FUZZY NEURAL NETWORK FOR PREDICTING 4-CBA CONCENTRATION OF PTA PROCESS

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Abstract: A fuzzy neural network model has been developed to predict the 4-CBA concentration of the oxidation unit in PTA process. Several technologies are used to deal with the process data before modeling. Suitable input variables set has been selected according to prior knowledge, experience and fuzzy curve method. Dead time delay has been considered in the fuzzy neural network model. The simulation results show that the model of the fuzzy neural network is better than that of AMOCO in prediction precision.

Key words: Purified Terephthalic acid (PTA), 4-CBA ,Fuzzy Neural Network, Fuzzy Curve, Soft Sensor

1. INTRODUCTION

PTA (Purified Terephthalic Acid) is the necessary material used widely in textile and packaging industries. It is made by purifying the TA (Terephthalic Acid) which is produced by oxidizing PX(para-xylene) with the catalyzer. The Catalytic Oxidation process of the PX is shown in figure 1. There are some mediproducts such as P-T(P-Toluic Acid) and 4-CBA (4-Carboxybenzaldchydc) in TA.

Concentration of 4-CBA is the main impurity and the important quality indicator. Reference (Cao,G,et al.1994) shows that the lower the 4-CBA concentration the more energy cost. So it is important to control the 4-CBA concentration of the oxidation unit on-line for saving energy and ensuring the purity of PTA.

In practice the 4-CBA concentration is sampled three times each day and measured by spectroscopic analysis. Since spectroscopic analysis is a laboratory technique with obvious time delay, the analysis values of the 4-CBA concentration are not available for timely control adjustment if required. An alternative method is to build a soft sensor for on-line control of the 4-CBA concentration. In soft sensor technique the 4-CBA concentration is inferred from the other measured process variables such as temperatures, pressures, flows and their relationship.

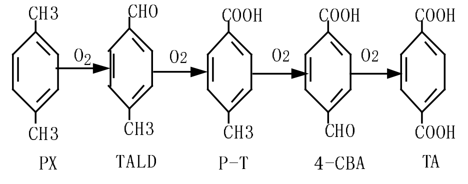

Fig. 1. The catalytic oxidation process of the PX

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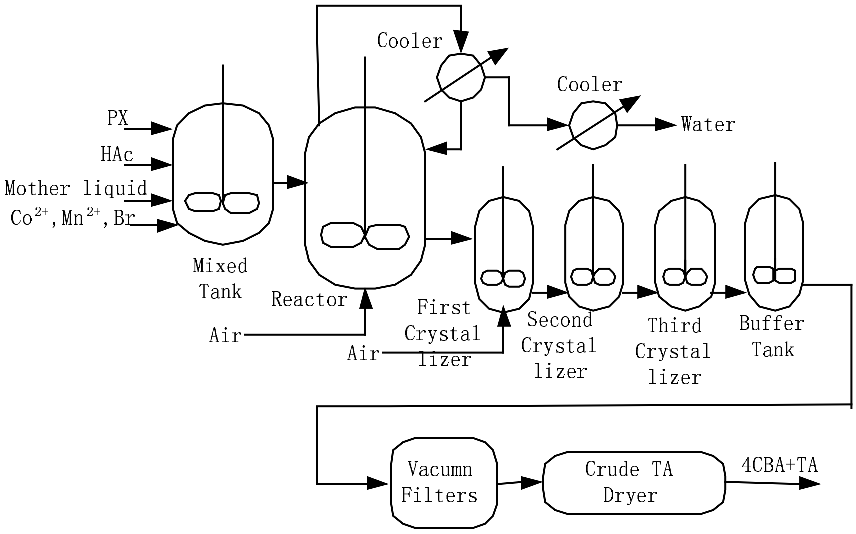

Fig. 2. Schematic diagram of the industry PTA oxidation process

The relationship between the measured process variables and 4-CBA concentration is modeled by a suitable technique.

Schematic diagram of the industry PTA oxidation process is shown in figure 2. The PTA oxidation process is very complex including heat transfer、mass transfer and solid crystal in gas and liquids phase. A complex dynamic model (Cao,G.,*et al.* 1994) about the PX oxidation process has been proposed firstly. However this model is highly nonlinear and its parameters have uncertainty. In order to forecast the 4-CBA concentration, some famous chemistry corporations have also developed different empirical regression models with patent rights (Harold,A.L,*et al.*1989). But the empirical models are only suitable to a limited operation region. In the present work fuzzy neural network based soft sensor is proposed to model the nonlinear relationship between the 4-CBA concentration and the measured process variables and accordingly predict the 4-CBA concentration in a timely manner.

The organization of the paper is as follows. Section 2 presents the architecture of the fuzzy neural network. Section 3 deals with a few practical issues including variable selection, dead time determination and data filtering. Section 4 presents simulation results. The final section gives conclusion.

2. FUZZY NEURAL NETWORK

The architecture of four layer fuzzy neural network with m inputs and one output is shown in figure 3, The four layers are input layer, fuzzification layer, inference layer and defuzzification layer respectively. There are m neurons connected with m input variables in the first layer, $m\times R$ neurons in the fuzzification layer, R neurons in the inference layer and one neuron in the output layer. Each m neurons in the fuzzification layer represents the premise part of one fuzzy rule, so there are R rules in total.

The ith IF-THEN rule is,

R^i :IF x_1 is $A_{i,1}$ and $\cdots$ and x_j is $A_{i,j}$ and $\ldots$ and x_m is $A_{i,m}$

THEN y is B_i

Where x_j is an input variable;

y is an output variable;

$A_{i,j}$ is a fuzzy set that characterized by the membership function $\mu A_{i,j}(x_j)$;

B_i is a fuzzy set that characterized by the membership function $\mu B_i(y)$;

Gaussian-type membership functions are used to calculate the values of $A_{i,j}$ and B_i as follows,

$$A_{i,j} = \mu A_{i,j}(x_j) = \exp(-(\frac{x_j - a_{i,j}}{c_{i,j}})^2) \tag{1}$$

$$B_i = \mu B_i(y) = \exp(-(\frac{y - b_i}{d_i})^2) \tag{2}$$

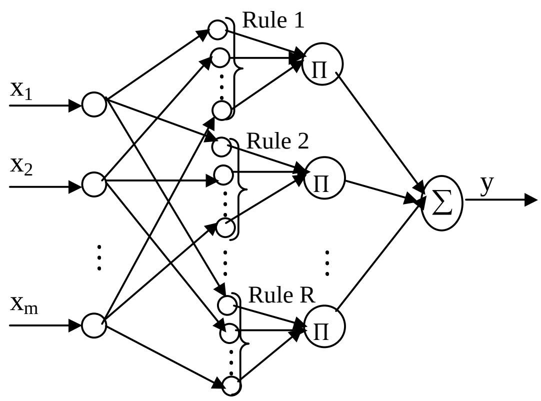

Fig. 3. The architecture of fuzzy neural network

where $a_{i,j}$, $c_{i,j}$, $i = 1, 2 \cdots R$; $j = 1, 2 \cdots m$ represent the center and width of input membership functions respectively. b_i and d_i reprensent the center and width of output membership function respectively. On the basis of multiplicative inference, we get

$$w_i = \prod_{j=1}^{m} \mu A_{i,j} \tag{3}$$

The inference result coming from R rules follows a standard center of gravity formla,

$$y_{out} = (\sum_{i=1}^{R} d_i b_i w_i) \Big/ (\sum_{i=1}^{R} d_i w_i) \tag{4}$$

the learning of FNN is accomplished by adjusting the input/output widths and centers of membership functions and follows gradient descent algorithm. in this study, we use an Euclidean distance, that is

$$E = \frac{1}{2}(y_{out} - y)^2 \tag{5}$$

where E is the error;
y_{out} is the actual output value;
y is the target output value.

We only take $a_{i,j}$ as an example for brevity. Using the BP (BackPropagation) algorithm, the following update formula can be derived

$$a_{i,j}(k+1) = a_{i,j}(k) - \eta \frac{\partial E}{\partial a_{i,j}} + \alpha(a_{i,j}(k) - a_{i,j}(k-1)) \tag{6}$$

$$\frac{\partial E}{\partial a_{i,j}} = \frac{\partial E}{\partial y_{out}} \frac{\partial y_{out}}{\partial w_i} \frac{\partial w_i}{\partial \mu A_{i,j}} \frac{\partial \mu A_{i,j}}{\partial a_{i,j}} \tag{7}$$

where η is the learning rate;
α represents the momentum coefficient.

It is important to initialize the parameters of fuzzy neural network because BP algorithm is sensitive to the initial parameters. In order to select a suitable parameters fuzzy C means clustering (FCM) algorithm (D.A.Linkens,Min-You Chen,1999) is applied to initialize the parameters. The centers of membership function, $a_{i,j}$, b_i , are initialized by the fuzzy clusters' centers; the initial width $c_{i,j}$ is given as follows,

$$c_{i,j} = \beta \times sqrt(\frac{\sum_{k=1}^{N} U_{i,k}(x_{k,i} - a_{i,j})^2}{\sum_{k=1}^{N} U_{i,k}}) \tag{8}$$

where U is the final fuzzy partition matrix calculated by FCM algorithm.
β is a constant.

d_i is initialized in the same way as $c_{i,j}$.

3. INPUT VARIABLES SELECTION AND DATA SET COLLECTION

3.1 Preliminary Selection of Process Variables

Hundreds of process variables affecting the 4_CBA concentration are recorded respectively one time per 30 seconds by the DCS system in PTA process. The selection of an appropriate subset from these variables is important. Too many unimportant variables included in the soft sensor model will lead to the difficulty of training and usage. On the other hand the model's accuracy can not be guaranteed if some important variables are not included.

According to prior knowledge and experience, ten variables are preliminarily selected including flow rates, reaction pressures, temperature, resident time, solvent ratio in the reactor and catalyzer liquid level. These ten process variables are measured in the reactor and the first crystallizer. Fuzzy curve method (Lin and Cunningham,1995) is applied to select the final variable subset in section 3.4.

3.2 Dead Time Determination

Dead time is the delay between the time when the value of a process variable changes and the time when the dependent variable begins to change in response which dependent on the structure and scale of the production equipment. It is obvious that the larger the scale of the production equipment and the longer the distance of materials transportation the longer the delay of dead time.

The schematic diagram of PTA oxidation process in figure 2 shows that the production equipment is of a large scale, so there are long dead time delays between the process variables and 4-CBA concentration. The different dead time of every process variable results from the fact that every tank has different residence time from 15 to 72 minutes and every sensor has its different position. Analysis indicated that the maximum dead time of the process variables is about 200 minutes while the minimum dead time is only about 70 minutes.

3.3 Data Collection and Preprocessing

As mentioned above, 4_CBA concentration is sampled only three times while the process variables are recorded about three thousand times each day. In other words, three samples at most are collected for training fuzzy neural network each day. The data set with 216 samples was collected according to the dead times of process variables and the sample time of 4-CBA concentration. That is

$$X = [x_1(t-\tau_1) \quad x_2(t-\tau_2) \quad \cdots \quad x_{10}(t-\tau_{10})] \tag{9}$$

$$Y = [y(t)] \tag{10}$$

Where X and Y represent process variables values and 4-CBA concentration collected, respectively, τ_i, $i = 1, 2, \cdots 10$,is the dead time of the i th process variable.

When data sets were collected, weighted moving average filtering method (Radhakrishnan V.R., Mahamed A.R. ,2000) is adopted to filter noise of the process data.

3.4 Reduce the Input Variables Using Fuzzy Curves method

The fuzzy curves method (Lin and Cunningham,1995) uses fuzzy logic to establish the relationship between the input variables and the output variable to identify the significant inputs. Suppose a multiple-input, single-output system has m inputs $X = [x_1 \quad x_2 \quad \cdots \quad x_m]$ and one output $Y = [y]$, We have N training data points. The algorithm is described briefly as follows,

1) Calculate the fuzzy membership function for the input variable x_i defined by

$$\Phi_{i,k}(x_i) = \exp(-(\frac{x_{i,k} - x_i}{b})^2) \tag{11}$$

where $i = 1, \cdots, m$; $k = 1, \cdots, N$;

$$b = 0.2 \times (\max(x_i) - \min(x_i))$$

2) Use centroid defuzzification to calculate the fuzzy curve c_i for each input variable x_i by

$$c_i(x_i) = \frac{\sum_{k=1}^{N} \phi_{i,k}(x_i).y_k}{\sum_{k=1}^{N} \phi_{i,k}(x_i)} \tag{12}$$

3) Calculate the range of each fuzzy curve by $R_i = Max(C_i(x_i)) - Min(C_i(x_i))$, the larger the R_i , the more important the corresponding variable x_i .

According to the approach the ranges of the fuzzy curves c_i in the PTA process, $i = 1, 2, \cdots 10$, are shown in table 1.

As shown in table 1, the range of the fuzzy curve for x_7 and x_9 is smaller than that of other variables. We delete these two variables for simplifying the model. However this does not mean that these two variables have no effect on the concentration of 4-CBA. It is just because that the range of these two variables is too small to produce any obvious error in the model prediction.

Table 1 The range of the fuzzy curves in PTA process

Input variables	The Range of c_i	Input variables	The Range of c_i
x_1	0.6188	x_6	0.5542
x_2	0.6030	x_7	0.0928
x_3	0.5822	x_8	0.4863
x_4	0.3318	x_9	0.1097
x_5	0.4921	x_{10}	0.3596

4. SIMULATION RESULTS

The data set with 216 samples is divided into two sets, one set has 150 samples used for training, the other set has 66 samples used for testing. After training FNN with different number of fuzzy rules, it is found that the most suitable number is 5. The training and testing relative errors after 250 iterations are shown in Fig 4. For comparison, the empirical nonlinear regression model of AMOCO is applied to the same data set. Under the same condition as in the FNN approach, the training and testing relative error are also given in Fig 4. Table 2 lists the two models' performances including maximum relative error, minimum relative error and root-mean-square-error (RMSE) in detail. It can be seen that not only the training results of the FNN model are better than that of the AMOCO model but also the better generalization results on the testing data.

The comparison of the predicted values of the two different models and the actual 4-CBAconcentration is given in Fig. 5. It can be seen that the FNN model has better prediction capability in the change trend of 4-CBA concentration while the AMOCO model just predicts the average of it.

Table 2 Training and testing performance for 4-CBA concentration using the FNN method and AMOCO model

	Training set			Testing set		
Model	max.rel.Error	min.rel.Error	RMSE	max.rel.Error	min.rel.Error	RMSE
FNN	0.0813	-0.0576	0.0248	0.0923	-0.0845	0.0342
AMOCO	0.1109	-0.0846	0.0357	0.0941	-0.0887	0.0373

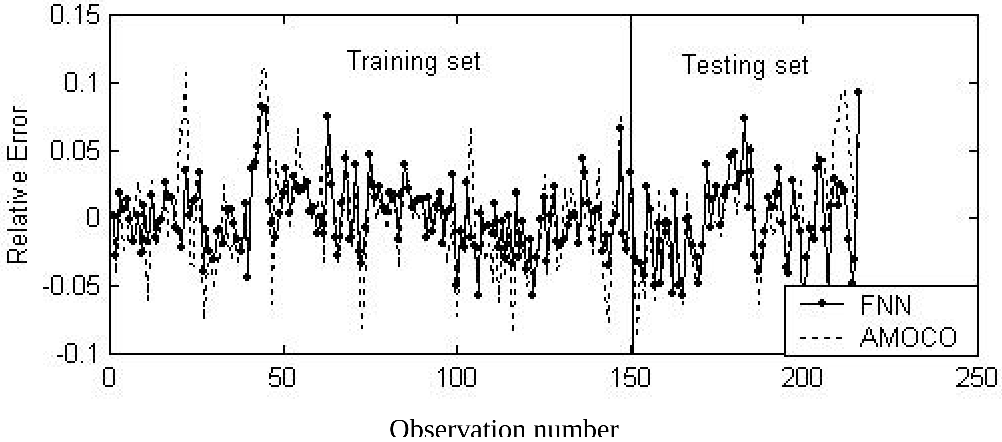

Fig. 4. Predicted relative errors for 4-CBA concentration using the fuzzy neural network model and AMOCO nonlinear regression model .

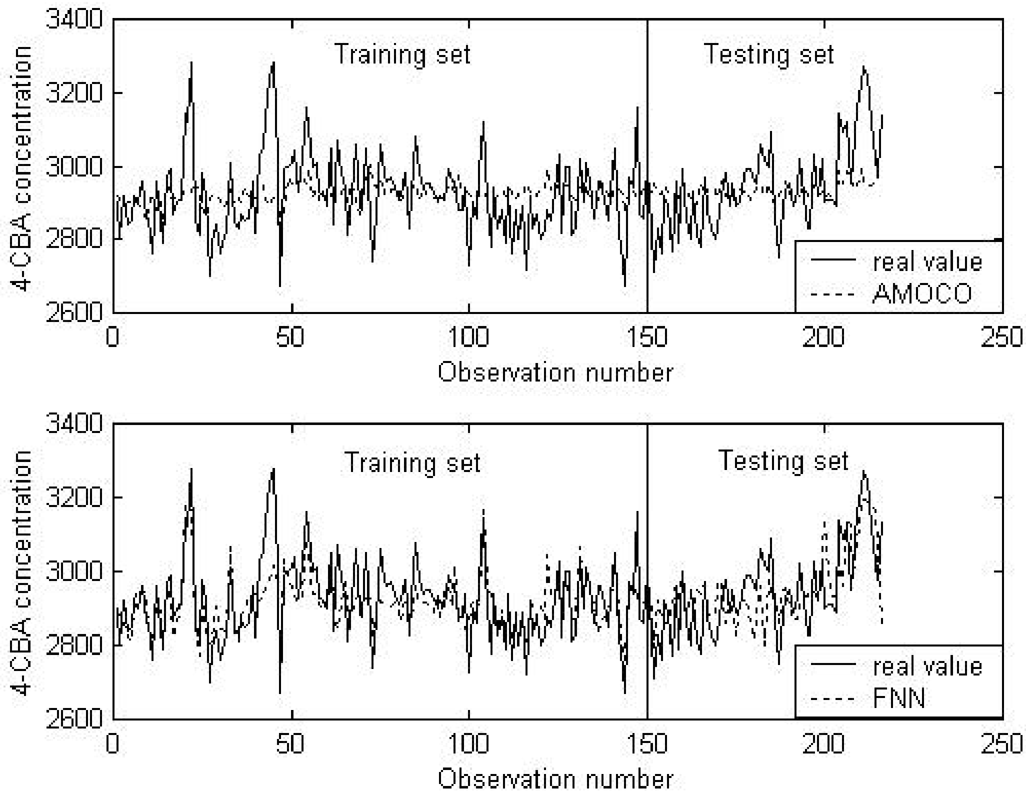

Fig. 5. Actual and predicted results of 4 CBA-concentration

5. CONCLUSION

In this paper, a fuzzy neural network model has been applied to predict the concentration of 4-CBA of the oxidation unit in PTA process. Several technologies are used to deal with the process data before modeling. Suitable input variable subset has been selected according to the prior knowledge and experience and fuzzy curve method. Dead time has been considered into the fuzzy neural network model. The simulation results show that the model of the fuzzy neural network is better than AMOCO model in prediction precision.

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