ANN based soft sensor model for reactive distillation column

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Abstract

To cope up with the strict emission and product quality standards the process industries are stern for the maintenance of the product quality and waste emission. For process industries, online hardware analyzers are costly alternate for analyzing the product quality, they are switching to online soft sensors which are cheap and efficient in use. In this work, soft sensor based on artificial neural network (ANN) has been developed. The motive of the sensor is to measure the immeasurable primary variables of the reactive distillation column i.e. product concentration, using the data of easily measurable secondary variables i.e. tray temperatures. ANN soft sensor has been trained using Levenberg-Marquardt algorithm. The predictions of the soft sensor are compared with the MATLAB mathematical model outputs.

Keywords

Soft sensor, ANN, Reactive distillation column, Levenberg-marquardt algorithm.

1.Introduction

In chemical industries quality standards and emission standards are getting strict. To meet the market and pollution control board demands, online monitoring of quality variables is essential for an industry. As concentration is a direct measure of product quality, so it is better to monitor the concentration of product in real time. The on-line measurement of concentration is not an easy and cheap task. Hardware estimators are costlier and also produce some time-lag. So, Soft sensors are suggested to measure the quality variable or concentration online. using easily measured variables such as tray temperatures, reboiler duty, etc.. Reactive distillation is a process that carries reaction and separation processes in a single still. Reversible reactions are operated in Reactive distillation column (RDC) so that equilibrium can be restricted in the process. The prime motive of RDC is to separate the products of the reaction so that Le-Chatelier's principle can restrain the backward reaction. It leads to better selectivity, better conversion, avoidance of Azeotropes formation and better heat utilization in the reactive distillation column. Esterification reaction is a reversible reaction which has been studied extensively in the RDC's. Esterification involves the formation of an ester from the reaction of carboxylic acid and alcohol in the presence of an acidic catalyst.

For maintaining the performance of an RDC, On-line monitoring of the product concentration in crucial for RDC's. Soft sensors can be developed using linear models or non-linear models. Linear model includes principle component analysis (PCA) [1-6] and partial least square (PLS) [2-8]. While, non-linear method includes artificial neural network (ANN) [7-15], and support vector regression (SVR) [5, 16-18]. Whereas, [19] and [20] proposed the first soft sensors for on-line monitoring in reactive distillation column's (RDC). They used extended Kalman Filter approach to estimate the product purity in the column.

An artificial neural network is an interesting approach for handling non-linearity in the process model. In this paper ANN has been used to estimate the product concentration for the reactive distillation column. ANN network is based on Levenberg-Marquardt algorithm for optimization of the network values.

2.Reactive distillation column model

The mathematical model for reactive distillation was developed using MATLAB Software. Butyl Acetate esterification was studied for the same. The reaction taking place in the column can be shown as:

Acetic Acid n-Butanol n-Butyl Acetate
Water Assumptions taken for the mathematical model are:

1. The reaction is proceeding only in the liquid phase

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2. Reaction is occurring only in the Reactive Section
3. Vapor holdup is assumed to be negligible
4. System is obeying UNIQUAC thermodynamic
5. Phase splitting is considered only in the decanter mode
6. Constant tray pressure drop is considered.

The stages are numbered from top to the bottom. Where, when 1st tray is condenser and NTth tray is reboiler.

Modeling equation [20] and [21] for the esterification reaction in reactive distillation column can be shown as:

Material Balance on ith tray

$$\frac{dM_i}{dt} = L_{i-1} + V_{i+1} - L_i - V_i + F_i \quad (1)$$

Component Material Balance on ith tray and jth element

$$\frac{dM_{ix_{i,j}}}{dt} = L_{i-1,j}x_{i-1,j} + V_{i+1,j}y_{i+1,j} - L_{i,j}x_{i,j} - V_{i,j}y_{i,j} + F_{i,j}x_{f,i,j} + \Delta R_i \quad (2)$$

Enthalpy Balance on ith tray

$$\frac{dM_i h_i}{dt} = L_{i-1}h_{i-1} + V_{i+1}H_{i+1} - L_i h_i - V_i H_i + F_i h_{f,i} \quad (3)$$

Material Balance on Condenser (1st Tray)

$$\frac{dM_1}{dt} = V_2 - R - D \quad (4)$$

Component Material Balance on Condenser

$$\frac{dM_{1,j}}{dt} = V_2 y_{2,j} - (R + D)x_{1,j} \quad (5)$$

Enthalpy Balance on Condenser

$$\frac{dM_1 h_1}{dt} = V_2 H_2 - (R + D)h_1 - Q_C \quad (6)$$

Material Balance on Reboiler (NTth tray)

$$\frac{dM_{NT}}{dt} = L_{NT-1} - V_{NT} - B \quad (7)$$

Component Material Balance on Reboiler

$$\frac{dM_{NT,j}}{dt} = L_{NT-1,j}x_{NT-1,j} - V_{NT,j}y_{NT,j} - Bx_{NT,j} \quad (8)$$

Enthalpy Balance on Reboiler

$$\frac{dM_{NT} h_{NT}}{dt} = L_{NT-1}h_{NT-1} - V_{NT}H_{NT} - Bh_{NT} + Q_B \quad (9)$$

The above mathematical model has been solved in MATLAB software for the collection of temperature and concentration data which is further used as input data for the soft sensor.

3. ANN soft sensor

Artificial neural network (ANN) is a reliable tool for dealing with complex nonlinear models. ANN architecture comprises of an input layer, hidden layer, and an output layer. Hidden layers contain various neurons which pass information through a weighted

signal from one neuron to other, and this continues until the output is obtained. The performance of the network can be regulated by adjusting the weights between the neurons.

The concentration of n-Butyl Acetate for a reactive distillation column has been estimated by a 3-layered artificial neural network. ANN based soft sensor used tray temperatures as input variables. The network was trained using Levenberg-Marquardt optimization technique. LM technique is opted as it can handle a complex model with a large number of parameters. LM also holds benefits of fast convergence as Gauss-Newton method and assured convergence as of steeper descent method.

The general model equation of a 3 layered Artificial Neural network can be shown as:

$$y = f^3(LW^3 f^2(LW^2 f^1(IW^1 x + b^1) + b^2) + b^3) \quad (10)$$

Where,

IW^1 = Input Weight at Layer 1

LW^2, LW^3 = Layer Weight at Layer 2 & 3

b^1, b^2, b^3 = bias values at Layer 1, 2 & 3

x = Input Vector

y = Output Vector

In this paper, input data for the soft sensor was obtained from MATLAB model of the reactive distillation column. Input data contain tray temperature data and n-Butyl Acetate concentration data at different reboiler duties. ANN developed using 80% of data for training the network, 10% for cross-validation of the network and rest 10% for testing the network [22]. Network was developed using 3 layer models with one input layer, one hidden layer and one output layer. Input layer contain 15 tray temperature variables, Hidden layer contain 5 neurons and output layer contain one output variable of n-Butyl Acetate mole fraction.

4. Results

An ANN based soft sensor was developed for estimation of product purity in RDC and results were obtained and compared with actual values. *Figure 1* shows the perfect fit of the training data when the network has been trained with the total of 55 set of tray temperature as input variables and 55 set mole fraction as target variables. After training the network, the network was validated with the cross-validation data as shown in *Figure 2*. It can be seen that the network has been cross-validated with MSE of 5.65×10^{-6} and R^2 value of 0.963 and network can be used for the testing purpose. In last, the network

has been tested with different sets of tray temperature data as shown in *Figure 3*. Testing data fitted finely

with a little MSE value of 4.12×10^{-6} .

Figure 1 Training curve of network

Figure 2 Cross validation curve of network

Figure 3 Testing curve of network

5. Conclusion and future work

Soft sensor was developed for the estimation of n-butyl acetate mole fraction in bottoms product of a reactive distillation column. The input data for the soft sensor was obtained from MATLAB model of RDC. A 3-layered ANN network was developed using Levenberg-Marquardt optimization technique. It has been observed that ANN based soft sensor worked perfect as an inferential estimator giving predictions with low mean square error and high R^2 value.

Acknowledgment

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Conflicts of interest

The authors have no conflicts of interest to declare.

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