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Correlation of Vapour-Liquid Equilibrium Data Using Neural Network for Hydrocarbon Ternary System (Ethane-n-Pentane-n-Hexane)

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Abstract

Correlation of vapour-liquid equilibrium data for hydrocarbon ternary system (ethane-n-pentane-n-heptane) is very useful in the design decision of separation process equipment such as separation columns, extractors etc. The tool used for the correlation is MATLAB: a very reliable software with adequate neural network conditions such as multi-layer feed forward, back propagation etc. A comprehensive Artificial Neural Network (A N N) training and simulation model and list of pre-existing vapour-liquid equilibrium data for ethane-n-pentane-n-heptane system was employed for this work. Neural network was trained in MATLAB 7.10.0 environment.Several iterations were carried out on the ternary system until the performance goal was met. From the analysis of the output result, regression and iteration graphs when compared with experimental data, artificial neural network offered very small deviation from the target. This confirms conclusively that artificial neural network is a consistent and reliable tool for predicting the vapour-liquid phase equilibrium for binary, ternary and quaternary system. The knowledge of correlation also establishes the basic background required for the understanding of the vapour-liquid phase behaviour of ternary systems which forms the basis of calculations of distillation, extraction and absorption processes etc.

Keywords: artificial neural network, back propagation, correlation, matlab, simulation model ternary system.

INTRODUCTION

The composition of vapour and liquid equilibrium phases is very important for calculations involving distillation, extraction and absorption processes which find useful application in the chemical process industry, petroleum and refining industries. Complete vapour-liquid equilibrium data for ternary systems are rare in the literature and quaternary data are practically non-existent. When designers need such information, they frequently attempt to predict the ternary or quaternary system from binary data by means of thermodynamics equation. Artificial Neural Network: a machine learning algorithm offers a more reliable and consistent means of correlating vapour-liquid equilibrium data for both ternary and quaternary systems. This is however done by training neural network using pre-existing vapour-liquid equilibrium, correlating and predicting the vapour-liquid equilibrium, comparing correlated and predicted values with pre-existing data and carrying out validity test to check for network efficiency.

LITERATURE REVIEW

The term “vapour-liquid equilibrium (V L E)” refers to systems in which single liquid phase is in equilibrium with its vapour (Mane and Shinde, 2012).

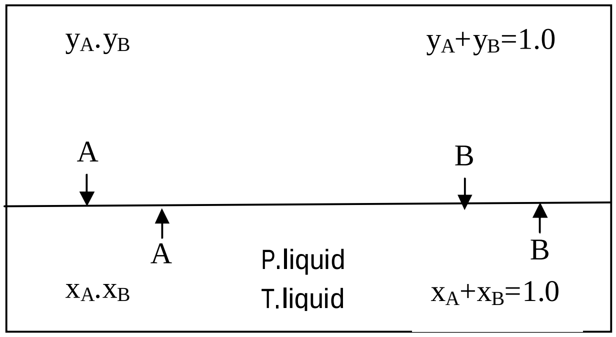

Fig. 1.0: Vapour and Liquid in Contact

Consider vapour and liquid in contact with each other as shown in Fig 1.0. Liquid molecules are continually vapourizing while vapour molecules are continually condensing. If three chemical species are present, they will generally condense and vapourize at different rates. When not in equilibrium, the liquid and vapour can be at different mole fractions. At equilibrium, the temperatures and pressures as well as fractions of different phases cease to change. Although, molecules continue to evaporate and condense, the rate at which each specie condenses is equal to the rate at which it evaporates. Although on a molecular scale nothing has stopped, on a macroscopic scale where processes are observed, there are no further changes in the temperature, pressure and composition.

Equilibrium conditions can be thermal, mechanical or chemical potential. In thermal equilibrium, heat transfer stops and the temperature of the two phases are equal

$$T_{liquid} = T_{vapour}\ (at\ equilibrium) \qquad (1)$$

In mechanical equilibrium, the forces between vapour and liquid balances. In other words, the pressures are equal (Seader and Ernest, 2001). In this case,

$$P_{liquid} = P_{vapour}\ (at\ equilibrium) \qquad (2)$$

A state of phase equilibrium is attained when the rate of vapourization of each specie is equal to the rate of condensation. Thus there is no change in compositions (mole fraction in Fig. 1.0). Ideally, the composition of liquid and vapour are not equal. If the compositions are equal, no separation can be achieved in any equilibrium process. If temperature and pressure are constant, equal rates of vapourization and condensation require a minimum in the fee energy of a system. The resulting condition for phase equilibrium is

$$(chemical\ \ potential\ \ i)_{liquid} = (chemical\ \ potential\ \ i)_{vapour} \qquad (3)$$

Experimental determinations of vapour-liquid equilibrium (V L E) are indispensable for the design of distillation columns and selection of solvents (Rattan et al., 2008). Ternary vapour-liquid equilibra is very complex with no reliable analytical or compact graphical way of representing experimental phase equilibrium hence the need to develop a neural network for the prediction of vapour-liquid equilibrium. For multi-component mixtures, as well as binary mixtures, the vapor–liquid equilibrium data are represented in terms of equilibrium constant (*K)* values (Kister and Henry, 1992; Perry and Green, 1997) defined by:

$$K = \frac{y_i}{x_i} \qquad (4)$$

where y_i and x_i are the mole fractions of component *i* in the vapour phase *y* and liquid phase *x* respectively. Equilibrium data supplies reliable and sufficient information regarding: feed F, equilibrium vapour V, equilibrium liquid L, feed mole fraction Z_i, vapour mole fraction y_i, liquid mole fraction x_i, equilibrium constant K, temperature and respective pressure.
Some equations are useful in deriving models for the correlating vapour-liquid equilibrium data, they are

Raoult's Law
This is particularly useful when composition of species is at high concentration

$$y_i P = x_i P^{Sat} \qquad (5)$$

P^{Sat} *is the saturation vapour pressure of pure component i*
Modified Raoult's is given as

$$y_i P = \gamma x_i P^{Sat} \qquad (6)$$

Equation 6 shows how vapour phase mole fraction y_i and liquid phase mole fraction x_i are related to total pressure P and activity coefficient γ .
From equation 6, equilibrium constant K is given as

$$K_i = \frac{\gamma_i P_i^{Sat}}{P} \qquad (7)$$

Activity coefficient can be used to relate fugacity of pure species in a mixture by:

$$F_i^L = \gamma_i x_i F_i^L \qquad (8)$$

Fugacity coefficient of pure component i is given as

$$F_i^L(T,P) = \Phi(T,P)P \qquad (9)$$

Fugacity of gas mixtures is also given as

$$F_i^V(T,P) = \Phi_i(T,P)P_p \qquad (10)$$

But

$$y_i P = P_p \qquad (11)$$

$$F_i^V(T,P) = \Phi_i(T,P)y_i P \qquad (12)$$

Where

γ_i *is the activity coefficient for specie i in the liquid mixture*

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

P *is the total pressure of the vapour mixture at equilibrium*

Henry's Law
This may apply when composition of species is at low concentration

$$K_i = H_i \qquad (13)$$

Where H is the Henry's law constant

Dalton's Law
For Dalton's law

$$P_{total} = P_1 + P_2 ....P_n \qquad (14)$$

$P_1\ P_2 ....P_n$ *are the partial pressures of each specie in the vapour phase*

Correlation of vapour-liquid equilibrium data is the process of comparing, contrasting and predicting various data obtained when there is no change in the composition of liquid and vapor at a certain temperature and pressure using approaches such as: graphical, analytical, statistical and artificial neural network. Vapour-liquid equilibrium (V L E) data is usually estimated by thermodynamics models based on the fundamental phase equilibrium criterion of equal chemical potential in both phases (Nguyena et al., 2007) cited by (Moghadassi et al., 2011).

Madagaran and Campanella, 2006, successfully used NRTL model in combination with (Harden and O' Connell 1975) second virial coefficient model for predicting the vapor - liquid equilibrium of the quaternary system containing acetic acid, isopropanol, water and isopropyl acetate. However, in this work prediction of VLE data was done with the aid of MATLAB (Matrix Laboratory) with neural network conditions. The experimental data are correlated to make the best possible interpolation using neural network. Neural network is designed by arranging neurons in various layers, deciding the type of connections among neurons for different layers as well as among neurons within a layer, deciding the way a neuron receives input and produces output and finally determining the strength of connections within the network by allowing the network learn the appropriate values of connection weights using the experimental data

According to (Shifmann et al., 1994; Rocha et al, Kumar and Zhang 2006; and Almeida et al., 2010 as cited by (Gunther and Fritsch, 2010), resilient back propagation is used in training network since this algorithm is one of the fastest algorithm for this purpose. Also, (Demuth and Beale, 2002) as cited (Moghadassi et al., 2011), explains, that the network is adjusted based on a comparison between the network, outputs and the targets (real values of output) until the network outputs match the target. It is important to note that the process of designing a neural network is an iterative process; developing a neural network entails series of trial and error in the design decision before coming up with a satisfactory design which enhances good correlation results. In the process of trial and error, model can be modified to facilitate discrimination among simulated system and the experiment is re-run. The second alternative is new search techniques or more powerful experiment designs (Adrian and Moshe, 1995) complex, linear and non-linear problems, thus, making results of data simulated this way to be very reliable.

The algorithm for training data set is the Levenberg Marquardt algorithm. The simulation is run as a loop for specific time and the output generated by simulation are compared with the target. This process is repetitive and continuous with the parameter changed and model run iteratively until there is high degree of coherence between the chosen target and the simulation result

Table 1.0: Experimental Vapour-liquid Equilibrium Data for the Ethane-Pentane-Hextane Ternary System at a Temperature of 338.555 K

Pressure (kPa)	Ethane vapour mole fraction (y_2)	Pentane vapour mole fraction (y_5)	Heptane vapour mole fraction (y_7)		Ethane liquid mole fraction (y_2)	Pentane liquid mole fraction (y_5)	Heptane liquid mole fraction (y_7)
1640.0	0.964	0.006	0.030		0.482	0.034	0.484
2050.0	0.973	0.005	0.022		0.575	0.026	0.399
2460.0	0.977	0.005	0.018		0.650	0.022	0.328
2870.0	0.979	0.005	0.016		0.715	0.020	0.328
3280.0	0.977	0.005	0.018		0.778	0.016	0.206
3690.0	0.973	0.005	0.022		0.840	0.014	0.146
3874.5	0.924	0.009	0.067		0.924	0.009	0.067
1640.0	0.972	0.013	0.015		0.461	0.076	0.463
2050.0	0.976	0.011	0.013		0.557	0.071	0.372
2460.0	0.978	0.010	0.012		0.642	0.065	0. 293
2870.0	0.978	0.010	0.012		0.721	0.055	0.224
3280.0	0.976	0.011	0.013		0.790	0.044	0.166
3690.0	0.971	0.011	0.018		0.859	0.030	0.111
3895.0	0.929	0.018	0.053		0.929	0.018	0.053
1640.0	0.940	0.044	0.016		0.440	0.200	0.360
2050.0	0.955	0.322	0.013		0.554	0.169	0.277
2460.0	0.961	0.028	0.011		0.639	0.147	0.214
2870.0	0.962	0.027	0.011		0.710	0.125	0.160
3280.0	0.962	0.027	0.011		0.780	0.100	0.120
3690.0	0.956	0.029	0.015		0.853	0.071	0.076
3874.5	0.914	0.046	0.040		0.914	0.046	0.040
1640.0	0.935	0.053	0.012		0.437	0.285	0.278
2050.0	0.949	0.042	0.009		0.536	0.242	0.222
2460.0	0.953	0.038	0.009		0.622	0.204	0.174
2870.0	0.955	0.035	0.010		0.703	0.166	0.131
3280.0	0.953	0.036	0.011		0.775	0.127	0.098
3690.0	0.944	0.044	0.012		0.846	0.098	0.056
3825.3	0.900	0.070	0.030		0.900	0.070	0.030

Source: (Dasturt and Thodos, 1964)

RESULTS AND DISCUSSION

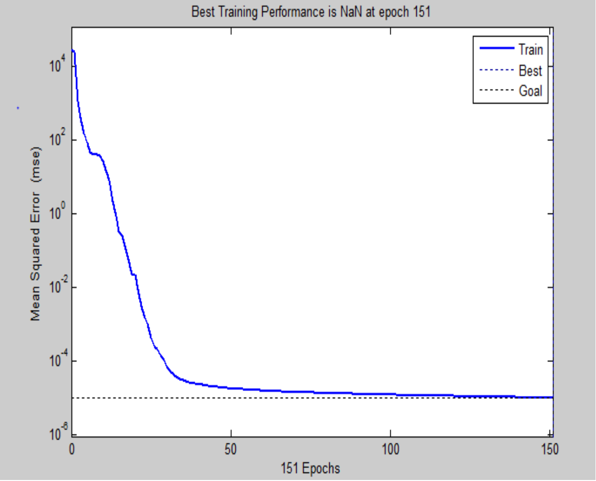

Fig. 1.0: Performance Trainlm Graph

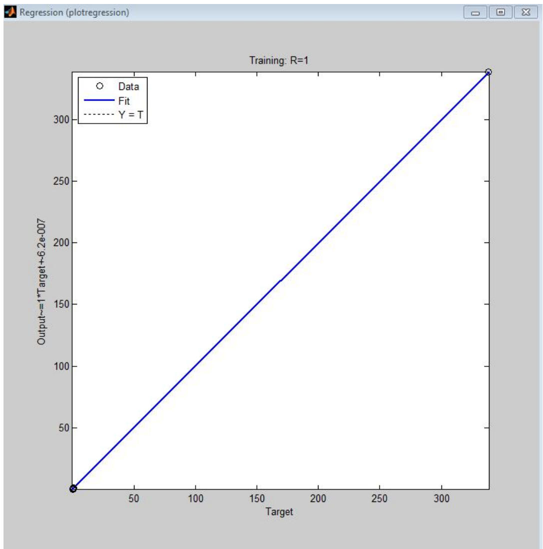

Fig. 2.0: Regression Graph

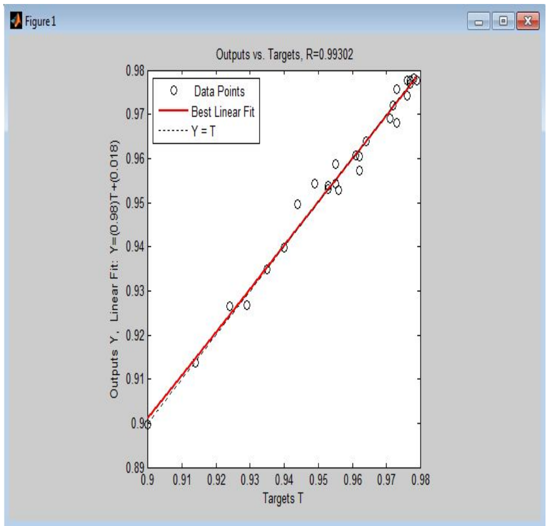

Fig. 3.0: Output-target Graph (Ethane)

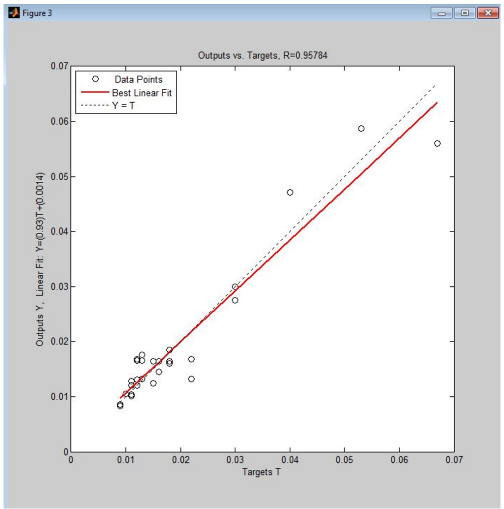

Fig. 5.0: Output-target Graph (Hexane)

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

Ethane (y_2)	Pentane (y_5)	Hexane (y_6)	Temperature (K)
0.964	0.006	0.030	338.555
0.973	0.005	0.022	338.555
0.977	0.005	0.018	338.555
0.979	0.005	0.016	338.555
0.977	0.005	0.018	338.555
0.973	0.005	0.016	338.555
0.924	0.009	0.067	338.555
0.972	0.013	0.015	338.555
0.976	0.011	0.013	338.555
0.978	0.010	0.012	338.555
0.978	0.010	0.012	338.555
0.976	0.011	0.013	338.555
0.971	0.011	0.018	338.555
0.929	0.018	0.053	338.555
0.940	0.044	0.016	338.555
0.955	0.322	0.013	338.555
0.961	0.028	0.011	338.555

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

Ethane (y_2)	Pentane (y_5)	Hexane (y_6)	Temperature (K)
0.9693	0.0062	0.0293	338.5552
0.9753	0.0056	0.0200	338.5550
0.9777	0.0048	0.0188	338.5551
0.9798	0.0051	0.0165	338.5551
0.9761	0.0050	0.0178	338.5549
0.9728	0.0050	0.0160	338.5550
0.9247	0.0087	0.0664	338.5552
0.9671	0.0126	0.0150	338.5551
0.9773	0.0100	0.0128	338.5550
0.9782	0.0096	0.0123	338.5550
0.9764	0.0104	0.0120	338.5551
0.9757	0.0107	0.0130	338.5549
0.9693	0.0109	0.0188	338.5548
0.9279	0.0186	0.0531	338.5545
0.9466	0.0441	0.0162	338.5553
0.9549	0.3200	0.0130	338.5549
0.9612	0.0279	0.0112	338.5550

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.

After 151 iterations, the performance goal was met (target reached) as shown in Fig. 1.0, with the trainlm line meeting the target line. The negligible value of the mean square error (M S E) as shown in Fig. 1.0 is an indication of the efficiency of the artificial neural network used since weights and biases which ensures good agreement between the output and the target has been fine tuned during the iteration process. 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).

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 are small. This indicates that there is agreement between correlation results and experimental data. The degree of correlation will only be significant when correlation coefficient R is 1 or close to 1.Correlation coefficient R in fig. 2.0 (Regression graph) is 1 while the values of R in Fig. 3.0, 4.0 and 5.0 are close to 1, confirming that there is good correlation between the input, target and output parameter. The linearity of regression graph (fig. 2.0) also indicates that that network is well trained and that the predicted values agree with the target. Liquid mole fraction of ethane, pentane and hexane picked at random at a particular pressure, [0.775; 0.127; 0.098;3280], were given as input to the trained network which predicted its equivalent composition of the vapour phase and temperature as [0.9532; 0.0359; 0.0111; 3380.555]. These values agree with the experimental data. In addition, in order to further affirm the predictive capability and efficiency of the developed network, arbitrary values of liquid mole fraction and pressure within the range of the experimental data were chosen for ethane, pentane and hexane as input to the network. P= [0.450 0.230 0.320 1845; 0.750 0.018 0.300 2666; 0.500 0.232 0.245 3419; 0.900 0.089 0.068 3698]. Simulation were carried out and the vapour phase composition and temperatures predicted as [0.9420 0.0400 0.0170 337.798; 0.9721 0.0048 0.0170 338.275; 0.9371 0.0933 0.0100 338.231; 0.9251 0.0890 0.0690 338.755] fell within the range of the experimental data, thus, confirming the reliability and efficiency of the network.

LIMITATION OF STUDY

Complete vapour-liquid equilibrium data for ternary systems are rare in the literature and quaternary data are practically non-existent.

CONCLUSION AND RECOMMENDATIONS

MATLAB software with neural network conditions and back propagation was used to correlate vapour-liquid equilibrium data for hydrocarbon ternary system. Training of network and experimental data was acheieved with the use of Levenbeberg algorithm. Observations from successive iterations reveal that neural network predicts more accurately when the network and experimental data are well trained.

Conclusively, good correlation results was achieved as predicted values agree reasonably with experimental data, hence, neural network is a viable correlation and prediction tool for vapour-liquid equilibrium data.

However, many research works on the correlation of vapour-liquid equilibrium data for binary systems have been reported, research can also be extended to the use of neural network in correlating of vapour-liquid equilibrium data for quaternary and multi-component systems.

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