



Prediction of Vapour-Liquid Equilibrium Data Using Neural Network for Hydrocarbon Ternary System (ETHANE-PROPANE-N-BUTANE)

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ABSTRACT

The prediction of vapour-liquid equilibrium is useful in process simulation and control as well making process engineering design decisions. Prediction of vapour-liquid equilibrium data was carried out using MATLAB software. Pre-existing data of hydrocarbon ternary system (ethane-propane-n-butane) in terms of phase composition, temperature and pressure was trained by iteratively adjusting networks, initializing weights and biases to minimize the network performance function net. MATLAB a software package containing artificial neural network was employed to predict the point where there is no change in composition of both liquid and vapour formed when liquid mixtures of ethane-propane-n-butane vapourises. Predicted values show reasonable and good correlation results when compared to the experimental data thus indicating that the network is an efficient and a good prediction tool for vapour-liquid equilibrium ternary systems.

Keywords: artificial neural network, biases, correlation, performance function net, vapour-liquid

INTRODUCTION

There are so many previous approaches to predicting and correlation vapour-liquid equilibrium data. Based on very good and reliable information and data, many attempts, methods and concept has been made to predict vapour-liquid equilibrium data before the advent of artificial neural network. Such attempts include: graphical method and analytical approaches.

The graphical method that have been employed include: Kellogg, De priester and Edminster monographs which were basically on fugacity and equation of state and Winn monographs which were based on convergence pressure.

The analytical approaches make provisions for the effect of variation of composition at constant pressure and temperature on equilibrium constant. Under this approach, the concept of thermodynamics is useful in correlating, predicting and interpreting available data.

Some of the analytical approaches are: Benedict Webb-Rubin equation of state, Redlich- kwong etc.

Vapour and liquid are said to be in a state of equilibrium when there is no change in the composition of both liquid and vapour formed when a liquid mixture vapourizes. Vapour-liquid equilibrium (V L E) data supplies the required information regarding the point where phase transition occurs which is useful

in the design and control of an evaporation or condensation process. Such V L E information is also useful in designing columns for distillation [1], [2], [3]. It is necessary to establish the basic background required for a better understanding of the vapour-liquid phase behavior of ternary systems. In an attempt to solve equilibrium stage problems, a model or a reliable correlation tool for vapour-liquid equilibrium and other physical properties of the system needed to be developed.

Early attempt to predict multi-component two-phase equilibria showed that the calculation based on binary equilibria only is not able to fit quantitatively the experimental multi-component equilibrium data [4]. In order to improve the consistency of experimental and computed

V L E data, also ternary equilibria should be regarded [5], [6]. Experimental V L E data were correlated using Redlich-Kister, Wilson and NRTL expression for excess Gibbs energy, GE. [7], [8], [9], as cited by [10].

Also, [11] have shown how NRTL equation can be used for simultaneous correlation of vapour-liquid equilibrium data. In this study, artificial neural network (A N N) was employed for predicting V L E data. Artificial neural network is an attempt at modeling the information processing capabilities of the nervous

system [12]. A N N is a simplified model of the brain which transforms inputs into outputs. One of the major advantages of the artificial neural network is efficient handling of non-linear relations in data even when the exact nature of such relation is unknown [13] cited by [14]. A N N has the ability to identify underlying highly complex relationships with input data. Infact, they define several empirical relations each for a part of the data. [15] cited by [14].

Determination of vapour-liquid equilibrium data can be achieved with the aid of the following:

Raoult's Law

It looks at equilibrium distribution of a liquid in a binary system component mostly between liquid and gas.

For a component, the fugacity of vapour phase F_i^V is related to fugacity of liquid phase F_i^L by

$$F_i^V = F_i^L \quad (1)$$

The vapour phase fugacity F_i^V at constant temperature and pressure is proportional to the mole fraction of vapour phase, thus,

$$F_i^V \propto y_i \quad (2)$$

$$F_i^V = y_i F^V \text{ pure } i \quad (3)$$

$F^V \text{ pure } i$ is the fugacity of pure component i as a vapour at temperature and pressure of a mixture.

The liquid phase fugacity of F_i^L is proportional to the liquid mole fraction x_i at constant temperature and pressure, hence,

$$F_i^L \propto x_i \quad (4)$$

$$F_i^L = x_i F^L \text{ pure } i \quad (5)$$

$F^L \text{ pure } i$ is the fugacity of pure component i as liquid at the temperature and pressure of a mixture. The vapour of pure component i to the temperature and pressure of a mixture is an ideal gas

$$F^V \text{ pure } i = P \quad (6)$$

The effect of pressure on the fugacity of a condensed phase is negligible at moderate pressure. Also, the vapour in equilibrium with pure liquid i at temperature is an ideal gas

$$F^L \text{ pure } i = P_i^{Sat} \quad (7)$$

Combining all equations 1-6

$$y_i F^V \text{ pure } i = x_i F^L \text{ pure } i \quad (8)$$

$$y_i P = x_i P^{Sat} \text{ (Raoult's Law)} \quad (9)$$

P^{Sat} is the saturation vapour pressure of pure component i

P is the total pressure of the equilibrium vapour mixture

Dalton's Law

For Dalton's law

$$P_{total} = \sum P_i \quad (10)$$

P_i is the partial pressure of species i in the vapour phase

Henry's Law

Henry's law is generally valid for solution of (dilute solution of a) provided that a does not dissociate, ionize or react in liquid phase. The law is often applied to solutions of non-condensable gases.

$$P_a = y_a P = x_a H_a(T) \quad (11)$$

Where $H_a(T)$ is the Henry's law constant for a in a specific solvent

Relative Volatilities

Volatility of most volatile component A is given as:

$$\alpha_A = \frac{P_A}{x_A} \quad (12)$$

Volatility of the less volatile component B is given as:

$$\alpha_B = \frac{P_B}{x_B} \quad (13)$$

$$\text{Relative Volatility } \alpha = \frac{P_A x_B}{x_A P_B} = \frac{P_A^0}{P_B^0} \quad (14)$$

P_A^0 = Partial pressure of the most volatile component

P_B^0 = Partial pressure of the less volatile component

Equilibrium Coefficient (K values)

Graphical representations of equilibrium data are difficult to adapt to programmed calculations and are not convenient for ternary systems. In these cases, equations are very useful. One way to represent equilibrium data is to define an equilibrium coefficient K values as

$$K_A = \frac{y_A}{x_A} \quad (15)$$

y_A and x_A are the vapour and liquid phase mole fractions respectively

In general, equilibrium coefficient values depend on temperature, pressure and composition. For many systems, the equilibrium coefficient values are independent of compositions thus,
 $K = K(T, P)$ approximate (16)

METHOD

Table 1.0: Experimental vapour-liquid equilibrium data for the ethane-n-propane-n-butane ternary system

Pressure (kPa)	Temperature (K)	Ethane vapour mole fraction (y_2)	Propane vapour mole fraction (y_3)	Butane vapour mole fraction (y_4)		Ethane liquid mole fraction (x_2)	Propane liquid mole fraction (x_3)	Butane liquid mole fraction (x_5)
4499.0	304.34	0.9679	0.0293	0.0028		0.9539	0.0410	0.0051
4507.9	304.34	0.9849	0.0031	0.0120		0.9738	0.0042	0.0220
4532.0	304.34	0.9804	0.0122	0.0074		0.9710	0.0160	0.0130
4550.0	304.34	0.9851	0.0110	0.0039		0.9719	0.0167	0.0114
4569.8	304.34	0.9838	0.0122	0.0040		0.9733	0.0176	0.0091
4574.1	304.34	0.9830	0.0126	0.0044		0.9748	0.0173	0.0079
4624.3	304.34	0.9876	0.0062	0.0062		0.9816	0.0078	0.0106
4631.8	304.34	0.9926	0.0017	0.0570		0.9864	0.0240	0.0112
4632.9	304.34	0.9891	0.0051	0.0058		0.9855	0.0062	0.0083
4656.2	304.34	0.9903	0.0069	0.0028		0.9846	0.0095	0.0059
4657.1	304.34	0.9930	0.0016	0.0054		0.9885	0.0020	0.0095
4671.1	304.34	0.9939	0.0029	0.0032		0.9904	0.0037	0.0059
4689.6	304.34	0.9948	0.0010	0.0042		0.9922	0.0012	0.0066
4717.8	304.34	0.9969	0.0007	0.0024		0.9952	0.0008	0.0004
4612.5	305.67	0.9862	0.0031	0.0107		0.9711	0.0044	0.0245
4617.1	305.67	0.9646	0.0320	0.0034		0.9837	0.0410	0.0053
4626.7	305.67	0.9715	0.0232	0.0053		0.9607	0.0305	0.0088
4648.4	305.67	0.9813	0.0117	0.0070		0.9703	0.0162	0.0135
4667.8	305.67	0.9736	0.0219	0.0045		0.9627	0.0293	0.008
4694.4	305.67	0.9832	0.0124	0.0044		0.9737	0.0075	0.0088
4737.4	305.67	0.9861	0.0068	0.0071		0.9837	0.0075	0.0088

4740.5	305.67	0.9809	0.00157	0.0034		0.9730	0.0206	0.0064
4743.6	305.67	0.9800	0.0167	0.0033		0.9719	0.0219	0.0062
4753.8	305.67	0.9915	0.0019	0.0066		0.9861	0.0025	0.0114
4756.1	305.67	0.9886	0.0053	0.0061		0.9859	0.0063	0.0078
4781.2	305.67	0.9922	0.0036	0.0042		0.9883	0.0045	0.0072
4781.5	305.67	0.9931	0.0013	0.0056		0.9882	0.0019	0.0099
4787.1	305.67	0.9901	0.0069	0.0030		0.9855	0.0091	0.0054
4817.1	305.67	0.9950	0.0011	0.0039		0.9917	0.0014	0.0069
4837.3	305.67	0.9966	0.0007	0.0027		0.9948	0.0009	0.0043
3743.1	307.04	0.9647	0.0317	0.0036		0.9538	0.0408	0.0054
4746.6	307.04	0.9688	0.0248	0.0064		0.9595	0.0309	0.0096
4746.7	307.04	0.9852	0.0030	0.0118		0.9722	0.0043	0.0235
4772.1	307.04	0.9796	0.0124	0.0080		0.0691	0.0166	0.0143
4789.0	307.04	0.9823	0.0123	0.054		0.9727	0.0164	0.0109
4791.7	307.04	0.9742	0.0211	0.0470		0.9626	0.0288	0.0086
4819.0	307.04	0.8919	0.0132	0.0049		0.9736	0.0174	0.0090
4868.1	307.04	0.9876	0.0062	0.0062		0.9840	0.0074	0.0086
4884.0	307.04	0.9903	0.0020	0.0077		0.9853	0.0026	0.0121
4888.2	307.04	0.9894	0.0050	0.0056		0.9855	0.0061	0.0084
4913.1	307.04	0.9919	0.0038	0.0043		0.9897	0.0044	0.0059
4915.1	307.04	0.9919	0.0017	0.0068		0.9885	0.0018	0.0097
4921.6	307.04	0.9884	0.0080	0.0036		0.9864	0.0087	0.0049

RESULTS AND DISCUSSION

In this study, correlation and prediction of vapour-liquid equilibrium data at different pressures and temperature for hydrocarbon ternary system was carried out with the aid of neural network. Correlation process was applied to three ternary systems (Table 1.0). The efficiency of network which in turn determines the accuracy of prediction was evaluated on the basis of the mean square error (M S E). The value of the mean square error (M S E) is negligible as shown in Fig. 1.0 indicating that the developed network is efficient and reliable for prediction and correlation purposes.

From the experimental data, the values of pressure and liquid phase composition of the ternary system were given as input to the network while the target was taken to be the respective temperatures and vapour phase composition.

The set target reached after 14 iterations (14 epochs) as shown in Fig. 1.0, with the performance goal line meets the target line. The accuracy of prediction by the network is summarized by comparing table 2.0 and 3.0, the output (predicted values) of vapour phase compositions and temperature gives set of data that is close to the target (experimental vapour phase compositions and temperature data).

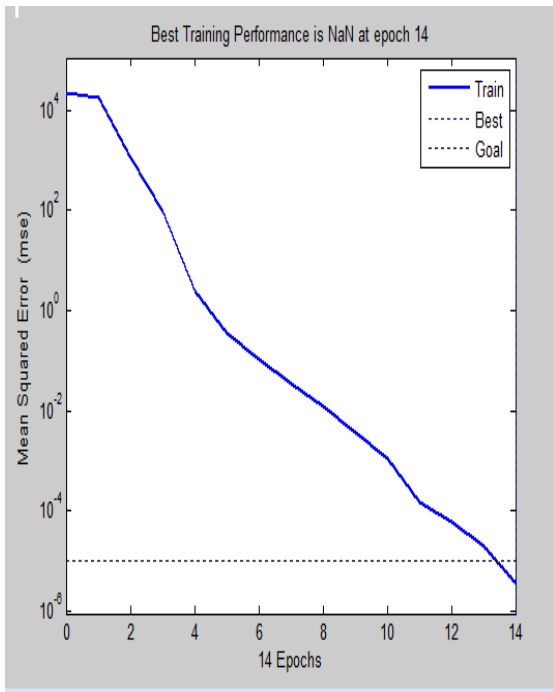


Fig. 1.0: Performance Trainlm Graph

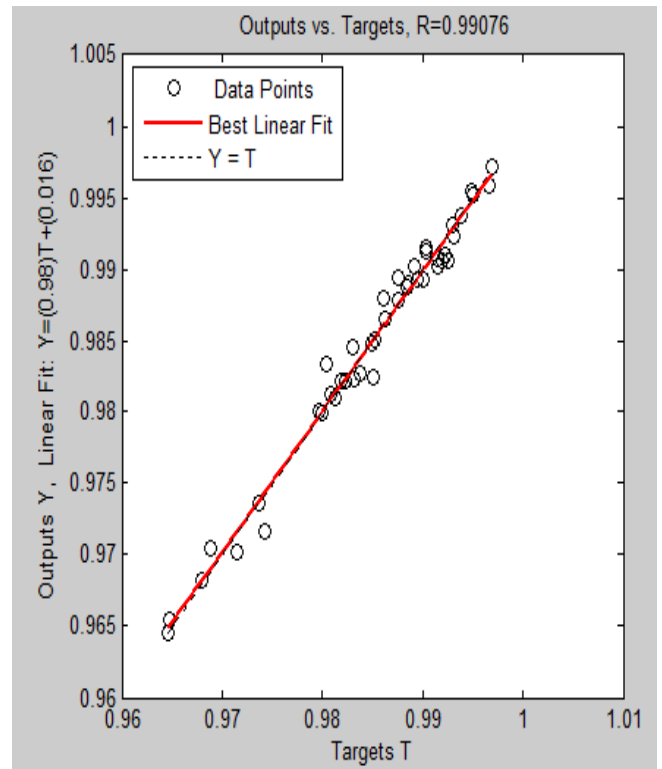


Fig. 3.0: Output-target Graph (Ethane)

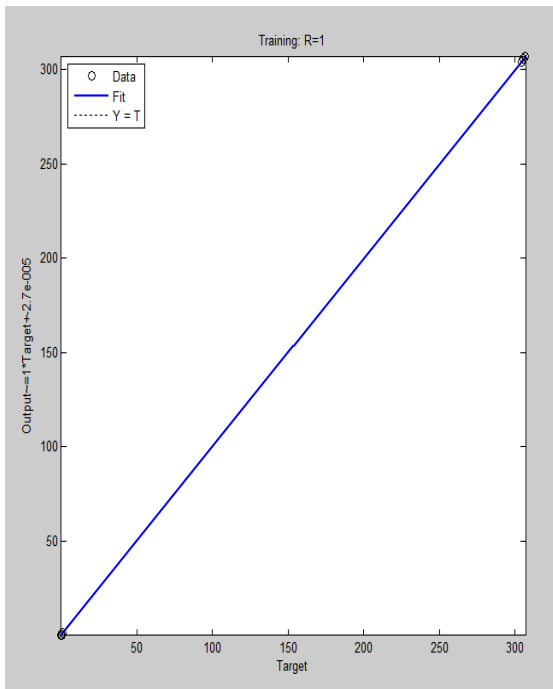


Fig. 2.0: Regression Graph

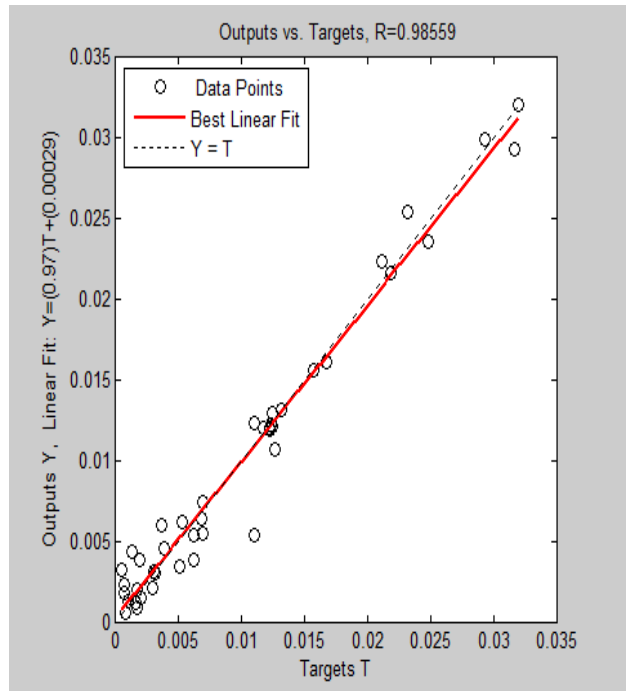


Fig. 4.0: Output-target Graph (Propane)

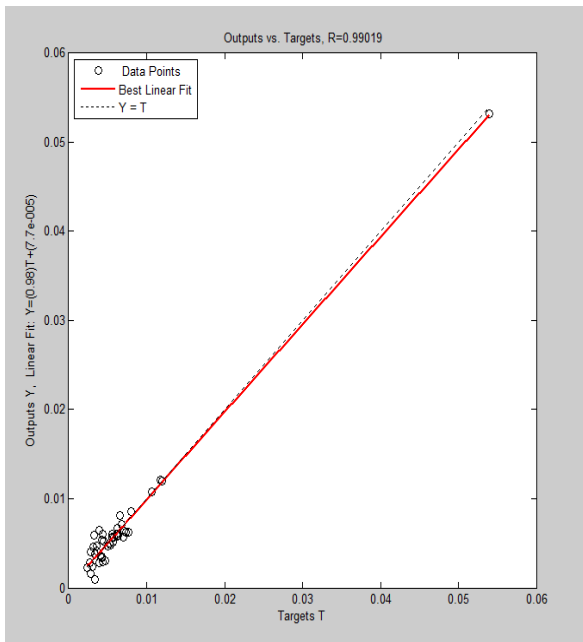


Fig. 5.0: Output-target Graph (Butane)

Table 2.0: Table showing vapour mole fraction and temperature values from experimental data (target)

Ethan e (y ₂)	Propan e (y ₃)	Butan e (y ₄)	Temperat ure (K)
0.9679	0.0293	0.0028	304.34
0.9849	0.0031	0.0120	304.34
0.9804	0.0122	0.0074	304.34
0.9851	0.0110	0.0039	304.34
0.9838	0.0122	0.0040	304.34
0.9830	0.0126	0.0044	304.34
0.9876	0.0062	0.0062	304.34
0.9926	0.0017	0.0570	304.34
0.9891	0.0051	0.0058	304.34
0.9903	0.0069	0.0028	304.34
0.9930	0.0016	0.0054	304.34
0.9939	0.0029	0.0032	304.34
0.9948	0.0010	0.0042	304.34
0.9969	0.0007	0.0024	304.34
0.9862	0.0031	0.0107	305.67
0.9646	0.0320	0.0034	305.67
0.9715	0.0232	0.0053	305.67
0.9813	0.0117	0.0070	305.67
0.9736	0.0219	0.0045	305.67
0.9832	0.0124	0.0044	305.67

From Fig. 2.0, 3.0, 4.0 and 5.0 (regression and output-target) graphs, deviations of data points from the line of best fit is small indicating good agreement between correlation values and experimental data. The degree of correlation is a measure of correlation coefficient R. In fig. 2.0 regression graph is linear and the correlation coefficient 1, meaning that the network is perfectly

trained. Also, for output-target graphs (Fig. 3.0, 4.0 and 5.0), as given by correlation

coefficient R, the degree of agreement between output and target are 99.076%, 98.559% and 99.019% for ethane, propane and butane systems respectively. This indicates that there is good correlation between the input, target and output parameter. The accuracy of prediction of the developed network was further tested when liquid mole fraction of ethane, propane and butane at a particular pressure, [0.9846; 0.0095 0.0059 4656.2], were given as input to the trained network which accurately predicted its equivalent composition of the vapour phase and temperature as [0.990310 0.006899 0.002800 304.3400] in agreement with the experimental data. In addition, with the predictive capability and efficiency of the developed network, vapour phase composition and temperatures of ethane, propane and butane system can be predicted by the network via interpolation when arbitrary values of liquid mole fraction and pressure within the range of the experimental data were chosen as input to the network.

Table 3.0: Table showing predicted values of vapour mole fraction and temperature with the use of Artificial Neural Network (A N N)

Ethan e (y ₂)	Propan e (y ₃)	Butan e (y ₄)	Temperat ure (K)
0.9665	0.0293	0.0029	304.33386
0.9883	0.0032	0.0119	304.3381
0.9821	0.0121	0.0075	304.3391
0.9837	0.0110	0.0039	304.3410
0.9862	0.0124	0.0042	304.3396
0.9831	0.0127	0.0044	304.3397
0.9874	0.0062	0.0062	304.3404
0.9927	0.0018	0.0570	304.3404
0.9894	0.0053	0.0058	304.3403
0.9900	0.0070	0.0028	304.3404
0.9940	0.0016	0.0054	304.3397
0.9938	0.0030	0.0032	304.3404
0.9948	0.0010	0.0042	304.3402
0.9970	0.0007	0.0024	304.3400
0.9863	0.0031	0.0109	305.6726
0.9645	0.0320	0.0034	305.6626
0.9715	0.0232	0.0052	305.6703
0.9813	0.0118	0.0071	305.6700
0.9738	0.0220	0.0045	305.6700
0.9831	0.0126	0.0044	305.6702

CONCLUSIONS AND RECOMMENDATION

In this study, correlation and prediction of vapour-liquid equilibrium data using neural network was efficiently carried out. Neural network correlates and predicts vapour-liquid equilibrium data with high degree of coherence when the network is iteratively trained. Predicted values were very close to the experimental target values, thus confirming conclusively that artificial neural network is a viable correlation and prediction tool for vapour-liquid equilibrium data. In addition, linear regression graphs and the values of correlation coefficient R, that is very close to unity confirms the network efficiency as well as the accuracy of predicted values. However, it is suggested that correlation and prediction of vapour-liquid should be extended to

alcohol ternary system, quaternary system and other multi-component systems.

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