by conventional thermodynamic methods is tedious and requires the determination of "constants" which is arbitrary in many ways hence the need to adopt ANFIS with its associative property and its ability to learn and recognize highly nonlinear and complex relationships. An empirical model was first developed to attempt predicting the highly nonlinear system. A Sugeno type ANFIS model having 5 layers with 9 hidden neurons representing the If then, the fuzzy logic rule was developed to predict the vapor phase fraction of the system. The inputs to the model were the temperature and pressure values simulated on Honeywell UNISIM® design software and the model was trained to calculate the mole fraction and vapor phase fraction of the system taken as outputs. The triangular membership function was used for the inputs and the constant membership function for the outputs. The ANFIS model returned R-square values of 0.9915 and 0.9981 for the mole fraction and molar flow rate respectively as against 0.7715 and 0.7733 respectively for the empirical model. The ANFIS model was further optimized using data-based particle swarm optimization to give a prediction of 89 mole% and flow rate of 2.11Kgmole/h at a temperature of 62.13^{o}C and pressure of 55.92KPa for the distillate. It can therefore be concluded that the ANFIS model gives a superior predictive capability than conventional thermodynamic models for system evaluation and design. This work is a basis for the design of flash columns to substitute conventional distillation columns in ethanol recovery.

Keywords: Optimization, prediction, ethanol, mixture, artificial, fuzzy-inference

INTRODUCTION

The development, design and operation of equilibrium stage processes require a detailed knowledge of the composition of coexisting phases at equilibrium, and the effect of temperature and pressure on this composition. However, such knowledge is limited, and usually not available when new systems are under consideration, because it is difficult and laborious to obtain the data experimentally. Classical thermodynamics of solutions provides us with ways and means of treating and testing experimental data, but it is of very little use in predicting system properties. Predictive methods are therefore valuable for process evaluation and design. Liquid state is highly complex for any general description, being in the in between ' state of 'orderly solids and disorderly gases. Our lack of knowledge of the liquid state precludes the prediction of solution properties from those of the pure components which are, in most cases, either readily available or easily estimated, and forces us to develop

empirical methods. With the rise of petrochemical industry and the rapid increase in the number and quantity of solvent type compounds, there is a concentrated attention on matters relating to distillation in general and vapor-phase fraction in particular. Vapor-phase fraction data are studied primarily with either one or both of the following objectives in mind:

(1) To collect the necessary equilibrium data for design of chemical process equipment.
(2) To provide the essential data needed to formulate models for the prediction of solution properties and test existing models.

To date, there has been virtually no first principles-based predictive method that can deal with the problem efficiently with an accuracy surpassing the widely utilized highly successful correlated models such as UNIQUAC Functional Group Activity Coefficients (UNIFAC). In spite of intensive theoretical efforts over the last few years to develop various physical and computational models to predict Vapor Phase Fraction (VPF), it appears that much more remains to be done in order to make the prediction reliable with accuracy comparable or superior to the experimental measurements. Thus, it is necessary to reduce and correlate the limited data to the best possible interpolations and extrapolation. This is the incentive for the application of various correlations to the calculation of phase equilibrium relationships. The Equations of State (EOS) fairly predicts the Vapor Liquid Equilibrium (VLE) data of hydrocarbon systems but is quite handicapped for systems containing polar compounds. Further, the EOSs are neither able to describe the critical region satisfactorily for mixtures nor estimate the liquid properties accurately. Activity coefficients are generally used for determining liquid properties and several estimation techniques exist in the literature (Smith and van Ness, 1995; Fredenslund *et al*., 1977). However, each has its limitations in its applicability to different systems; for instance, even though the UNIFAC method (Fredenslund *et al*., 1977) is applicable even to systems containing water, it has its limitations with regard to hydrocarbon mixtures. So, thermodynamics of mixtures are more complicated than for pure compounds and the difficulty in mixture analysis increases with the extent of non-ideality. To speed up flash calculation, attentions have been paid to other numerical tools, such as sparse grids technology and artificial neural networks (ANN). Sparse grids technology is often considered preferable in coupling with flow as the surrogate model created in the offline phase can be used repeatedly (Yuanqing *et al*., 2015). However, the generation of the surrogate model is still time- consuming. On the other hand, due to its ability to capture the relationship among large number of variables, especially for non-linear correlations, ANN has attracted considerable attention for performing acceleration. Artificial Neural Network (ANN) can be cited as‘ algorithmic equivalent’ of the human learning process and information processing scheme at a modest scale. They are pattern recognition architecture which can identify patterns between complex sets of input and output data (Hagan and Demuth, 1996). The chief advantage of ANNs lies in the fact that ANN uses a generic model which covers a wide class of problems. Thus, they are gaining a rapid interest within engineering, medical, financial and various other fields. ANNs being purely “numeric” in nature do not require thermodynamic modeling; and hence, are convenient for VPF data prediction (Sharma *et al*., 1999). It has been reported that ANN has been used in the thermodynamic property’s calculation successfully, including compressibility factor, vapor pressure and viscosity. For example, ANN has shown the efficiency, as well as the ability to estimate the shape factors and density of regenerates, which is a function of temperature, and then been extended to solve the corresponding state model (Viet *et al*., 2007; Nikkholgh *et al*., 2010; Ahmad *et al*., 2013). Mehmet (2004), employed a neural network model to calculate the isobaric vapor-liquid equilibrium of binary systems composed of different chemical structures, which do not show azeotropic behavior. Results generated by the ANN model were compared to those generated by the UNIFAC and the Margules model. In all cases, the deviations between the experimental activity coefficients and those calculated by the neural network were less than those obtained by the Margules and the UNIFAC models.

Although, ANN can predict the VLE successfully, traditional neural network schemes still have several limitations that result from the possibility of getting trapped in local minimum, and the choice of model architecture. If the predicting performance can be further promoted, a better operation strategy can be formed. To overcome these limitations of traditional ANNs, and to increase their reliability, many new training algorithms have been proposed such as ANFIS (Jang, 1993). ANFIS stands for Adaptive Neuro-Fuzzy Inference System. It is a hybrid neuro-fuzzy technique that brings learning capabilities of neural networks to fuzzy inference systems. The learning algorithm tunes the membership functions of a Sugeno-type Fuzzy Inference System using the training input-output data which allows the fuzzy systems to learn from the data they are modeling. The basic structure of a fuzzy inference system is a model that maps input characteristics to input membership functions, input membership functions to rules, rules to a set of output characteristics, output characteristics to output membership functions, and the output membership functions to a single-valued output or a decision associated with the output. Such a system uses fixed membership functions that are chosen arbitrarily and a rule structure that is essentially predetermined by the user's interpretation of the characteristics of the variables in the model. The neuro-adaptive learning method works similarly to that of neural networks.

Neuro-adaptive learning techniques provide a method for the fuzzy modeling procedure to learn information about a data set. Fuzzy Logic Toolbox software computes the membership function parameters that best allow the associated fuzzy inference system to track the given input/output data. The Fuzzy Logic Toolbox function that accomplishes this membership function parameter adjustment is called ANFIS (Neural Networks Toolbox User's Guide, 1994). The computation of these parameters (or their adjustment) is facilitated by a gradient vector. This gradient vector provides a measure of how well the fuzzy inference system is modeling the input/output data for a given set of parameters. When the gradient vector is obtained, any of several optimization routines can be applied in order to adjust the parameters to reduce some error measure. This error measure is usually defined by the sum of the squared difference between actual and desired outputs. ANFIS uses either back propagation or a combination of least squares estimation and back propagation for membership function parameter estimation. At the end of training, the trained ANFIS network would have learned the input-output map and be ready to be deployed into the larger control system solution. ANFIS has been successfully applied in many fields such as automated control, water resource management, fishing catch (Kalyanaraman and Akilandeswari, 2005; Karthikeyan *et al*., 2005; Chang and Chang, 2006; Cakmakci, 2007; Firat and Güngör, 2007). Hosseini-Nasab *et al*. (2013) investigated the accuracy of an ANFIS for the three binary refrigerant systems for prediction the vapor liquid equilibria. Their results demonstrated that the ANFIS can be applied successfully and provide high accuracy and reliability for prediction of VLE. Furthermore, the performance of the proposed model was compared with SRK-EoS by using statistic parameters in terms of mean MAPE, MSE, RMSE, and R^2 for error estimation. The comparison of the prediction accuracies of the ANFIS and SRK-EoS indicated that the neuro-fuzzy approach was more accurate in predicting VLE (Hosseini-Nasab *et al*., 2013). Development of ANFIS model for predicting VLE is less cumbersome than methods based on EoS, because ANFIS does not require parameters such as the critical properties of the component, and the binary interaction parameters and the mixing rules as required by conventional methods (EoS). In this present work, application of ANFIS for predicting and optimizing VPF data will be explored. According to Gibbs phase rule, two intensive properties are required to completely describe a binary two-phase system at equilibrium. Thus, two intensive properties can be selected to describe all the properties of the system irrespective of the methodology used. Pressure (P) and Temperature (T) are two convenient intensive properties, since they can be easily measured and controlled. Therefore, the ANFIS to be developed will use P and T as the inputs and will give mole fraction and molar flow rate of the distillate as the outputs. Ethanol-water system was selected to explore the use of ANFIS as an alternative VLE data prediction.

MATERIALS AND METHODS

The materials utilized for this study were mainly software which was projected with a personal computer. The software includes:

(i) Honeywell UNISIM design: software widely used by processing engineers for the design of chemical engineering process routes, schedules of the equipment design and processing of raw materials into finished goods (steady state and dynamic process).
(ii) MATLAB: mainly used for mathematical computation and modeling. It is vast in various areas of model generation, optimization and artificial intelligence modeling.
(iii) MICROSOFT WORD: used to create professional looking documents.

The vapor-phase fraction, the molar flow rate and the mole fraction of the volatile component were obtained using UNISIM design software at varying temperature and pressure values shown in Table1 for an equimolar mixture of ethanol and water (inlet mole fraction of ethanol = inlet mole fraction of water = 0.5) and feed stream molar flow rate of 100kgmole/h.

Table 1: Data for UNISIM design software simulation.

Temperature (ºC)	Pressure (KPa)
60.6	53.33
65.9	57.00
67.6	61.00
70.3	68.00
72.5	74.00
74.6	80.00
77.5	87.00
80.0	95.00
83.7	105.00
88.0	120.00
91.0	128.00

The empirical modeling

The empirical model is an exponential model given as:

$$\left(Y_{frac}, Y_{flow}\right) = e^{a_0 + a_1 T + a_2 P} \quad (1)$$

Taking the natural logarithm of both sides of equation 1 gives

$$\ln\left(Y_{frac}, Y_{flow}\right) = a_0 + a_1 T + a_2 P \quad (2)$$

Where;

Y_{frac}, Y_{flow} = ethanol mole fraction and molar flow rate at the top product of the flash column respectively,

T = inlet temperature,
P = inlet pressure and
a_0 to a_2 = regression coefficients
Inserting the error parameter into equation 2 to obtain:

$$Y_{fract} = a_0 + a_1T + a_2P + \varepsilon \quad (3)$$

Making the error parameter ε the subject of the formula:

$$\varepsilon = Y_{fract} - a_0 - a_1T - a_2P \quad (4)$$

Squaring and summing ε from equation 4 gives:

$$\sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(Y_{fract} - a_0 - a_1T - a_2P\right)^2 \quad (5)$$

Let $S = \sum_{i=1}^{n} \varepsilon_i^2$

Equation 5 becomes: $S = \sum_{i=1}^{n} \left(Y_{fract} - a_0 - a_1T\, a_2P\right)^2$

Differentiating S with respect to a_0, a_1 and a_2 and solving for the resultant matrix gives:

$$y = A \times a \quad (6)$$

$$Where \begin{bmatrix} \sum_{i=1}^{n} Y_{fract} \\ \sum_{i=1}^{n} Y_{fract}T \\ \sum_{i=1}^{n} Y_{fract}P \end{bmatrix} = y, \begin{bmatrix} n & \sum_{i=1}^{n} T & \sum_{i=1}^{n} P \\ \sum_{i=1}^{n} T & \sum_{i=1}^{n} T^2 & \sum_{i=1}^{n} PT \\ \sum_{i=1}^{n} P & \sum_{i=1}^{n} PT & \sum_{i=1}^{n} P^2 \end{bmatrix} = A, \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = a$$

Making a the subject of the formula gives:

$$a = A^{-1} \times y \quad (7)$$

Equation 7 was used to determine the regression coefficient values a_0 to a_2 in MATLAB.

The ANFIS model

Adaptive Neuro Fuzzy Inference System (ANFIS) is the adaptive combination of artificial neural network and fuzzy inference system. It is believed by past works to be the best in terms of handling of stochastic data that yields high prediction accuracy. MATLAB 2015a was used for the model because it is the only software that has an application for modeling ANFIS. In this structure, the Takagi-Sugeno fuzzy system was employed as FIS. In the architecture used in this study, to simplify the model used, it is assumed that the framework of ANFIS includes two inputs (x, y) representing temperature and pressure and one output (F) representing the mole fraction or molar flow rate. Thus, a fuzzy rule based on the Takagi–Sugeno type can be represented as below: (Rezakazemi *et al.*, 2017; Ausati and Amanollahi, 2016).

Rule 1: If x is A_1 and y is B_1 then

$F_1 = a_1x + b_1y + r_1$. (8)

Rule 2: If x is A_2 and y is B_2 then

$F_2 = a_2x + b_2y + r_2$. (9)

where, A_1, A_2, B_1 and B_2 are nonlinear parameters and membership functions for inputs (x and y) and a_1, a_2, b_1, b_2, r_1, and r_2 are linear, and output's (F) function parameters. The ANFIS architecture includes five layers with different functions. These layers can be named as a fuzzy layer, product layer, normalized layer, de-fuzzy layer and output layer, respectively. The function of each layer is shown in equations (10) - (15). Each node 'i' in this layer produces a membership grade of a linguistic label. The membership relationship including the input and output functions of this layer can be written as:

$Fi^1 = \mu Ai(x);$ i=1, 2… (10)

$Fi^1 = \mu Bi(y);$ i=1, 2… (11)

Where Fi^1 and Fi^1 show membership functions and μAi(x) and μBi(y) indicate the output functions. Each node in this layer is a fixed node which calculates the 'firing strength' (w_i) of each rule. In the second layer, output is the input signal's product that is referred to as:

$F_i^2 = w_i = \mu A_i(x) \times \mu B_i(y)$, i=1,2,… (12)

Where F_i^2 shows the output.

In layer 3, the weight function is under normalization as:

$F_i^3 = w = \frac{Wi}{W1+W2}$ i=1,2,… (13)

Where F_i^3 was called normalized firing strength.

In layer 4, the output from the prior layer is multiplied with the Sugeno fuzzy rule's function:

$F_i^4 = \overline{wi}f_i = wi(a_ix+b_iy+r_i), \quad i=1,2,\ldots$ (14)

where F_i^4 indicates the output of the layer 4.

In layer 5, the sum of all outputs of every rule is computed and overall output can be calculated as follows:

$$F_i^5 = \text{overall output} = \sum \overline{wi}\, fi = \frac{\sum_i WiPi}{\sum_i Wi} \quad (15)$$

In the ANFIS structure, the first layer and the fourth layer include parameters that can be changed over time. The first layer contains the nonlinearities of the precursor parameters, while the fourth layer contains the linear result parameters. Both of these parameters can be modified and updated with a learning method that trains both of these parameters and also adapts to their conditions. Particle swarm optimization was used in this study in ensuring that the optimum (maximum) value of the vapor-phase fraction of ethanol in ethanol water mixture was achieved with the required temperature and pressure values obtained. ANFIS model, being the best model for the prediction of VPF with respect to temperature and pressure as the independent variables was used as an objective function to particle swarm optimization technique (PSO). Since ANFIS model is not empirical model but an intelligent model, a MATLAB program was developed to proceed based on the data format of the PSO. This program selects the best point (optimum value of the response) and prints the independent variables associated with the best point. It should be noted that the best point is not always part of the ANFIS predicted data but part of the direction of prediction performed by the ANFIS.

RESULTS AND DISCUSSION

In this work to predict and optimize the flash calculation, an ANFIS was used to model input and output process of the NPT flash column for an equimolar ethanol/water system. An empirical method was first developed to be used as a comparison. Essentially, as the Gibbs phase rule stipulates, two intensive properties are required to completely describe a binary two-phase system at equilibrium conditions. Temperature and pressure were two such thermodynamic intensive properties conventionally selected as inputs to the model, because of the relative ease with which they can be measured. Molar flow rate and mole fraction values of the distillate for a total of 11 temperature/pressure data points were gotten from the UNISIM software flash simulation for training the ANFIS model. The aim function which was used to select the ANFIS as the best model is the root squared error. Furthermore, the ANFIS prediction was optimized using PSO.

Data selection

NPT flash simulation was carried out using 11 data points of variable temperature and pressure values as presented in (Table 1). The temperature range considered were those within the boiling points of the components of the mixture (78°C and 100°C for ethanol and water respectively) and the pressure range that gave tangible mole fractions of ethanol at the top. Notwithstanding the stochastic nature of the data set, it was expected of the model to give a robust performance after training as ANNs are proven to model even stochastic data with great accuracy.

Empirical model

An empirical model was developed using data generated from the NPT flash simulation on UniSim design software. An exponential model was chosen considering the highly non-linear behavior of the system. Table 2 shows the corresponding VLE data for the system as simulated using UNISIM software. Equations 16 and 17are the empirical models developed for the prediction of the mole.

$$\ln Yflow = 4.0479 + 0.0079T - 0.0066P \quad (16)$$

$$\ln Yfrac. = -41.1938 + 0.9056T - 0.2903P \quad (17)$$

Data which shows the actual and predicted values for the molar flow rate and mole fraction of the distillate for the 11 data pairs were used to plot (Figures 1- 6) using the MATLAB graphing tool. Generally as seen from (Figures 1 and 3), the mole fraction of ethanol decreased as the values for the input variables (temperature and pressure) correspondingly increased. This could be because of the approach towards the boiling point of water which increases the volatility of water since volatility is a function of temperature and pressure.

Also, Figure 5 shows that although the data line of the empirical model predicted mole fraction followed a similar path with the actual (UniSim) data, the fit was not satisfactorily close.

The plot of the empirical model predicted data compared with the actual data of molar flow rate for the distillate followed an increasing trajectory up to the eight data point (between temperature/pressure range of 60.6°C/53.33KPa and 83.7°C/105.00KPa). Hence, it is inferred that although the developed empirical model is somewhat capable of describing the liquid system, its prediction is not highly robust.

Table 2: UNISM data for VLE of equimolar ethanol/water mixture.

Temperature (ºC)	Pressure (KPa)	Vapor Phase Fraction VPF	Ethanol flow rate at the top Y_{flow} (kgmole/h)	Ethanol mole Fraction at the top $Y_{frac.}$ (%)
60.6	53.33	0.0000	0.0000	0.0000
65.9	57.00	0.0758	4.9394	65.19
67.6	61.00	0.1742	11.2340	64.48
70.3	68.00	0.2641	16.8364	63.75
72.5	74.00	0.3585	22.5455	62.89
74.6	80.00	0.4491	27.8275	61.96
77.5	87.00	0.6848	40.2157	58.72
80.0	95.00	0.7348	42.4227	57.74
83.7	105.00	0.8724	47.3264	54.25
88.0	120.00	0.9420	48.9781	51.99
91.0	128.00	1.0000	50.0000	50.00

ANFIS model

The ANFIS modeling was a supervised learning algorithm as the algorithm was provided with not only the inputs, but also the targets (desired outputs). The hybrid training algorithm was used for the ANFIS with the following configurations; 5 layers representing the fuzzy membership functions with 9 hidden neurons. As shown in Figure 7, the model took the two variables (temperature and pressure) as inputs and the value of mole fraction and molar flow rate for the distillate as the output. The key parameters of the model are the weights of each layer, which determines the outputs from the model given the input. At first, those weights were initialized randomly, which meant that the model gave insignificant output values with the given inputs. To make the model useful for this problem, those weight parameters were trained with the fuzzy inference system to fit our problem. In doing so, an iterative optimization process was run on the model's parameters to make the loss (error) as small as possible. The difference between the model's output and the expected value is referred to as loss. Here, for this regression problem, R-squared was used as the loss function. As the training progressed, the loss of the model on the validation dataset decreased gradually, which implies that the difference between the model's output and the expected value became smaller, and the model became increasingly useful.

In this study, using the programming language of MATLAB 2015a software, ANFIS and PSO-ANFIS were proposed for VLE prediction. In the first step of modeling, temperature and pressure were set as input factors, and mole fraction and molar flow rate of the distillate were set as output factors. In order to obtain enough prediction capability using ANFIS, it be provided with an adequate number of clusters for the model. The developed ANFIS model uses fuzzy c-means clustering to form a fuzzy inference system. This process depends on the number of data that are evaluated for training. The rule extraction method first uses the Fuzzy c- means (FCM) clustering function, known as genfis3, to determine the number of rules and membership functions for the antecedents and consequents. The Fuzzy c-means (FCM) clustering techniques (genfis3) were also used to optimize the result by extracting a set of rules that models the data and generate an initial FIS for ANFIS training. In order to construct a fuzzy system using ANFIS, the genfis3 function in MATLAB is first run to create a Sugeno-type FIS structure using fuzzy c-means clustering to extract a set of rules and membership functions that model the training data. This function allows the specification of the number of clusters used to model the data.

In PSO-ANFIS, ANFIS provides the search space while PSO seeks the best solution by comparing objective function at each solution point. The difference between the actual data and the model output can be minimized by iterating the PSO algorithm (Sajjadi *et al*., 2017). The main benefit of the PSO is that this algorithm has a high degree of stability and does not depend on the derivative nature of the objective function and can achieve the optimal solution by tuning the membership functions. Data based PSO-ANFIS model was applied by using a code developed in MATLAB software. Figures 8 and 9 show the intelligence model prediction results for the mole fraction and molar flow rate of the distillate for the various temperature/pressure data pairs. The predictions for the data sets followed similar trajectory of the actual data gotten from UNISIM simulation for both mole fraction and molar flow rate values. To demonstrate the relative accuracy of the ANFIS model with UniSim data (seen as real data).

Figures 10 and 11 show the validation plot for the actual and predicted values of the mole fraction and molar flow rate of the distillate; where the blue solid curve is the UniSim values and the red curve denotes the neural network model prediction. The intelligence model gave very robust predictions of the mole fractions and molar flow rates with just very slight deviations between the second and third points. Also, the coefficient of determination (R-square) of 0.99 as seen in (Table 3) validates the robustness of the ANFIS model in predicting the thermodynamic properties of interest.

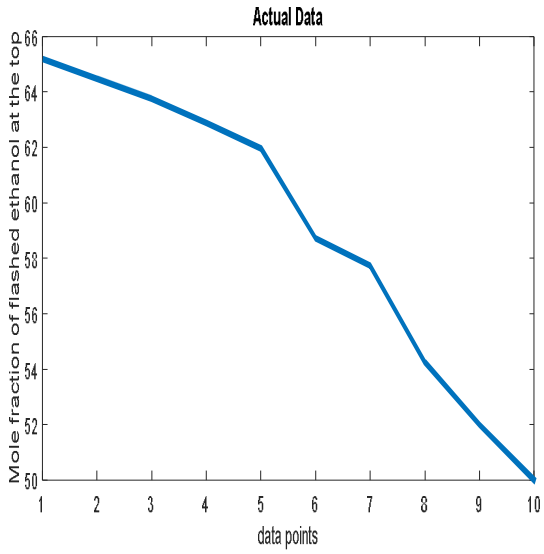

Figure 1: Actual Data of Mole Fraction of ethanol at the top (%).

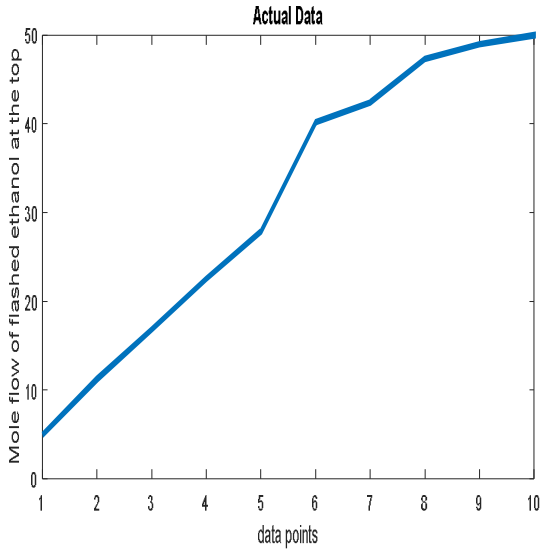

Figure 2: Actual Data of Molar Flow Rate of ethanol at the top (Kgmole/h).

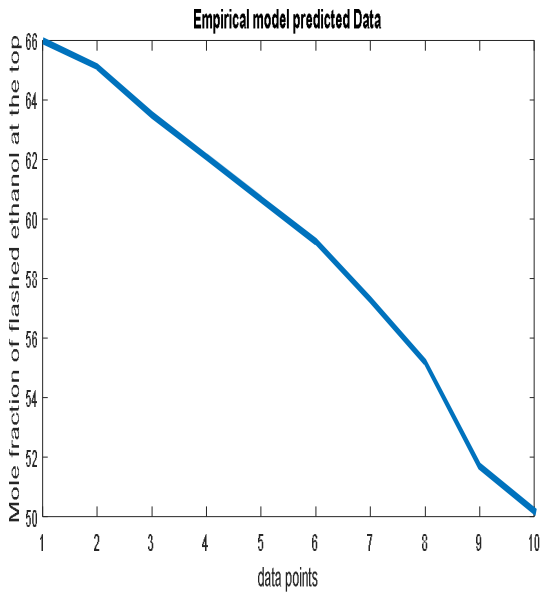

Figure 3: Empirical Model Predicted Data Fraction of Ethanol at the top (%).

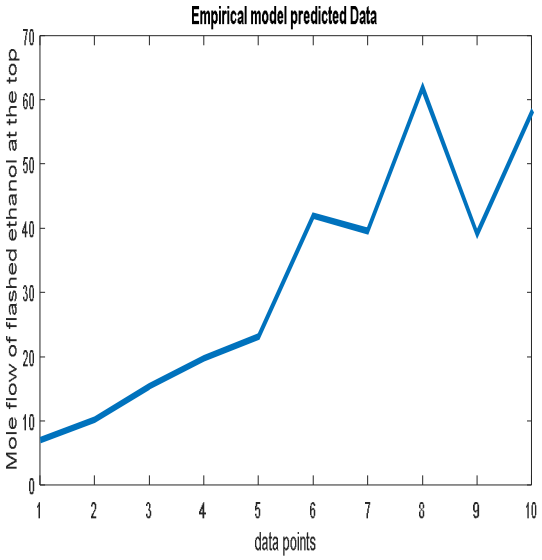

Figure 4: Empirical model Predicted data of Mole Mole flow of ethanol at the top (kgmole/h).

Comparism between the empirical and intelligence model

To show the convenience of the developed ANFIS model on VLE prediction, an empirical model has also been developed as a comparison. Overall, it can be seen from Figures 12 and 13 that the VLE prediction using ANFIS model can always preserve the accuracy while empirical models may result in large error. Phase equilibrium properties usually exhibit nonlinearity, with the first-principles models often inaccurate and demanding modifications. This is because of its assumption that the relative volatility is a constant, although studies from literature have shown it is not so with varying feed conditions. The developed ANFIS model on the other hand, helped such predictions and eliminated the need for determining these constants by finding the functional relationship all at once. As a result, the machine learning method was used to achieve a better model to represent the properties. An ethanol purity of 89 mole % at a flow rate of 2.11Kmol/h was achieved in the flash column after optimization using PSO with the optimal parameters of 62.13^{o}C and 55.92 KPa.

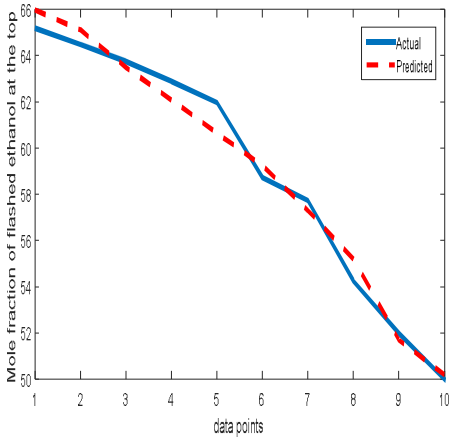

Figure 5: Empirical model predicted versus mole fraction of ethanol (%).

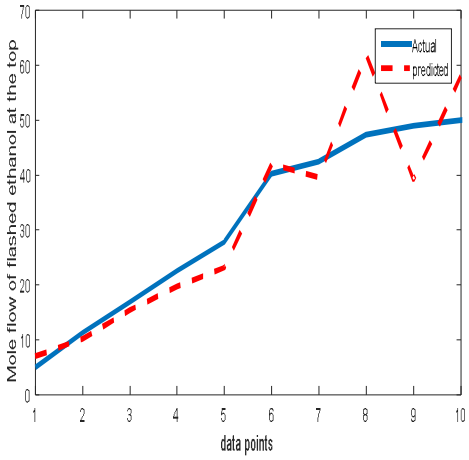

Figure 6: Empirical model predicted actual data versus actual data of molar flow rate of ethanol at the top (Kgmole/h).

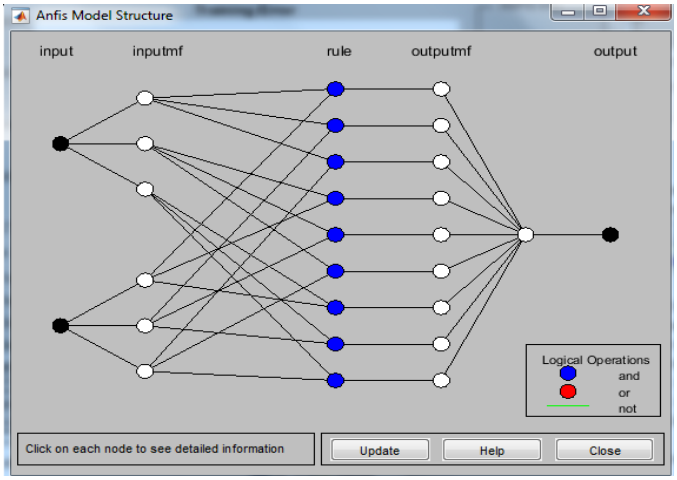

Figure 7: Architectural structure of the ANFIS model.

Table 3: Prediction Performance Evaluation.

	Mole fraction (%)		Molar Flow Rate (Kgmol/h)	
	Empirical	**Intelligence**	**Empirical**	**Intelligence**
SSE	30534	0.63719	10141	2.064
SSR	30274	269.45	7841.7	2512.7
R-square	0.77149	0.99149	0.77325	0.99806

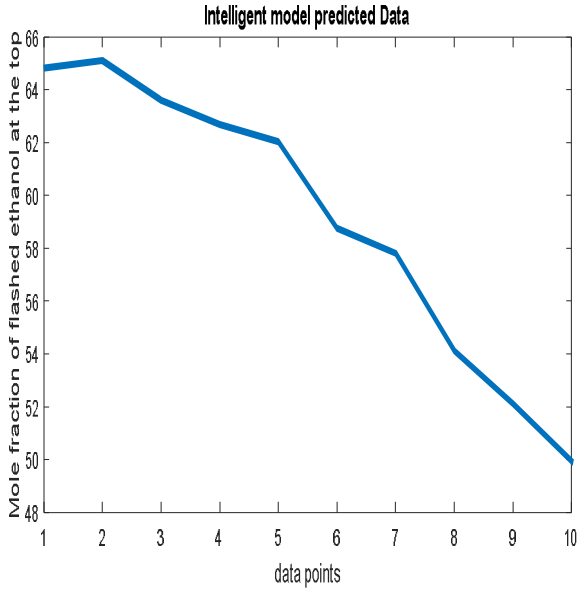

Figure 8: Intelligence model predicted data of mole fraction of ethanol at the top (%).

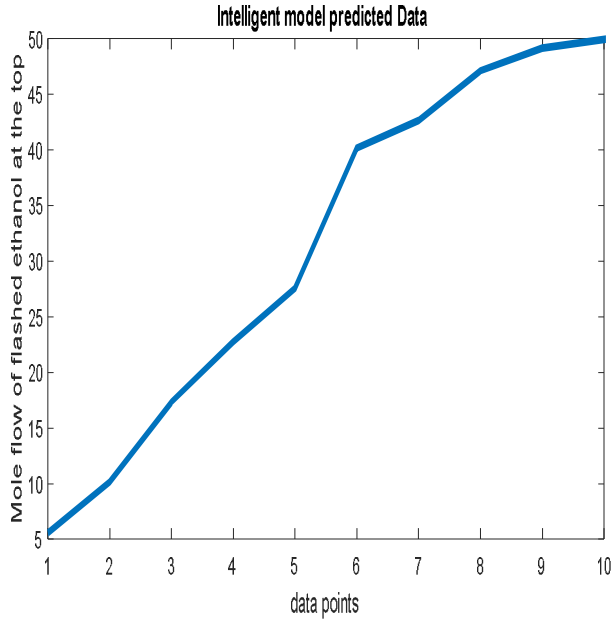

Figure 9: Intelligence model Predicted data of Mole flow of ethanol at the top (Kgmole/h).

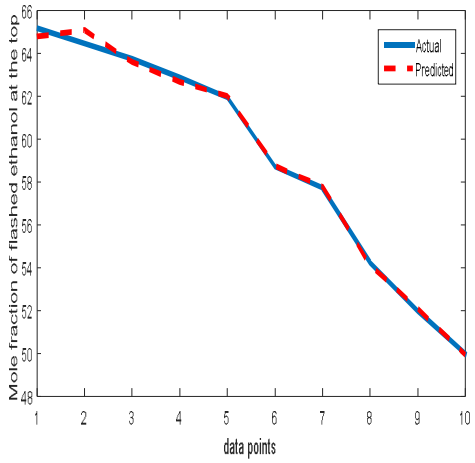

Figure 10: Intelligence model predicted data compared to the actual data of ethanol mole fraction at the top (%).

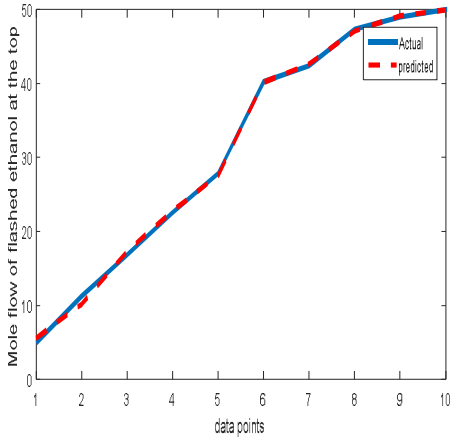

Figure 11: Intelligence model predicted data compared to the actual data of ethanol molar flow rate at the top (Kgmole/h).

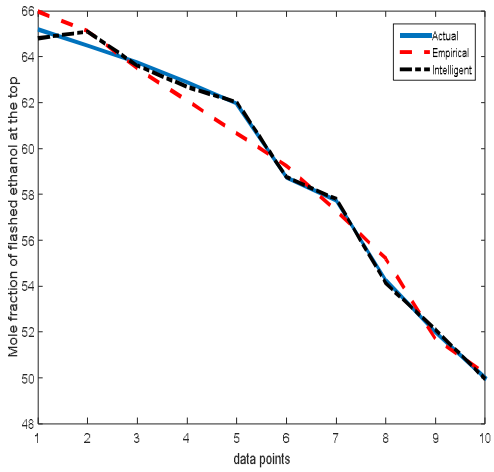

Figure 12: Comparative analysis for mole ethanol at the top (%).

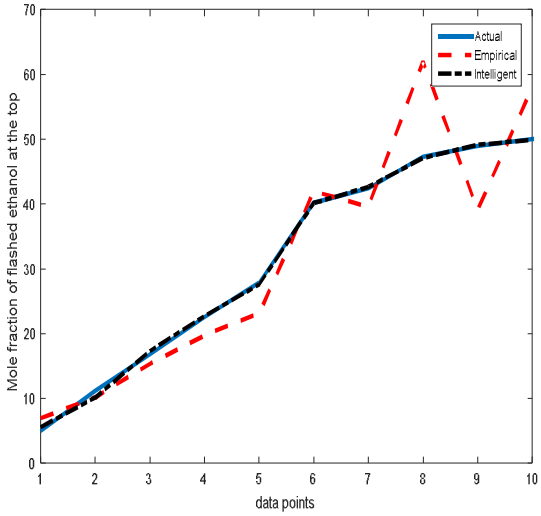

Figure 13: Comparative analysis for molar fraction of flow rate of ethanol at the top (Kgmole/h).

Conclusion

An artificial neuro fuzzy inference system has been developed for the prediction of VLE data in a non-linear binary system (ethanol/water) and the model predicts the composition and flow rate of ethanol in vapor phase for an equimolar mixture of ethanol and water. Sets of 11 experimental data pairs were used for the network training. The best architecture is the feed forward neural network, which consists of one hidden layer with 9 neurons. The performance of the proposed ANFIS model was also tested through its application to a test data set consisting of one-third of the experimental data not used in the training. The results of this estimation indicate that the developed ANFIS will be able to predict VLE data with lower errors than that of the other well- known thermodynamic models. An even spread of the data seemed to be essential for better predictions. Thus, in principle ANFIS hold promise as a strategy for solving the tedious VLE data generation problem.

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