

Original Research Article

Artificial Neural Network Model for the Prediction of the Products of a Crude Distillation Column

Abstract

An artificial neural network (ANN) model for predicting the flowrates and temperatures of the products of a crude distillation column in a refinery in West Africa was developed. The ANN model was based on the Bayesian Regularization Back Propagation (BRBP) algorithm, with 16 input and 10 output variables. Ninety sets of plant data were used for training and validating the model, while ten sets of data, different from those used for training, were used for testing the model. Another five sets of data with ± 2 or more standard deviations from the mean of a variable were then used to evaluate the extrapolation capacity of the model. Model predictions for the testing dataset showed average percentage deviations between 0.08 and 0.49 for product flowrates, and between 0.04 and 0.09 for temperatures, respectively. Regression analysis on these data also indicated a good model fit for the predicted variables. For the sets of extrapolation data, average percentage deviations were between 2.67 and 19.95 for predicted flowrates, and between 0.67 and 1.98 for temperatures, respectively. Regression analysis showed a lack of model fit for both flowrates and temperatures. While the ANN model accurately predicted product flowrates and temperature for interpolating data, its limited capacity for extrapolation suggests potential challenges beyond the training dataset. These findings emphasise the importance of cautious interpretation and application of the model in scenarios beyond the scope of the training data.

Keywords: Neural network modeling, Crude distillation column, Distillation product prediction, Model extrapolation capacity

1. Introduction

Crude oil distillation is the process of separating crude oil into fractions based on their boiling points, for further processing into various petroleum products. The Atmospheric Crude Distillation Unit (CDU) is one of the largest and most important processing units in a petroleum refinery, providing feeds to other process units in the refinery plant. The separation process of crude oil involves many complex physical

phenomena, while the operating variables of a CDU interact with the system output variables in a non-linear manner. Hence, the efficient operation of a CDU process requires simulation schemes that incorporate models capable of accurately predicting the products of the CDU column.

Mechanistic models such as the rigorous and shortcut distillation models are derived based on the knowledge of the underlying physical laws which govern the operation of the process. They are usually built on certain simplifying assumptions; hence, the accuracy of the model depends on the simplifying assumptions applied, and the complexity of the modeled process. The rigorous and the shortcut distillation models usually do not capture all the complexities of a crude oil distillation process. Statistical models such as the Artificial Neural Network (ANN) models, which serve as function approximators, can represent the relationships between the variables of a process in a simplified manner (Smith et al., 2013). These models approximate the unknown functional relationships in a process by relying entirely on experimentally gathered information from the system. Hence, the drawbacks of these models are that they are only valid for specific equipment within an experimental domain where the parameters were determined (Rasmuson et al., 2014).

In recent times, ANN modeling has been widely applied to model and optimize process operating conditions (Boger 1997; Liau et al., 2004; Jami et al., 2012). Some authors have also investigated the application of neural networks to CDU column modeling. Yusof et al. (2002) developed ANN models of a CDU column that can be used for real-time optimization. Motlaghi et al. (2008) also used an ANN model to design an expert system of a crude oil distillation column capable of predicting unknown output values from required inputs. A review of expert systems for CDU columns, incorporating an ANN model and a genetic algorithm framework for optimization and control, was carried out by Popoola et al. (2013a). Popoola et al. (2013b) additionally developed an expert system for the design and control of a Nigerian refinery CDU column, using ANN model. In this paper, the application of an ANN model in predicting the products of an existing CDU column in a refinery in West Africa, as well as the capacity of the model to extrapolate were investigated.

2. Methodology

2.1 The Modeled CDU Column

The modeled column is the atmospheric CDU column of a refinery in West Africa, which was designed to process 125,000 bpd (830 m³/hr) of crude oil. The CDU consists of a main column with 46 trays, 3 side-strippers (each with 5 trays) and 3 pump-around circuits. In all, the atmospheric column produces five products: top distillate (a mixture of naphtha and LPG), kerosene (KERO), light atmospheric gas oil (LAGO), heavy atmospheric gas oil (HAGO) and Atmospheric Residue.

2.2 Model Architecture

The architecture of the ANN model consists of one (1) input layer, two (2) hidden layers and one (1) output layer. The network has a total of sixteen (16) input variables and ten (10) output variables. The hidden layers have 20 and 14 nodes, respectively, thereby giving a total of 60 nodes distributed over the 4 layers. In the hidden layers, the inputs to the network are multiplied by adjustable random weights, then summed and transferred in the processing elements (neurons) to produce an output. The model inputs include crude feed rate, crude feed temperature, crude feed pressure, steam flow to main column, steam flow to side strippers, pump around flow rates, pump around temperature drops, and temperature of the draw stages. The model outputs are the flowrates and the temperatures of the five products of the column.

2.3 The ANN Modeling Equations

The Bayesian Regularization Back Propagation (BRBP) neural network algorithm was employed in modeling the atmospheric distillation process. The activation function for each neuron in the network is the sum of input (x_i) multiplied by their respective weights (w_{ji}).

$$A_j = \sum_{i=0}^m x_i w_{ji} \quad 1$$

The sigmoidal transfer function below (Equation 2), was used as the output function of the network neurons.

$$O_j = \frac{1}{1 + \exp(-A_j)} \quad 2$$

The Mean-Square-Error (MSE) was selected as the error function to be minimized, and was defined as

$$E = \frac{1}{m} \sum_{i=1}^m (d_j - O_j)^2 \quad 3$$

Where,

O_j = computed data of the j th output neuron

d_j = practical data of the j th output neuron

m = number of data sets

The errors are back propagated through the layers of the network, and weight adjustments are made. The formular used for updating the weights is given below (Kayri (2016); Araromi, Afolabi and Aloko (2007); Popoola et al. (2013)).

$$w_{K+1} = w_K - \eta \nabla V_K(w)$$

Where;

η = learning rate

K = number of iterations

$\nabla V_K(\mathbf{w})$ = function of the gradient of the errors

The gradient of the errors was defined by the Jacobian matrix that contains first derivatives of the network errors with respect to network parameters, as given below

$$\nabla V_K(\mathbf{w}) = J^T(\mathbf{w})E(\mathbf{w}) \quad 5$$

Where,

$$J(\mathbf{w}) = \begin{bmatrix} \frac{\delta E_1(\mathbf{w})}{\delta w_1} & \dots & \frac{\delta E_1(\mathbf{w})}{\delta w_K} \\ \vdots & \ddots & \vdots \\ \frac{\delta E_m(\mathbf{w})}{\delta w_1} & \dots & \frac{\delta E_m(\mathbf{w})}{\delta w_K} \end{bmatrix} \quad 6$$

and, $E(\mathbf{w})$ is the error for all inputs (Kayri (2016)).

2.4 Implementation of the BRBP Algorithm on the CDU Column

In the BRBP algorithm used to develop the ANN model of the CDU process, the coefficients of the model were determined by training the network on ninety (90) sets of plant data (80 sets of data for training and 10 sets of data for validation). This involved adjusting the weight coefficients until the difference between the predicted values and plant values fell within acceptable limits. Subsequently, these coefficients were applied to ten (10) sets of plant data, which were not used in determining the coefficients, for the purpose of testing the model. Additionally, these coefficients were applied to another five (5) sets of plant data with variable values in the range of ± 2 to ± 3 standard deviations from the mean of the variables, for evaluating the model's capacity to extrapolate. In total, a hundred and five (105) sets of plant data were used.

3. Results and Discussions

3.1 Performance of ANN Model on Test Data

Table 1: ANN model predicted product flowrates on test data

Parameter		Test No										Avg.
		1	2	3	4	5	6	7	8	9	10	
RESDF (m ³ /h)	M _v	151.1	152.3	154.2	143.7	152.3	155.7	151.8	151.6	158.0	154.3	0.26
	P _v	151.0	152.3	154.2	143.7	154.1	155.7	151.8	153.6	158.0	154.3	
	ADV (%)	0.07	0.00	0.00	0.00	1.18	0.00	0.00	1.32	0.00	0.00	
HAGOF (m ³ /h)	M _v	26.5	25.7	26.0	25.7	27.2	28.0	26.8	27.9	27.4	25.4	1.29
	P _v	26.4	25.7	26.1	25.6	24.6	27.9	26.8	27.4	27.3	25.5	
	ADV (%)	0.23	0.00	0.35	0.19	9.56	0.25	0.19	1.62	0.18	0.28	
LAGOF (m ³ /h)	M _v	124.9	123.9	125.0	120.7	123.1	124.8	125.0	125.0	122.9	125.0	0.23
	P _v	124.8	124.0	125.1	120.7	124.5	124.7	124.9	124.1	122.9	125.0	
	ADV (%)	0.08	0.08	0.08	0.00	1.14	0.08	0.08	0.72	0.00	0.00	
KEROF (m ³ /h)	M _v	91.0	91.0	91.0	95.0	91.0	91.0	91.0	91.0	91.0	91.0	0.08
	P _v	91.1	90.9	91.0	94.8	91.0	90.8	91.0	91.0	90.9	91.0	
	ADV (%)	0.11	0.11	0.00	0.21	0.00	0.22	0.00	0.00	0.11	0.00	
NAPHF (m ³ /h)	M _v	86.6	86.7	83.4	91.4	87.6	86.8	86.9	85.8	87.4	86.2	0.49
	P _v	86.5	86.7	83.4	91.4	86.0	86.8	86.9	88.3	87.4	86.2	
	ADV (%)	0.12	0.00	0.00	0.00	1.83	0.00	0.00	2.91	0.00	0.00	

Table 2: ANN model predicted product temperatures on test data

Parameter		Test No										Avg.
		1	2	3	4	5	6	7	8	9	10	
RESDT (°C)	M _v	338.6	339.4	339.3	338.6	338.5	340.1	339.8	339.8	339.9	339.9	0.04
	P _v	339.0	339.4	339.3	338.6	339.2	340.1	339.8	340.1	339.9	339.9	
	ADV (%)	0.12	0.00	0.00	0.00	0.21	0.00	0.00	0.09	0.00	0.00	
HAGOT (°C)	M _v	334.6	333.6	332.9	328.3	334.0	333.2	333.5	332.4	332.4	332.8	0.08
	P _v	334.2	333.6	332.8	328.3	333.2	333.3	333.4	331.2	332.4	332.7	
	ADV (%)	0.12	0.00	0.03	0.00	0.24	0.03	0.03	0.36	0.00	0.03	
LAGOT (°C)	M _v	284.9	284.0	285.9	287.5	285.1	285.6	287.0	286.8	287.4	286.4	0.04
	P _v	284.6	284.1	286.0	287.5	285.0	285.6	287.0	286.3	287.5	286.4	
	ADV (%)	0.11	0.04	0.03	0.00	0.04	0.00	0.00	0.17	0.03	0.00	
KEROT (°C)	M _v	192.0	192.4	192.1	192.1	193.5	192.6	193.1	192.6	193.0	193.8	0.09
	P _v	192.3	192.3	192.2	192.1	193.1	192.6	193.2	191.9	193.0	193.7	
	ADV (%)	0.16	0.05	0.05	0.00	0.21	0.00	0.05	0.36	0.00	0.05	
NAPHT (°C)	M _v	136.7	136.5	134.8	133.7	137.1	135.3	136.3	135.6	134.0	134.8	0.09
	P _v	136.6	136.4	134.8	133.7	137.2	135.1	136.3	135.0	134.1	134.9	
	ADV (%)	0.07	0.07	0.00	0.00	0.07	0.15	0.00	0.44	0.07	0.07	

The results obtained for the test data (Table 1.) show that the maximum percentage deviations for product flowrates were 1.32%, 9.56%, 1.14%, 0.22% and 2.91%, while the corresponding average values were 0.26%, 1.29%, 0.23%, 0.08% and 0.49% for residue, heavy atmospheric gas oil, light atmospheric gas oil, kerosene and naphtha respectively. The percentage deviations for predicted flowrates were all below 10%, while the average percentage deviations were all below 2%. Percentage deviations below 10% are generally acceptable. The maximum percentage deviations for product

temperatures (Table 2) were 0.21%, 0.36%, 0.17%, 0.36% and 0.44% for residue, heavy atmospheric gas oil, light atmospheric gas oil, kerosene and naphtha, respectively. The observed maximum percentage deviations for temperatures were below 1%, while the average values were all within 0.10%. The temperature deviations were also generally below 2 °C. These low deviation values clearly indicate that the ANN model is able to accurately model the existing atmospheric CDU process when applied to the set of data for testing.

The linear regression analysis between the plant data and the output of the ANN model, for the set of test data are shown in Figures 1. and 2.

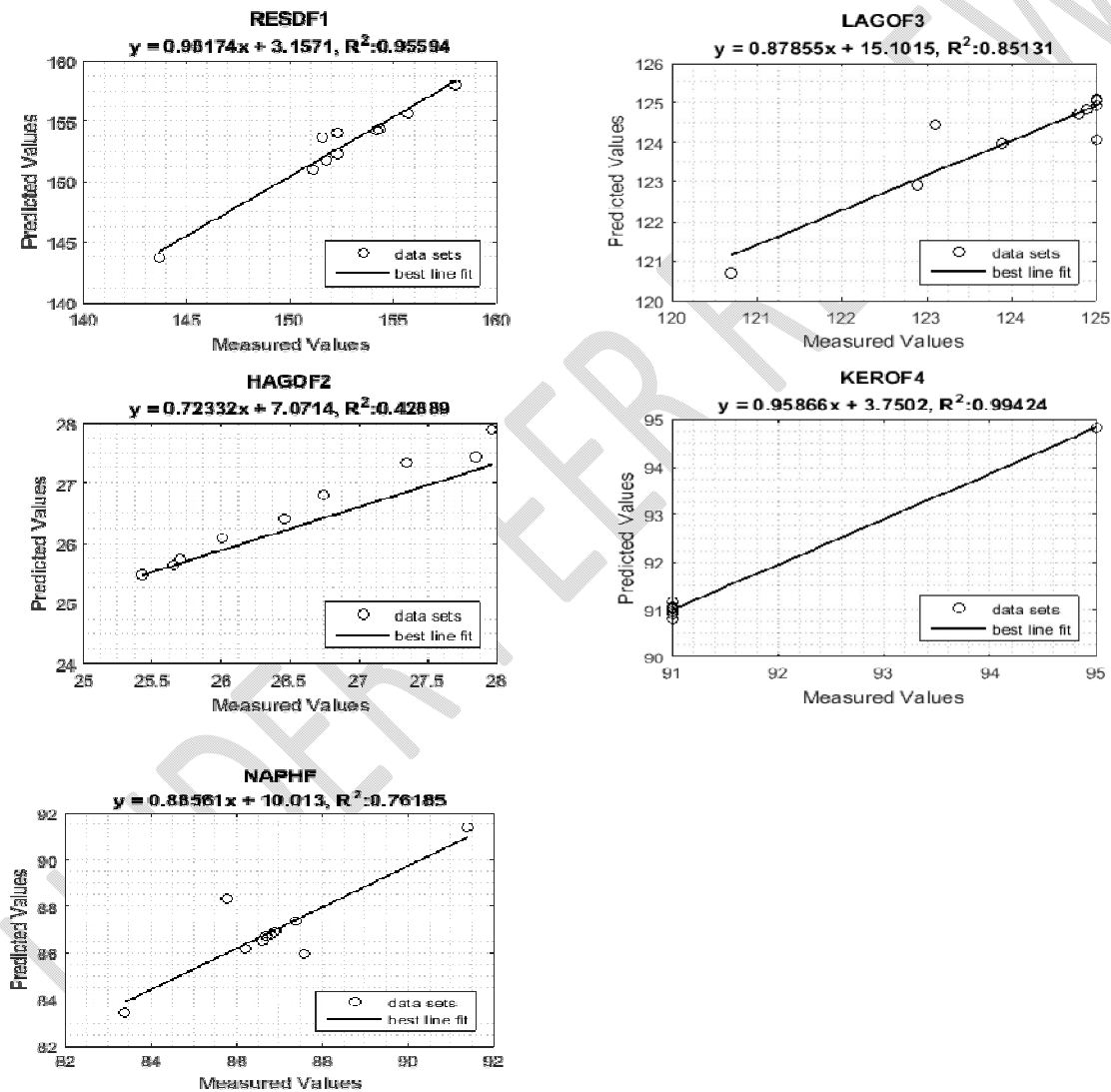


Figure 1: Linear regression for predicted flowrates from ANNmodel on test data

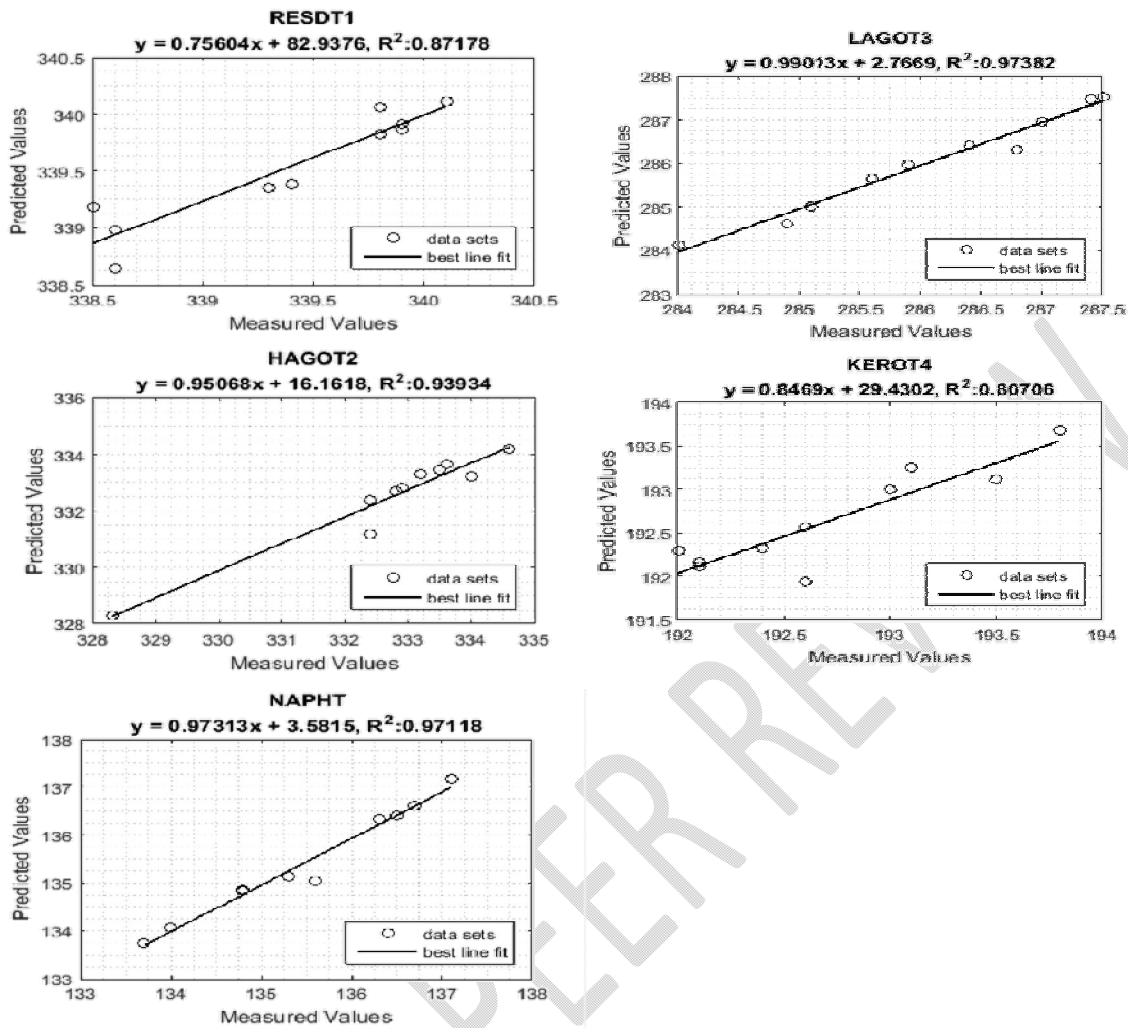


Figure 2: Linear regression for predicted temperatures from ANN model on test data

The regression plots of the ANN model output on the set of test data (Figures 1. and 2.) also indicate a good model fit to the plant data. Except for the flowrate of HAGO, all other predicted variables show high coefficients of determination (R^2), ranging from 0.76165 to 0.99424. The low value ($R^2 = 0.42889$) observed for HAGO flowrate may have resulted from the magnitude of the values of the HAGO flowrates, which were relatively small compared with those of the other process variables. Hence, small deviations from the plant values may have been magnified by the regression analysis. Additionally, though the observed deviations were small, the ANN model generally predicted lower values for the HAGO flowrates than the plant values; hence, the data points lay above the line of best fit on the regression plot for HAGO flowrate. The ANN model generally provide accurate predictions for the product flowrates and temperatures of the atmospheric CDU column when applied to the set of data for testing.

3.2 Performance of ANN Model on Extrapolation Data

Table 3: ANN model predicted product flowrates on extrapolation data

Parameter		Test No					Avg.
		1	2	3	4	5	
RESDF (m ³ /h)	M _V	146.3	153.6	152.2	155.0	143.2	
	P _V	153.7	145.6	144.1	125.5	144.1	
	ADV (%)	5.06	5.21	5.32	19.03	0.63	7.05
HAGOF (m ³ /h)	M _V	22.4	25.3	24.1	28.0	25.0	
	P _V	20.6	20.3	17.3	31.8	17.3	
	ADV (%)	7.87	19.64	28.13	13.45	30.69	19.95
LAGOF (m ³ /h)	M _V	121.9	126.0	126.0	125.0	123.0	
	P _V	120.0	123.3	117.3	124.1	117.3	
	ADV (%)	1.56	2.14	6.90	0.72	4.63	3.19
KEROF (m ³ /h)	M _V	91.0	92.0	92.0	92.0	91.0	
	P _V	94.0	93.2	94.2	94.6	94.2	
	ADV (%)	3.30	1.30	2.39	2.83	3.52	2.67
NAPHF (m ³ /h)	M _V	82.3	76.6	72.9	77.4	79.0	
	P _V	76.0	83.0	81.3	84.2	81.3	
	ADV (%)	7.65	8.36	11.52	8.79	2.91	7.85

Table 4: ANN model predicted product temperatures on extrapolation data

Parameter		Test No					Avg.
		1	2	3	4	5	
RESDT (°C)	M _V	334.8	339.5	338.9	338.9	336.6	
	P _V	333.5	335.6	337.3	335.1	337.3	
	ADV (%)	0.39	1.15	0.47	1.12	0.21	0.67
HAGOT (°C)	M _V	323.5	329.6	327.7	331.4	328.5	
	P _V	326.6	323.0	322.3	327.7	322.3	
	ADV (%)	0.96	2.00	1.65	1.12	1.89	1.52
LAGOT (°C)	M _V	286.6	286.4	285.5	286.2	285.7	
	P _V	284.3	281.9	283.6	288.8	283.6	
	ADV (%)	0.80	1.57	0.67	0.91	0.74	0.94
KEROT (°C)	M _V	194.0	193.1	191.1	191.1	189.4	
	P _V	187.8	188.2	187.5	193.5	187.5	
	ADV (%)	3.20	2.54	1.88	1.26	1.00	1.98
NAPHT (°C)	M _V	138.8	135.4	134.9	134.3	133.0	
	P _V	135.8	133.3	134.1	134.8	134.1	
	ADV (%)	2.16	1.55	0.59	0.37	0.83	1.10

The results in Table 3 show that the order of magnitude of both the maximum and the average percentage deviations increased for all predicted flowrates, compared with those of the test data. The maximum percentage deviations were 19.03%, 28.13%, 6.90%, 3.52% and 11.52% for residue, heavy atmospheric gas oil, light atmospheric gas oil,

kerosene and naphtha, respectively. The average percentage deviation ranged between 2.67% and 19.95%, compared to 0.08% and 1.29% recorded for the test data. The ANN model poorly predicted the flowrates of residue, heavy atmospheric gas oil and naphtha for the set of data for extrapolation. The predicted product temperatures (Table 4.) were also worse than those recorded for the test data. The observed maximum percentage deviations for temperatures were between 1.15% and 3.20%, as against 0.17% and 0.44% for the test data. The corresponding average values were between 0.67% and 1.98%, compared with values between 0.04% and 0.10% recorded for the test data.

The regression analyses of the ANN model output for the set of extrapolation data are presented in Figures 3. and 4.

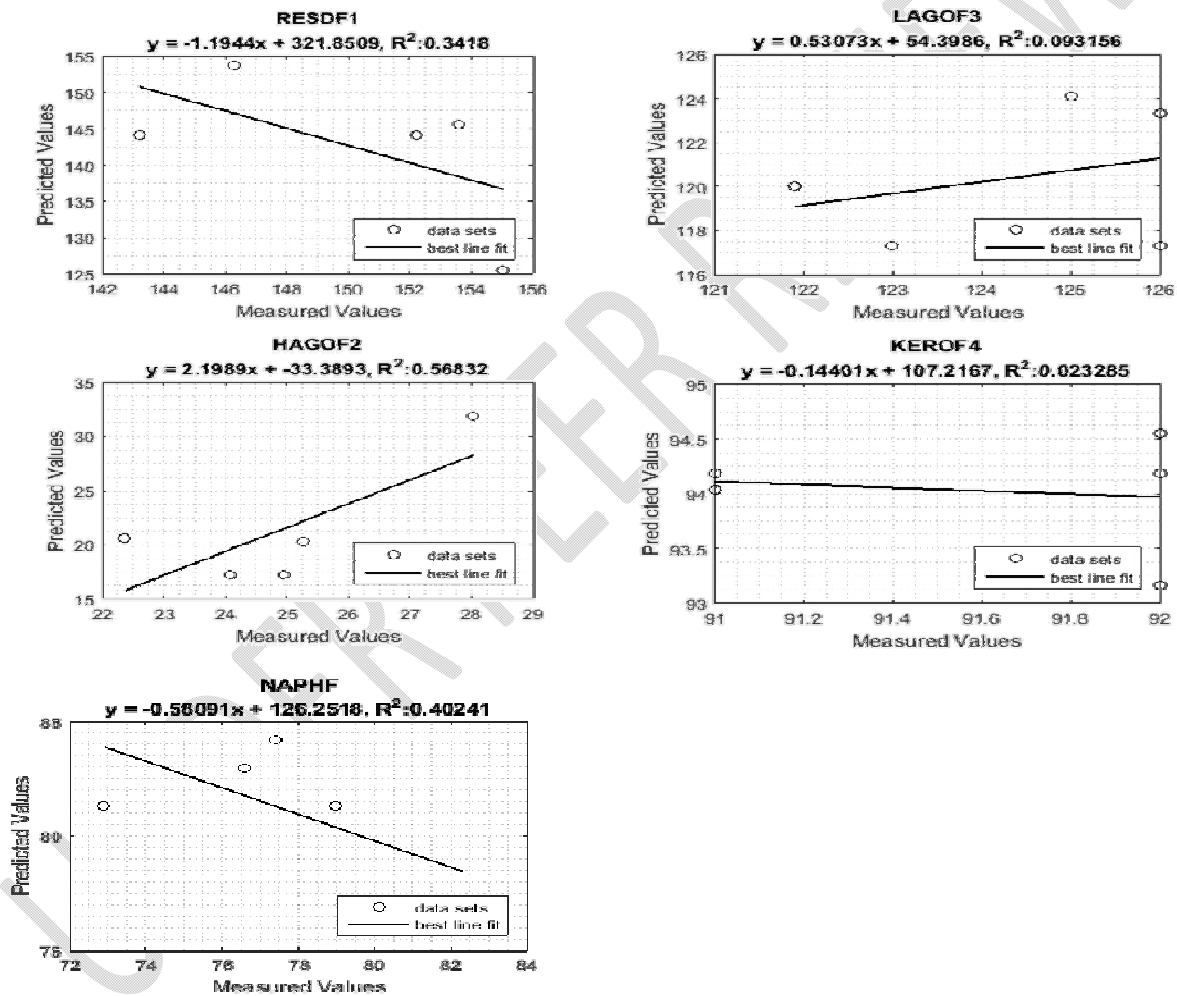


Figure 3: Linear regression for predicted flowrates from ANN model on extrapolation data

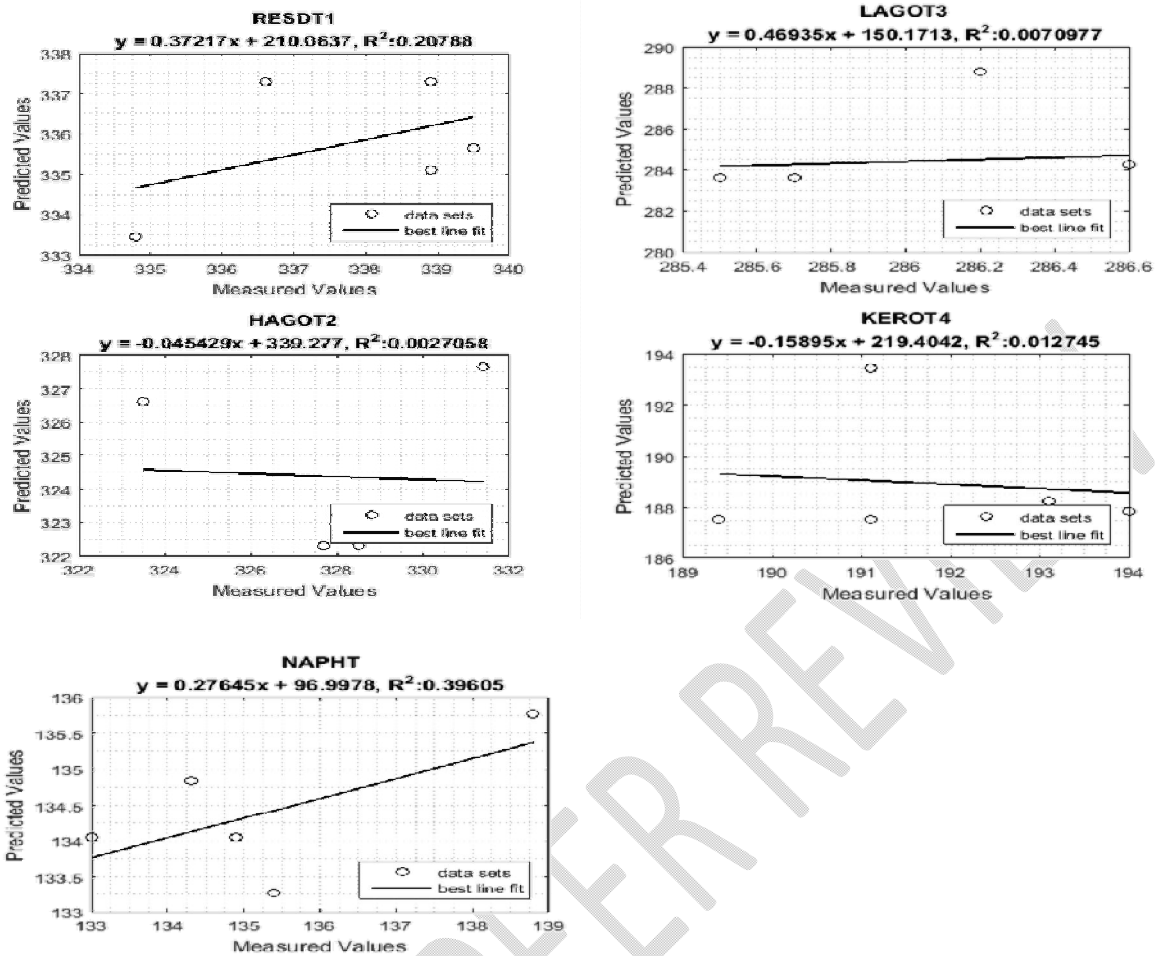


Figure 4: Linear regression for predicted temperatures from ANN model on extrapolation data

The regression analysis of the ANN model output (Figures 3. and 4.) suggests a poor fit of the model on these sets of data. The plots were characterized by low values of R^2 , ranging from 0.00710 to 0.56832, for the predicted flowrates and temperatures.

The trained ANN model was able to accurately predict the product flowrates and temperatures of the atmospheric CDU column when applied to a set of interpolation data (test data), but showed a poor capacity for predicting the process when implemented on a set of extrapolation data. Poor capacity for extrapolation has been identified as a drawback of conventional ANN modeling (Lee et al (2005); Thompson and Kramer (1994); Psychogios and Ungar (1992)).

4. Conclusion

An ANN model of an atmospheric crude distillation column has been developed. When the model was implemented on a set of data for testing, average percentage deviations for predicted flowrates were observed to be between 0.08 and 0.49, while the values for product temperatures were between 0.04 and 0.09. The regression plots for

these data also showed a good model fit with high R^2 values for both the flowrates and temperatures. Hence, the ANN model can accurately predict product flowrates and temperatures of the modeled CDU column when implemented on a set of interpolating data. However, the model performed poorly when implemented on the set of data for evaluating model extrapolation capacity. The average percentage deviations for the sets of extrapolation data were between 2.67 and 19.95 for flowrates, and between 0.67 and 1.98 for temperatures. Regression plots for these sets of data also showed a lack of model fit for both predicted flowrates and temperatures. This clearly suggests that the ANN model lacks the capacity for extrapolation.

Notations

HAGOF	Flowrate of heavy gas oil product
HAGOT	Temperature of heavy gas oil product
KEROF	Flowrate of kerosene product
KEROT	Temperature of kerosene product
LAGOF	Flowrate of light gas oil product
LAGOT	Temperature of light gas oil product
NAPHF	Flowrate of naphtha product
NAPHT	Temperature of naphtha product
RESDF	Flowrate of atmospheric residue
RESDT	Temperature of atmospheric residue

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