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MIMO Soft-sensor Model of Nutrient Content for Compound Fertilizer Based on Hybrid Modeling Technique*

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Abstract In compound fertilizer production, several quality variables need to be monitored and controlled simultaneously. It is very difficult to measure these variables on-line by existing instruments and sensors. So, soft-sensor technique becomes an indispensable method to implement real-time quality control. In this article, a new model of multi-inputs multi-outputs (MIMO) soft-sensor, which is constructed based on hybrid modeling technique, is proposed for these interactional variables. Data-driven modeling method and simplified first principle modeling method are combined in this model. Data-driven modeling method based on limited memory partial least squares (LM-PLS) algorithm is used to build soft-senor models for some secondary variables; then, the simplified first principle model is used to compute three primary variables on line. The proposed model has been used in practical process; the results indicate that the proposed model is precise and efficient, and it is possible to realize on line quality control for compound fertilizer process.
Keywords multi-inputs multi-outputs, soft-sensor, limited memory partial least squares, simplified first principle model, nutrient content of compound fertilizer

1 INTRODUCTION

In chemical industrial process, some variables cannot be measured on line. Soft-sensor technique is a very effective method to implement real-time estimation of these variables. Overcoming many deficiencies of artificial analysis and on line analytical instrumentation, soft-sensor technique has become an important method for implementing on line quality control, advanced process control, and optimization control[1,2].

The most popular methods of soft-sensor modeling are first principle modeling method[3], data-driven modeling method, and hybrid modeling method[4]. Data-driven modeling method includes partial least squares (PLS) regression method[5], artificial neural network method[6], and support vector regression method[7]. First principle model and data-driven modeling method have advantages and disadvantages. Essentially, the former can reflect the industrial process; it can be propagated and explained. Its disadvantage is that the modeling process is very complicated. The complete first principle model cannot be obtained for some complicated process; only the simplified first principle model can be obtained. The latter can build soft-sensor model directly according to the input and output data and it almost does not need prior knowledge of the process. However, it is time-consuming and is very easily prone to overfitting; furthermore, the model built by this method cannot be explained. Hybrid modeling method combines the simplified first principle modeling method and the data-driven modeling method. The prior knowledge offered by the simplified first principle model can save training samples for the data-driven model and the data-driven model can compensate the non modeling characters of the simplified first principle model. So, hybrid modeling method has been widely used and satisfactory results have been obtained[8—10].

In multivariate process control, it is very common to study multi-input single-output (MISO) process control problems; however, multi-input multi-output (MIMO) objects are seldom researched[11]. But in many industrial processes, several variables need to be monitored and controlled simultaneously. In compound fertilizer process, there are three quality variables: nitrogen content, P_2O_5 content, and K_2O content. These three nutrient content must be maintained over a certain range. If the content of one of these three variables is under the request range, the compound fertilizer product is defective and must be reprocessed, thereby increasing the cost of production; but if the content of one of these three variables is very high, the costs will also increase. To ensure that the compound fertilizer products are of good quality and has lower energy consumption, these three nutrient content must be maintained over a certain range, so real-time control of the nutrient content of compound fertilizer is very important. But in practice, the content of these three nutrients cannot be measured on line. They are sampled thrice each day and measured by manual analysis. Manual analysis is a laboratory technique that is highly time-consuming, so it cannot meet the requirement of real-time control. To implement on line quality control, the real-time estimate values of these quality variables must be obtained. Building a soft-sensor model is a good alternative method. The common idea is to build a MISO model for each variable separately and then combine the individual models into a final MIMO model. This approach is not suitable for compound fertilizer process because there are strong coupling and interaction between these

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three quality variables. In such circumstances, building a joint MIMO soft-sensor model to predict the three quality variables simultaneously will make the model simpler and more robust[12].

In this article, data-driven modeling method and simplified first principle modeling method are combined to build the MIMO soft-sensor model of the three nutrient content for compound fertilizer. First, data-driven modeling approach based on LM-PLS algorithm is used to build soft-sensor models for some key secondary variables that cannot be measured on line, and then simplified first principle modeling method is used to compute the three primary variables on line. LM-PLS algorithm not only has the traditional PLS algorithm's advantages in overcoming the deficiencies of variable relevance and noise interference but also can be updated on line and can effectively track real-time changes of the system. Furthermore, it can overcome the saturation of the samples[13]. Simplified first principle model has the advantages of saving training samples for data-driven model. This hybrid model is being used in practical process to predict the three nutrient content of compound fertilizer on line; the results that were obtained indicate that the predicted results are good; the trends of model predicted values and manual analysis values almost coincide; therefore, the soft-sensor modeling method is effective.

2 LM-PLS ALGORITHM

Compared with the traditional multiple linear regression (MLR) and principal component regression (PCR), PLS algorithm is more robust. In this case, robustness indicates that when a new sample joins, model parameters do not change very acutely. It is a very important method for building soft-sensor model[14—16].

2.1 PLS algorithm description

The PLS model is built based on the properties of the nonlinear iterative partial least squares (NIPLS) algorithm. Suppose, there are two data matrix $\boldsymbol{X}$ and $\boldsymbol{Y}$, called independent $\boldsymbol{X}$(size $n\times m$) and dependent $\boldsymbol{Y}$(size $n\times l$), the relationship between them can be represented mathematically as

$$\boldsymbol{Y}=\boldsymbol{X\beta}+\boldsymbol{e} \tag{1}$$

The estimate $\hat{\boldsymbol{\beta}}$ of parameter $\boldsymbol{\beta}$ can be obtained by least-squares regression as

$$\hat{\boldsymbol{\beta}}=\left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{Y} \tag{2}$$

The PLS model can be considered as consisting of two outer relations ($\boldsymbol{X}$ and $\boldsymbol{Y}$ block individually) and an inner relation (linking both blocks). The outer relation for the $\boldsymbol{X}$ block is

$$\boldsymbol{X}=\boldsymbol{TP}^{\mathrm{T}}+\boldsymbol{E}=\sum_{h=1}^{a}\boldsymbol{t}_h\boldsymbol{p}_h^{\mathrm{T}}+\boldsymbol{E} \tag{3}$$

The outer relation for the $\boldsymbol{Y}$ block is

$$\boldsymbol{Y}=\boldsymbol{UQ}^{\mathrm{T}}+\boldsymbol{F}=\sum_{h=1}^{a}\boldsymbol{u}_h\boldsymbol{q}_h^{\mathrm{T}}+\boldsymbol{F} \tag{4}$$

where matrix $\boldsymbol{T}=\left[\boldsymbol{t}_1,\boldsymbol{t}_2,\cdots,\boldsymbol{t}_a\right]$ and matrix $\boldsymbol{U}=\left[\boldsymbol{u}_1,\boldsymbol{u}_2,\cdots,\boldsymbol{u}_a\right]$ are called score matrix, a is the quantity of hidden variables. $\boldsymbol{P}=\left[\boldsymbol{p}_1,\boldsymbol{p}_2,\cdots,\boldsymbol{p}_a\right]$ and $\boldsymbol{Q}=\left[\boldsymbol{q}_1,\boldsymbol{q}_2,\cdots,\boldsymbol{q}_a\right]$ are called loading matrix. The inner relation between $\boldsymbol{U}$ and $\boldsymbol{T}$ is

$$\boldsymbol{U}=\boldsymbol{TB}+\boldsymbol{R}=\sum_{h=1}^{a}\boldsymbol{b}_h\boldsymbol{t}_h+\boldsymbol{R} \tag{5}$$

$\boldsymbol{E}$, $\boldsymbol{F}$, $\boldsymbol{R}$ are residual matrix.

See related Refs.[17—19] about the details of PLS algorithm.

2.2 LM-PLS algorithm

LM-PLS algorithm [20] is a rolling modeling algorithm. It simultaneously deals with the time-varying property of the process parameters and the saturation of samples. The approach discards an old sample when a new one joins, so the quantity of the samples used in building the soft-sensor model remains unchanged. In general, the data window length is not very long when PLS algorithm was used to build model, so some useful information might be lost if old samples are discarded directly. The basic idea of LM-PLS algorithm is on line modification of the variances and means of samples; accordingly, the useful information in old samples can be introduced to the model by the variances and means. The modifying representation is

$$\bar{\boldsymbol{x}}_{i,N+1}=\frac{N}{N+1}\bar{\boldsymbol{x}}_{i,N}+\frac{1}{N+1}\boldsymbol{x}_{i,N+1} \tag{6}$$

$$\sigma_{i,N+1}^2=\frac{N-1}{N}\sigma_{i,N}^2+\frac{1}{N+1}\left(\boldsymbol{x}_{i,N+1}-\bar{\boldsymbol{x}}_{i,N+1}\right)^2 \tag{7}$$

Equation (6) is the on line modifying equation of means, and Eq.(7) is the on line modifying equation of variances, where $\bar{\boldsymbol{x}}_{i,N}$ and $\sigma_{i,N}^2$ are the means and variances, respectively, when the data window length is N; $\bar{\boldsymbol{x}}_{i,N+1}$ and $\sigma_{i,N+1}^2$ are the means and variances, respectively, when the data window length is $N+1$.

The LM-PLS algorithm is described as follows:

(1) Determine the window length N of sample data, and calculate its means and variances;

(2) Standardize the samples;

(3) Use PLS algorithm to these N samples and calculate the regression parameter $\hat{\boldsymbol{\beta}}$ of the model;

(4) Estimate the quality variables based on $\hat{\boldsymbol{\beta}}$ and the measurement values of the secondary variables;

(5) Judge whether a new sample is collected; if yes, then go to step (6); if no, go to step (4);

(6) Modify the means and variances of the samples according to Eqs.(6) and (7), then discard the oldest sample and join the newest sample to the training set. Go to step (2).

3 PROCESS DESCRIPTION OF COMPOUND FERTILIZER

The simplified compound fertilizer process flow sheet is shown in Fig.1. This product line adopts a

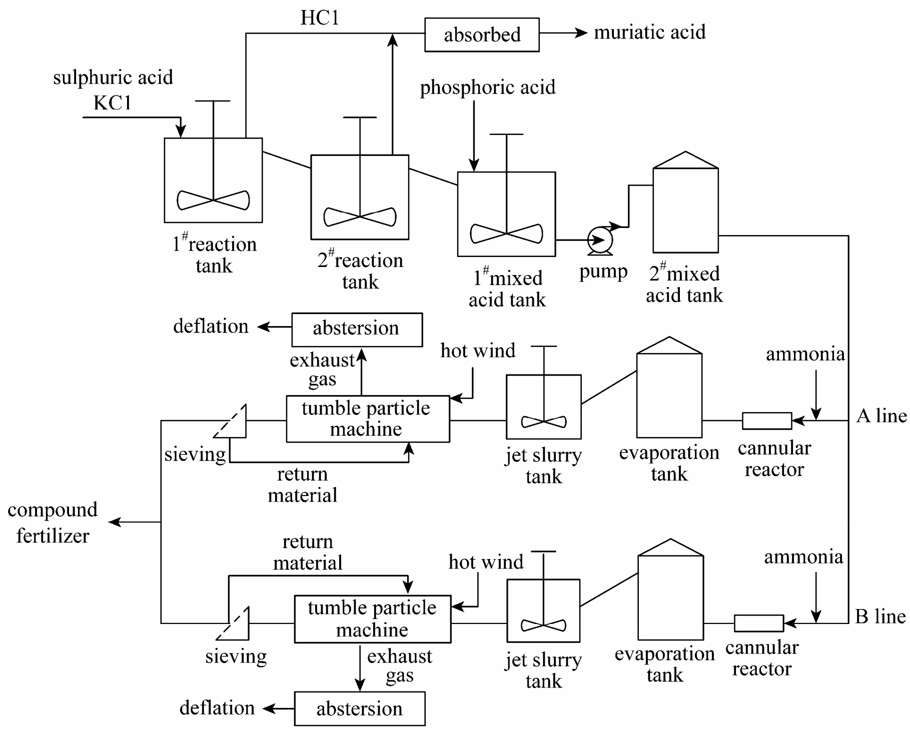

Figure 1 Schematic layout of compound fertilizer process

new technique-potassium chloride cryogenic transformation to produce sulfur-based nitrogen, phosphorus, and potassium compound fertilizer. This technique combines the processes of producing phosphoric acid, ammonium phosphate, and potassium sulfate, so it not only avoids the use of the phosphoric acid concentrate equipment or serous concentrate equipment but also the process of producing potassium sulfate at very high temperature. It can produce high-quality and effective compound fertilizer. This product line is divided into A line and B line after the $2^{\#}$ mixed acid tank and is united into one line after sieving. A line is the same as B line. The purpose of dividing into two lines is to regulate the production and facilitate overhaul.

There are three quality indicators in compound fertilizer process—the content of nutrients, nitrogen, P_2O_5, and K_2O. The primary method to ensure quality control is maintaining the three nutrient content in a certain range. In practical process, these three quality indicators are measured by off-line manual analysis because they cannot be measured on line by instrument. But off-line analysis is a laboratory technique with considerable delay and samples only three times each day; it is inadequate for timely control adjustment if required. To estimate the nutrient content on line, building a soft-sensor model for these quality indicators by measurable variables that can affect the nutrient content is an alternative choice.

The compound fertilizer process is very long. It is easily blocked and easily eroded. In the process, there is gas, secure, liquid three-phase response. Between production devices, interaction is considerably large; relevance is strong; and there are many interference sources. The devices generally have considerable lag, strong coupling, and nonlinear characters. For these reasons, the predict precision of the nutrient content soft-sensor model built by only using traditional data-driven modeling method is unsatisfactory. Also for these reasons, building a high-precision first principle model to estimate the nutrient content of compound fertilizer is unattainable. In this paper, data-driven modeling method and simplified first principle modeling method are combined to build the joint MIMO soft-sensor model for the three nutrient content of compound fertilizer. This joint MIMO soft-sensor model can predict the three quality indicators simultaneously. The soft-sensor model has been used in practical process, and good results have been obtained.

4 MODELING FOR NUTRIENT CONTENT OF COMPOUND FERTILIZER

4.1 Data pre-processing

In this industrial process, the flow is very long, so it is necessary to determine the lag time of each secondary variable relative to the primary variable. Through discussions with the technical engineers, lag times of the secondary variables are determined by equipment analysis and stay time calculation. When lag times are determined, weighted moving average filtering method is adopted to filter noise of the data set. The algorithm is described as

$$\bar{\boldsymbol{x}}_n = \frac{1}{M}\sum_{i=0}^{M-1} c_i \boldsymbol{x}_{n-i} \tag{8}$$

where M is the number of the average terms, $\bar{\boldsymbol{x}}_n$ is the output of the nth sample after filtering, $\boldsymbol{x}_{n-i}$ is the $(n-i)$th sample, c_i is constant. After filtering, the data set are standardized and then sent to the soft-sensor model.

4.2 Building soft-sensor model

Although a high-precision first principle model cannot be built because of the complexity of the process, it is realized that the mechanism of the compound fertilizer process is simple. There are only two chemical reactions in the whole process as follows.

The reaction between potassium chloride and sulfuric acid is

$$KCl + H_2SO_4 = KHSO_4 + HCl\uparrow \tag{9}$$

The counteractive reaction between mixed acid and ammonia is

$$\begin{gathered} NH_3 + H_3PO_4 = (NH_4)H_2PO_4 \\ NH_3 + (NH_4)H_2PO_4 = (NH_4)_2HPO_4 \\ NH_3 + KHSO_4 = KNH_4SO_4 \\ 2NH_3 + H_2SO_4 = (NH_4)_2SO_4 \end{gathered} \tag{10}$$

No other chemical reactions, except for those mentioned above and the corresponding physical processes occur, so the nutrient content of the compound fertilizer can be calculated by making full use of these two chemical reaction formulae. This process poses two problems. One is the reaction degree between potassium chloride and sulfuric acid. Because potassium chloride and sulfuric acid cannot react completely, their reaction degree would directly impact the mass of ammonia integrated by the reaction products and residues, thereby affecting the nitrogen content and other nutrient content in compound fertilizer products. The other is determining the mass of $(NH_4)H_2PO_4$ and $(NH_4)_2HPO_4$ produced in the counteractive reaction between mixed acid and ammonia. The counteractive reaction would be affected by ammonia flow, pressure and other factors, so how much $(NH_4)H_2PO_4$ would integrate ammonia and thereby produce $(NH_4)_2HPO_4$ is time-varying and cannot be measured on line. Therefore, it is difficult to determine the whole mass of the final product and thereby determine the three nutrient content.

If the two problems can be resolved, the measurable variables such as potassium consumption, sulfuric acid flow, and phosphoric acid flow can be used to calculate the three nutrient content by Eqs.(9) and (10). The solution to these two problems is as follows:

(1) The reaction degree between potassium chloride and sulfuric acid is relevant to the reaction tanks temperature, the ratio of the consumption of potassium to sulfuric acid, and the particle size of potassium; so potassium consumption, sulfuric acid flow, 1# reaction tank temperature and 2# reaction tank temperature are chosen as the secondary variable set ($\boldsymbol{X}_1$) and LM-PLS algorithm is used to build the soft-sensor model for the reaction degree. At the same time, according to the chlorine ion content in compound fertilizer products that is analyzed every eight hours and material balance, the degree of reaction can be calculated and the calculated value can be used to do soft-sensor model rectification.

(2) The indicator of counteractive degree reflects the ratio of $(NH_4)H_2PO_4$ to $(NH_4)_2HPO_4$ in the products of the counteractive reaction. According to the value and the measurement method of the counteractive degree, the mass of $(NH_4)H_2PO_4$ and $(NH_4)_2HPO_4$ in the products of the counteractive reaction can be calculated, and thereby the final mass of the overall products can be determined. Counteractive degree is obtained by manual analysis every two hours because it cannot be measured on line. To achieve its real-time estimate, potassium consumption, sulfuric acid flow, phosphoric acid flow, concentration, and density, mixed acid flow of A line, ammonia flow of A line, and ammonia pressure are chosen as the secondary variable set ($\boldsymbol{X}_2$); then, LM-PLS algorithm is used to build the soft-sensor model for the counteractive degree of A line. The every two-hour analytical value of A line counteractive degree is used to do soft-sensor model rectification. Similarly, potassium consumption, sulfuric acid flow, phosphoric acid flow, concentration, and density, mixed acid flow of B line, ammonia flow of B line, and ammonia pressure are chosen as the secondary variable set ($\boldsymbol{X}_3$); then, LM-PLS algorithm is used to build the soft-sensor model for the counteractive degree of B line. The every two-hour analytical value of B line counteractive degree is used to do soft-sensor model rectification. After calculating the A line counteractive degree and the B line counteractive degree by corresponding soft-senor models, weighted average method is used to calculate the counteractive degree of the whole production line according to A line mixed acid flow and B line mixed acid flow.

After deriving the reaction degree and the counteractive degree according to the above mentioned methods, the measured variables such as potassium consumption, sulfuric acid flow, phosphoric acid flow, *etc*., can be used to do calculation. First, the overall mass of the final products is calculated according to Eqs.(9) and (10); then the impurities contained in potassium and phosphoric acid are added to it and thereby the overall mass of the final compound fertilizer products is obtained. Because the potassium consumption, the mass of P_2O_5, and the mass of nitrogen in the consumed ammonia have been obtained, these variables are divided by the overall mass of the final compound fertilizer products and then the contents of nitrogen, P_2O_5 and K_2O can be calculated.

The whole soft-sensor model architecture is shown in Fig.2. In this Figure, $\boldsymbol{X}_1$ is the secondary variable set of the soft-sensor model for the reaction degree; $\boldsymbol{X}_2$ and $\boldsymbol{X}_3$ are the secondary variable sets of the soft-sensor models for A line counteractive degree and B line counteractive degree, respectively; $\boldsymbol{X}_4$ is the secondary variable set that is used in the simplified first principle model other than the reaction degree, the A line counteractive degree and the B line counteractive degree and includes sulphate density in phosphoric acid, A line mixed acid flow and B line mixed acid flow.

4.3 Model rectification

Because there are many factors that cannot be described in practical industrial process, the influencing factors of the secondary variables to the primary variable are not very complete in the practical process

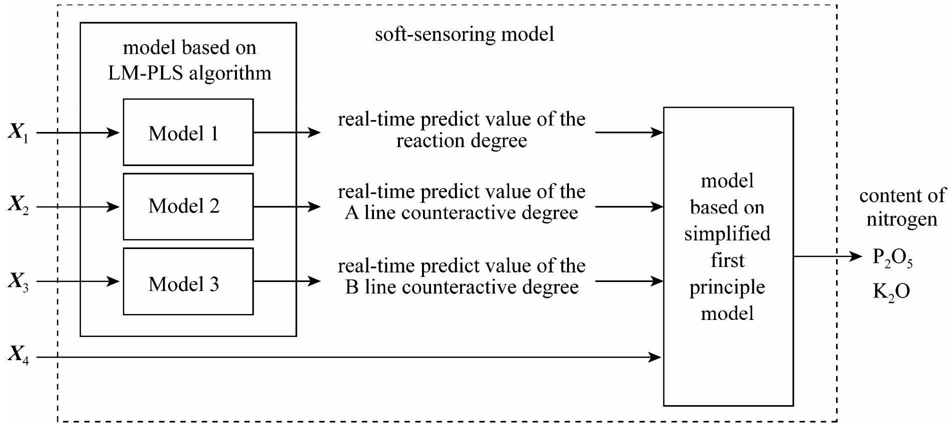

Figure 2 Architecture of the MIMO soft-senor model
Model 1—The soft-sensor model of the reaction degree based on LM-PLS algorithm;
Model 2—The soft-sensor model of the A line counteractive degree based on LM-PLS algorithm;
Model 3—The soft-sensor model of the B line counteractive degree based on LM-PLS algorithm;
Model 4—The soft-sensor model of nutrient content model based on simplified first principle model

expressed by the soft-sensor model. Furthermore, there are other error factors existing in the model calculation. These reasons make the results calculated by the model only an approximation. It can only express the changing trend of the quality of the product. There exits some error between this model computed value and the laboratory analyzed value; therefore, the model computed results should be rectified to eliminate the errors.

The errors between the model computed value and the laboratory analyzed value can be used to rectify the output of the model online. First, the model computed value at the sample moment and the model computed value at present moment should be obtained. Then, the error used in rectification can be obtained by weight adding the error of the sample moment and the error of the present moment. The final rectified value of the model can be obtained by adding the model computed value at present moment and the error obtained in last step.

5 RESULTS AND DISCUSSION

The soft-sensor model built according to the above mentioned method has been used in practical process. To illustrate the effectiveness of the soft-sensor model, the predicted values of the soft-sensor model are compared with the laboratory analysis values. Data were collected from 2:00 on October 1, 2005 to 10:00 on October 25, 2005. There are three samples each day, which are sampled at 2:00, 10:00 and 18:00. After discarding the invalid data caused by temporary non production, 61 data were collected.

Comparison of the predicted values of the soft-sensor model and the values of laboratory analysis is given in Fig.3. The relative errors of the soft-sensor model are shown in Fig.4. Table 1 lists the soft-sensor model's performances including maximum relative error, minimum relative error, and root-mean-square-error (RMSE) in detail.

From Fig.3 and 4 and Table 1, it can be seen that all outputs of the soft-sensor model have good

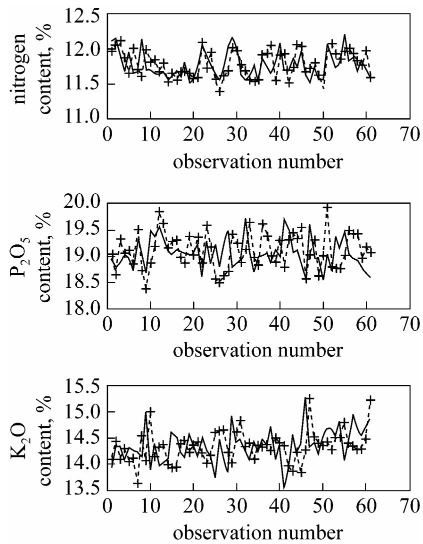

Figure 3 Comparison of the predicted values of the soft-sensor model and the values of laboratory analysis
—— analysis value; - - + - - predict value

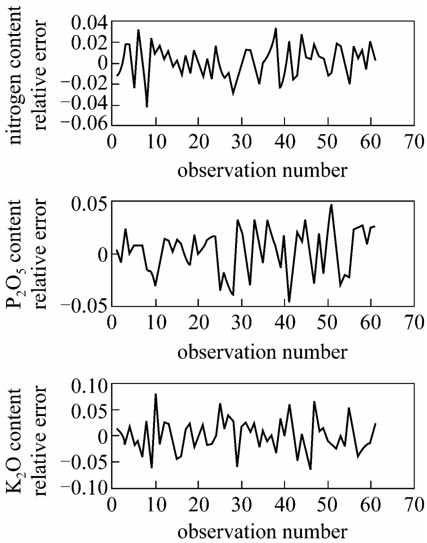

Figure 4 Relative errors of the soft-sensor model

Table 1 The performance of the soft-sensor model

Quality variable	Max. rel. error	Min. rel. error	RMSE
nitrogen	0.0341	−0.0425	0.0157
P_2O_5	0.0489	−0.0466	0.0212
K_2O	0.0802	−0.0660	0.0312

prediction capability. The built model is a joint MIMO soft-sensor model, so it is much simpler than building three MISO soft-sensor models. Furthermore, it can greatly reduce calculating time, so it can fully meet on line measurement requirement of nutrient content in compound fertilizer production.

6 CONCLUSIONS

As an important auxiliary method in process monitoring and optimization control, soft-sensor technique is used more widely now. Because three quality variables need to be monitored and controlled simultaneously in compound fertilizer production, the hybrid modeling method combined with data-driven modeling method and simplified first principle modeling method is used to build the joint MIMO soft-sensor model of the nutrient content in this study. The entire process is treated as a whole to analysis, so some redundant information can be eliminated from the internal structure of the proposed model, thereby simplifying the modeling process. The model built in this paper makes full use of the existing knowledge of the mechanism of the process. The LM-PLS algorithm possesses the advantages of rapid calculation and less training data and can update the model parameters on line, so it can track the time-varying characters of the system effectively. The hybrid model has been used in on line prediction of the nutrient content of the practical process. The operating results indicate that the model has better precision for prediction, and the curve of the predicted values of the model almost coincides with the curve of the laboratory analysis values. So, the built model can achieve on line measurement of the nutrient content of compound fertilizer. It can provide a reference for soft-sensor modeling used in other industrial process.

NOMENCLATURE

a	quantity of hidden variables
$\boldsymbol{E},\boldsymbol{F},\boldsymbol{R}$	residual matrix
N	data window length
$\boldsymbol{P},\boldsymbol{Q}$	loading matrix
$\boldsymbol{T},\boldsymbol{U}$	score matrix
$\boldsymbol{X}$	independent matrix
$\bar{\boldsymbol{x}}_{i,N}$, $\bar{\boldsymbol{x}}_{i,N+1}$	means when the data window length is N, N+1, respectively
$\boldsymbol{Y}$	dependent matrix
$\boldsymbol{\beta}$	regression parameter
$\hat{\boldsymbol{\beta}}$	estimate of $\boldsymbol{\beta}$
$\sigma_{i,N}^2$, $\sigma_{i,N+1}^2$	variances when the data window length is N, N+1, respectively

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