A Neural Network Based Soft Sensor for Online Vapor Product Quality Estimation of a Refinery Debutanizer Column

Bordin Wanichodom, Nont Neamsuwan, and Pornchai Bumroongsri

Abstract—In order to keep crude oil refining products within the specifications, online monitoring and laboratory testing are usually required. Time delay in process monitoring and control may occur since the products from distillation columns must be analyzed in the laboratory. To overcome this problem, a neural network based soft sensor for online measurement of product quality was developed in this paper. A refinery debutanizer was chosen as a study case. Various structures of neural networks with different numbers of neurons in each hidden layer were created and tested for their performance on the estimation of propane composition in the distillate stream. The simulation results showed that the neural network containing 5 and 10 neurons in the first and second hidden layers, respectively, gave the best performance as compared to real industrial data.

Index Terms—Artificial neural network, debutanizer column, online soft sensor, vapor product quality estimation.

I. INTRODUCTION

Distillation column is one of the important units in various chemical industries such as petroleum, petrochemical and plastic [1], [2]. A major problem observed in controlling the distillation process is the difficulty in online measurement of product quality. Laboratory analysis must be conducted periodically and continually for quality inspection which may cause time delay in process monitoring and control [3]. For this reason, soft sensor technology has been extensively studied in academia and industry. Jana et al. [4] collected the temperature at various points in the distillation column for water and ethanol separation. The collected data were then used to develop the relationship between the temperature and the product composition using the phase equilibrium model. Although the developed method was able to predict the composition in distillate stream, the model was only valid for separation of two components. Motlaghi et al. [5] designed an expert system based on neural network model to predict the required operating variables of crude oil distillation column. The operating data of the refinery such as flow rate and temperature were collected to predict the product quality. The developed system can be used by operators and engineers to obtain the operational values for the distillation column.

Rani et al. [6] developed an adaptive soft sensor for multicomponent distillation process. The developed soft sensor was trained online using past measurements. The results showed that the developed soft sensor can be implemented in an industrial process. Rogina et al. [7] conducted an experiment which applied an artificial neural network (ANN) to predict the Reid vapor pressure (RVP) of light naphtha based on reflux flowrate, temperature, and pressure of the distillation column. The results showed that the developed ANN was able to accurately predict the RVP.

From the literature review, it is seen that a reliable online measuring device has been required in the operation of the distillation column. This research aimed to develop a neural network based soft sensor for online measurement of product composition in the distillate stream.

II. PROCESS DESCRIPTION

Petroleum products such as diesel fuel, gasoline and naphtha can be produced from crude oil refinery which is a large industrial plant consisting of several processes including purification and separation. Propane, a natural gas by-product from crude oil distillation, is vastly used as a vehicle fuel. To yield high purity propane, a feed stream composed of propane and some heavy residue gases is fed to the 14th tray of the 28-tray debutanizer column with total condenser and thermosiphon reboiler as shown in Fig. 1. High purity propane is produced at the top of the column while butane is separated as a bottom product. The normal operating
condition of the debutanizer was monitored. The following operating variables of the debutanizer are observed and collected every 2 hours:
- Feed rate
- Feed pressure
- Bottom rate
- Boil up rate
- Reflux ratio
- Reboiler duty
- Propane composition

\[ b_j = \text{the bias value of each neuron} \]
\[ N = \text{the number of input variables}. \]

The net input of each neuron \( n_j \) was then converted to the output of each neuron \( a_j \) by a transfer function. The following tan-sigmoid function was used as a transfer function in the hidden layer:
\[
\text{tanh}(n_j) = \frac{e^{n_j} - e^{-n_j}}{e^{n_j} + e^{-n_j}}
\]

After all neuron outputs in the same hidden layer were calculated, the similar procedures were repeated for all neurons in the next hidden layer. The outputs of the last hidden layer were transferred to the output layer where the output of the network was calculated. The linear function was used as the transfer function in the output layer. The following mean squared error (MSE) function was used to test the performance of the developed neural network:
\[
\text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2
\]

where \( n = \text{the total number of data} \)
\( y_i = \text{the actual value} \)
\( \hat{y}_i = \text{the predicted value.} \)

III. NEURAL NETWORK MODELING

In order to estimate the propane composition in the distillate stream, the relationship between the operating data of debutanizer and the propane composition must be studied. The standard back-propagation (BP) technique was used for ANN learning and the Levenberg Marquardt (LM) algorithm was used as a training function \([8]\). A network structure developed in this research was shown in Fig. 2.

![Fig. 2. An artificial neural network structure with two hidden layers and one output layer.](image)

A set of 12 inputs \( (p_{1}, p_{2}, p_{3}, \ldots, p_{12}) \) was fed to the first hidden layer containing various numbers of neurons. Each neuron has its bias value \( (b_j) \) and the individual weight for each input \( (w_{i,j}) \) as shown in Fig. 3.

![Fig. 3. The first hidden layer containing neurons with tan-sigmoid functions.](image)

The net input of each neuron \( (n_j) \) can be written as
\[
n_j = \sum_{i=1}^{N} (w_{i,j} * p_i) + b_j
\]

where \( w_{i,j} = \text{the individual weight for each input variable} \)
\( p_i = \text{the input variable} \)

IV. CASE STUDY

A. Preparation of Training Data

Due to the difficulty in collecting the operating data from the industrial-scale debutanizer column at various operating conditions, an Aspen Plus model of the debutanizer column was developed and compared with the real industrial column. The normal operating condition of the industrial debutanizer column was shown in Table I.

| TABLE I: THE NORMAL OPERATING CONDITION OF THE INDUSTRIAL DEBUTANIZER COLUMN |
|---------------------------------------------|-----------------|----------------|
| Variable | Unit | Value |
| Feed flowrate | kmol/h | 126.36 |
| Feed temperature | K | 342.10 |
| Feed pressure | MPa | 1.77 |
| Distillate rate | kmol/h | 18.46 |
| Reflux ratio | | 3.28 |
| Reboiler vapor fraction | | 0.33 |
| Feed stage | | 14th |
| Overall column pressure | MPa | 1.51 |

| TABLE II: COMPARISON BETWEEN THE ACTUAL AND SIMULATION DATA |
|---------------------------------------------|-----------------|----------------|
| Component | Actual Data | Simulation Data |
| Distillate Stream | (kmol/h) | (kmol/h) |
| Ethane | 0.160 | 0.160 |
| Propane | 18.000 | 18.002 |
| i-Butane | 0.230 | 0.224 |
| n-Butane | 0.070 | 0.074 |

The developed debutanizer model was validated with the real industrial data at the normal operating condition. The
actual data agreed well with the simulation data as shown in Table II so this model can be used as a representative of the debutanizer column.

To provide sufficient amount of data for ANN training, upper and lower boundaries of some manipulated variables were determined as shown in Table III to generate input and output data from the developed debutanizer model.

### TABLE III: BOUNDARIES OF MANIPULATED VARIABLES

<table>
<thead>
<tr>
<th>Manipulated Variable</th>
<th>Unit</th>
<th>Lower Boundary</th>
<th>Upper Boundary</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed flowrate</td>
<td>kmol/h</td>
<td>119.36</td>
<td>133.36</td>
</tr>
<tr>
<td>Feed temperature</td>
<td>K</td>
<td>332.10</td>
<td>352.10</td>
</tr>
<tr>
<td>Feed pressure</td>
<td>MPa</td>
<td>1.67</td>
<td>1.87</td>
</tr>
<tr>
<td>Distillate rate</td>
<td>kmol/h</td>
<td>13.46</td>
<td>23.46</td>
</tr>
<tr>
<td>Bottom rate</td>
<td>kmol/h</td>
<td>105.90</td>
<td>109.90</td>
</tr>
<tr>
<td>Reflux ratio</td>
<td></td>
<td>2.28</td>
<td>4.28</td>
</tr>
<tr>
<td>Reboiler duty</td>
<td>GJ/h</td>
<td>0.08</td>
<td>0.11</td>
</tr>
<tr>
<td>Reboiler vapor fraction</td>
<td></td>
<td>0.23</td>
<td>0.43</td>
</tr>
</tbody>
</table>

Total 257 sets of data were collected from the simulation. The 12 input variables for ANN training were feed flow rate, feed temperature, feed pressure, distillate rate, bottom rate, reflux rate, boil up rate, boil up ratio, reflux ratio, condenser duty, reboiler duty, and reboiler vapor fraction. The output variable was the propane composition. The collected data were subsequently divided into 3 main groups for network training: training set 60%, validating set 20% and testing set 20%.

B. Performance Test for Neuron Networks

The performance test was conducted to find the most efficient network structure which possibly gave the lowest MSE value. The neural networks containing 1 and 2 hidden layers were created and classified as the network types I and II, respectively. Then, each network type was separately examined by varying the number of neurons in each hidden layer as shown in Table IV.

### TABLE IV: NETWORK TYPES OF ANN STRUCTURES

<table>
<thead>
<tr>
<th>Network Type</th>
<th>1st Hidden Layer</th>
<th>2nd Hidden Layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>5 to 50</td>
<td></td>
</tr>
<tr>
<td>II</td>
<td>5 to 30</td>
<td>5 to 30</td>
</tr>
</tbody>
</table>

Each ANN structure was examined for its performance. The lowest MSE value obtained from each network type was compared to find the best ANN structure.

V. RESULTS AND DISCUSSION

The results of network types I and II were separately discussed as follows:

A. A Neural Network with One Hidden Layer (Network Type I)

Network type I was the ANN structure containing only 1 hidden layer. The number of neurons was varied from 5 to 50. The MSE values of different number of neurons were calculated as shown in Fig. 4.

The MSE value shown in Fig. 4 decreased drastically as the number of neurons were added. However, the MSE value increased when the number of neurons added was more than 30. Therefore, the best ANN structure for network type I was consisted of 30 neurons in one hidden layer. The corresponding MSE value was 0.0010.

B. A Neural Network with Two Hidden Layers (Network Type II)

In this case, a neuron network with two hidden layers was considered. The numbers of neurons in the first and second hidden layers were both varied from 5 to 30. The MSE values of each ANN structure were calculated as shown in Fig. 5.

The MSE values tended to decrease as a few neurons were added to the second hidden layer. However, the MSE values increased when the number of neurons was more than 10. The lowest MSE value at 0.000832 was obtained for the neural network containing 5 and 10 neurons in the first and second hidden layers, respectively. As a result, this ANN structure was chosen as the best structure for the network type II.

The lowest MSE values from the best ANN structures of network types I and II were compared. The neural network with two hidden layers gave lower MSE value so this structure was used to predict the propane composition in the distillate stream of the actual debutanizer column. The results were in good agreement with the actual values obtained from the industrial debutanizer column as shown in Fig. 6. The relationship between the actual and predicted values was

\[ y = 0.9641x + 0.0307 \]  

(4)
where $y$ is the predicted propane composition  

$x$ is the actual propane composition.

The $R^2$ value is equal to 0.9629 indicating that the developed soft sensor can accurately predict the actual propane composition in the distillate stream.

![Fig. 6. The comparison between the predicted propane composition and the actual data.](image)

**VI. CONCLUSION**

In order to estimate the product composition of the debutanizer column, a neural network based soft sensor was developed in this paper. Various network structures with different numbers of neurons in the hidden layers were generated and compared. It was found that the neural network with 5 and 10 neurons in the first and second hidden layers, respectively, gave the lowest value of mean squared error. This network structure was then used to predict the propane composition in the distillate stream of the refinery debutanizer column. The results were in good agreement with the real industrial data.

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REFERENCES


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