A NOVEL SOFT SENSOR MODELING

FOR GASOLINE ENDPOINT OF THE CRUDE UNIT

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ABSTRACT: This paper presents a novel soft sensor model for identifying the gasoline endpoint of a crude unit. A hybrid model was developed, by combining in series a first principle model with a neural network. A nonlinear observer based on the prior knowledge of the process is designed to estimate the composition C of the upper unit. The neural network is used to predict the gasoline endpoint with C and other process parameters as its inputs. The error between real measurement and the network prediction is fedback for the network correction. Industrial applications of the proposed model indicate that the proposed model is accurate and adaptable.

KEYWORDS: soft sensor modeling, gasoline endpoint, first principle models, neural network, hybrid model

1. INTRODUCTION

Soft sensing technique has been increasingly used as an attractive and effective method for process modeling (McAvoy, 1992) and for the replacement of expensive and inefficient analytical instrumentation (Santen A, et al, 1997). First principle modeling and empirical modeling are the common two methods that are used in the soft sensor modeling of a chemical process. First principle model (FPM) is based on the analysis of the mass, momentum, and energy balance as well as empirical state equations. However, only major characteristics and trends of the process can be well described by the FPM. In developing such a model, certain assumptions that may be strong have to be made. Also, disturbances that are common in a practical process are difficult to be modeled. These can often lead to poor model precision. Empirical models (EM) (T.Montin, 1998), on the other hand, are computationally efficient. Data-driven models, such as statistical analysis, neural network and fuzzy deduction, can model a nonlinear process accurately in the domain covered by the data, even if unmeasured disturbances are present. But, they often lack of good process interpretability for the dynamic behaviors of the system.

In this paper, we propose a soft sensor model, by combining a first principle model with a neural network, to overcome the drawbacks of these two approaches in their separate forms. Industrial application to the gasoline endpoint prediction shows that this model is more accurate and adaptable.

2. PROCESS DESCRIPTION

The crude distillation unit is a front operation for a refinery. This unit performs the initial distillation of crude oil into several fractions of different boiling ranges. The products of the crude distillation unit are either feedstock for other processing units or a part of product blending pool. The lighter fraction distilled from the upper section of the crude unit (Fig.1.) can be used as gasoline. End point is an important quality indicator for the gasoline produced from the unit. The operating economics of the crude unit generally dictate that the units run as close as possible to the product specifications (end point). A soft sensor for the endpoint measurement needs to be constructed due to the lack of an effective online analytic instrument.

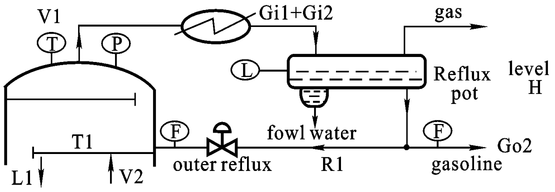

Fig.1. Schema of the upper section of a crude distillation unit

3. SOFT SENSOR MODELING SCHEME

A hybrid model is developed to identify the endpoint of gasoline for the crude unit, by combining, in series, a FPM model that predicts the upper section composition factor C and a multilayer neural network that predicts the gasoline endpoint by taking the composition C and a number process parameters as the network input. The error between the real value and the prediction is feedback to the network for correction. The general structure is illustrated as Fig.2. below.

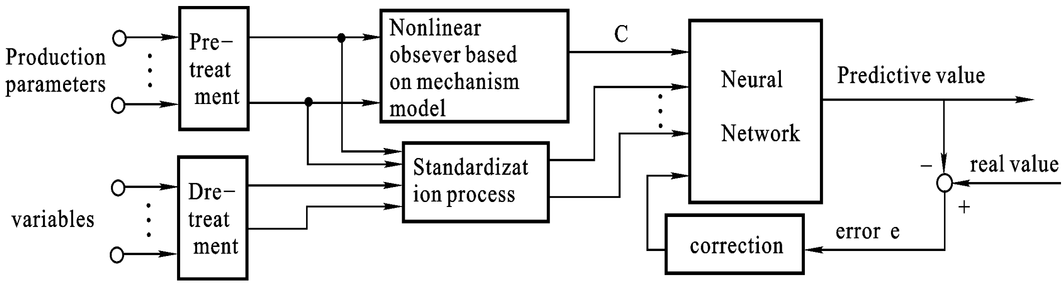

Fig.2. General structure of soft sensor model for gasoline endpoint

In the crude distillation operation, it is a common knowledge that the composition of the top inner section will affect the product quality. Disturbances can change the cut points of the fractions. There lacks an on-line measurement of the upper inner composition, a nonlinear observer is proposed to estimate it. We define that the composition of the top inner section as $C=L_1/V_2$. C increases, when the composition of the feed becomes heavier. The condensed liquid phase increases, as the inner reflux liquid phase L_1 increases, with an unchanged upper unit vapor phase V_2. For the similar reasons, C decreases with a lighter feed. So, C, as defined, can reflect the changes in the cut fraction composition of the upper unit. For this reason, C is referred as a composition factor.

4. ESTIMATIOR DESIGN FOR COMPOSITION FACTOR C

The composition estimator, developed for the crude distillation based on FPM, is derived from the first principles of the material and energy equations. The model equation for the process, based on the separation process principles, is:

$$A_0 \rho_0 \frac{dH}{dt} = G_{i2} - G_{02} - R_1 \qquad (1)$$

The energy conservation of the upper unit results in:

$$\frac{dT_1}{dt} = \frac{R_1\left(H_1^R - H_1^L\right) + V_2\left(H_2^V - H_1^L\right) - V_1\left(H_1^V - H_1^L\right)}{n_1 A \rho_1 \left(a_{11} + 2a_{12}T_1\right)\left[0.00284\left(\frac{L_1}{\rho_1 l_w}\right)^{2/3} + h_w\right]} \qquad (2)$$

By rearranging Eq. (1), the observation equation for V_1 is given as:

$$\begin{cases} Z_1(k+1) = (1-g_1 d_1)Z_1(k) - g_1^2 d_1 H(k) + g_1 d_1 (G_{02}(k) + R_1(k)) \\ \hat{G}_{i2}(k) = Z_1(k) + g_1 H(k) \\ V_1(k) = G_{i1} + \hat{G}_{i2}(k) \end{cases} \qquad (3)$$

By rearranging Eq. (2), the observation equation for V_2 is given as:

$$\begin{cases} Z_2(k+1) = (1-g_2 d_2)Z_2(k) - g_2^2 d_2 T_1(k) - g_2 f_1 R_1(k) + g_2 f_2 V_1(k) \\ \hat{V}_2(k) = Z_2(k) + g_2 T_1(k) \end{cases} \qquad (4)$$

Since the change of the retaining flow in the tower tray is much faster than the change of the temperature, the dynamic behavior of the retaining flow can be neglected. By observing V_1 and V_2, we get the observation equations for the liquid flow L_1 and the composition factor C of the upper unit:

$$\begin{cases} L_1(k) = R_1(k) + V_2(k) - V_1(k) \\ C(k) = L_1(k) / V_2(k) \end{cases} \tag{5}$$

5. NEURAL NETWORK MODELS

Artificial Neural Network (ANN) is widely used for its ability in modeling complex nonlinear processes, with a minimal requirement of the process knowledge. BP network is one of the most widely used among numerous networks, so it is adopted here to construct the soft sensor model for the gasoline endpoint.

In the network, the output is the gasoline endpoint, the number of hidden layers is one and the number of nodes in the hidden layer is I, the number of nodes in the input layer is n, the input signal is $x_1^{kk} \sim x_n^{kk}$ （kk=1, 2, ⋯, np, np is the total number of the samples）, the weight between the input nodes and hidden nodes is W1(n, i), the weight between hidden nodes and output nodes is W2(i). They are determined by the net transfer function Φ and the training data sets. The structure of this network is illustrated as in Figure.3.

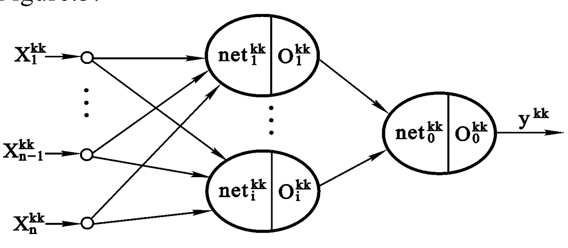

Fig.3. Network structure (NN1)

After setting the structure and the initial weights of the network, BP algorithm (Chen, 2000) can be used to train NN1, using the sample data of the inputs and outputs, to obtain the network weights.

In the production, there always exist uncertain disturbances and time-variance process factors that can influence the network prediction accuracy. A standard BP network is only suitable within a certain range of operation conditions. To improve its prediction, we need to make correction to the network model. Correction includes real-time dynamic correction and updating model periodically. Updating model means that, when sufficient new samples are accumulated, the system model is re-constructed based on these new training samples. Real-time dynamic correction refers to correct the model according to the difference between the real value and the model predictive value. In this paper, we would use the dynamic correction for the soft sensor modeling, by error-feedback correction.

The error correction structure is formed by adding an error feedback element to the structure of the BP network (NN1). With the basic structure of NN1 unchanged, an additional input node and its relevant weights are added. The added input node f_1^{kk}, i.e. the correction input, can be estimated by the error feedback. The new network (NN2) contains the new weights, and the weights of the previous network NN1.

6. INDUSTRIAL EXAMPLE

6.1 BPNN Model

By analyzing the crude unit process, we can determine the input variables that are relevant to the gasoline endpoint. They are the pressure of the crude unit x1, the top temperature of the crude unit x2, the temperature of reflux x3, the outer reflux flow x4, the distillation temperature of the first section x5, the flow of the first section x6, the flow of the first middle part x7, the pressure of input material x8, the temperature of input material x9, and the composition factor C of the upper section x10. The output is gasoline endpoint.

In order to show the effect of introducing composition factor C to the soft sensor model of the gasoline endpoint, a model is also constructed for comparison by deleting the composition factor C and its related weights from the above-developed model. By comparing the prediction results of these two models, with C and without C, we can obviously see the effect of estimating C.

The trained network has the following structure. The number of hidden layer is 1, and in the hidden layer, the number of nodes is 8. NN1 represents the following nonlinear relationship:

$$y(k) = f(x1(k), x2(k), \cdots, x10(k)) \qquad (6)$$

Where, $f(\cdot)$ indicates the nonlinear function and k is sampling moment.

6.2 Results And Analysis

Comparison of learning results 170 pairs of samples are used, after pretreatment of error testing, filtering and normalization, to train three different soft sensor models as described above (see table 1)

Table 1 the contrast of the results of three models after learning

<table>
<tr><td colspan="2"></td><td>average</td><td>Mini-Mum</td><td>maximum</td><td>|e|</td><td>|e|<1</td><td>1<|e|<2</td><td>|e|>2</td></tr>
<tr><td colspan="2">Real value（℃）</td><td>185.8</td><td>178</td><td>193</td><td>total</td><td colspan="3">170</td></tr>
<tr><td rowspan="3">Com-putation value</td><td>without C</td><td>186.0</td><td>179.5</td><td>192.3</td><td>no.</td><td>141</td><td>21</td><td>8</td></tr>
<tr><td>No Correction</td><td>185.9</td><td>178.8</td><td>192.99</td><td>no.</td><td>159</td><td>10</td><td>1</td></tr>
<tr><td>Corrected</td><td>185.85</td><td>178.5</td><td>192.6</td><td>no.</td><td>169</td><td>1</td><td>0</td></tr>
<tr><td rowspan="3">Absolute average error</td><td>without C</td><td colspan="3">1.15（℃）</td><td rowspan="3">deviation</td><td>without C</td><td colspan="2">2.145（℃）</td></tr>
<tr><td>No Correction</td><td colspan="3">0.881（℃）</td><td>No correction</td><td colspan="2">1.223（℃）</td></tr>
<tr><td>Corrected</td><td colspan="3">0.159（℃）</td><td>Corrected</td><td colspan="2">0.064（℃）</td></tr>
</table>

Comparison of validation results 50 pairs of samples are used to test the three trained models (see Table 2). The deviation of model prediction with C and error correction is less than 1℃. In Figures 4, and 5, solid lines stands for the real value of the gasoline endpoint, dotted-line stands for the model prediction. The abscissa stands for sample number and the vertical coordinate indicates gasoline endpoint (℃).

Table 2 the contrast of the results of industrial validation

<table>
<tr><td colspan="2"></td><td>average</td><td>Mini-mum</td><td>Maxi-mum</td><td>|e|</td><td>|e|<1</td><td>1<|e|<2</td><td>|e|>2</td></tr>
<tr><td colspan="2">Real value（℃）</td><td>185.7</td><td>178</td><td>190</td><td>total</td><td colspan="3">50</td></tr>
<tr><td rowspan="3">computation value</td><td>Without C</td><td>185.8</td><td>178.5</td><td>192.0</td><td>no.</td><td>35</td><td>9</td><td>6</td></tr>
<tr><td>No correction</td><td>185.5</td><td>179.0</td><td>189.8</td><td>no.</td><td>39</td><td>7</td><td>4</td></tr>
<tr><td>Corrected</td><td>185.7</td><td>178.6</td><td>190.0</td><td>no.</td><td>49</td><td>1</td><td>0</td></tr>
<tr><td rowspan="3">Absolute average error</td><td>Without C</td><td colspan="3">1.61 (℃)</td><td rowspan="3">deviation</td><td>Without C</td><td colspan="2">4.78 (℃)</td></tr>
<tr><td>No correction</td><td colspan="3">1.241（℃）</td><td>No correction</td><td colspan="2">2.583（℃）</td></tr>
<tr><td>Corrected</td><td colspan="3">0.165（℃）</td><td>Corrected</td><td colspan="2">0.077（℃）</td></tr>
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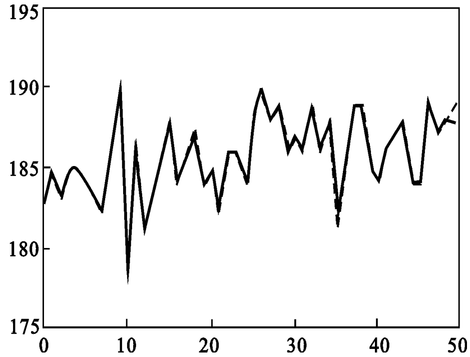

Fig.4. Industrial validation results with C and Error correction

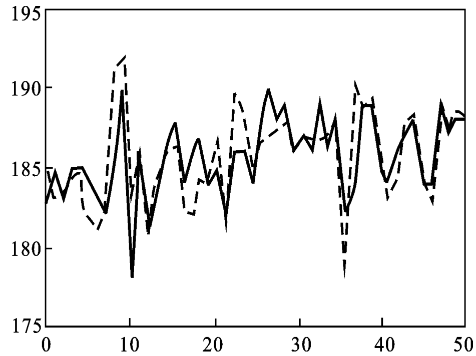

Fig.5. Industrial validation result without C

From Tables 1 and 2 and Figures 4 and 5, it is obvious that the average error and standard deviation of the soft sensor model with C is far smaller than those of the model without C. It is also shown that the modeling with correction has much better precision than the one without correction. The generalization performance of the model with error correction is also better than that of the model without the correction.

7 CONCLUSIONS

A modeling method has been proposed by combining a first principle model with a neural network to form a hybrid model. A soft sensor model with composition C and error correction has been presented for the endpoint prediction for a crude distillation with superior performance to the models without error correction or composition C estimation.

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