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Process Feature Change Recognition Based on Model Performance Monitoring and Adaptive Model Correction for the Gold Cyanidation Leaching Process

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ABSTRACT The gold cyanidation leaching process (GCLP) is the central unit operation in hydrometallurgy, and satisfactory gold recovery is highly significant in practice. However, GCLP faces the challenge of an irregular slow time-varying feature (STVF), which seriously affects gold recovery, and blind treatment for STVF also has drawbacks, which results in the need for the recognition of STVF for purposeful, rather than blind, treatment. Meanwhile, it also faces the problem of change of working condition (COWC) due to the variability of mineral resources. Both STVF and COWC may cause degradation of the soft-measuring model, which presents the need for model correction. Therefore, a coping strategy is proposed to solve these existing problems. First, an improved model-based principal component analysis monitoring is proposed to detect model mismatch and monitor the change of process feature. Next, a support vector machine-based process feature change recognition method is presented to recognize change type, which not only provides guidance in treating STVF but also makes it possible to implement targeted model correction for STVF and COWC. Finally, an adaptive model correction strategy that combines case-based correction and just-in-time learning-based correction is proposed. The simulation studies have verified the validity of the proposed coping strategy.

INDEX TERMS Gold cyanidation leaching process, model-based principal component analysis, process feature change recognition, adaptive model correction.

I. INTRODUCTION

The gold cyanidation leaching process (GCLP) has been the dominant process for the extraction of gold from ores in alkaline cyanide pulp due to its advantages of simple structure, little occupied space, ease of adjustment and low cost for construction and maintenance [1]–[5]. Actually, GCLP usually occurs in a cascade of continuous stirred tank reactors (CSTRs) to ensure longer residence time of pulp and higher gold recovery [1]–[4], [6]. As the most significant production target, gold recovery rate has an important influence on total gold production, production efficiency and so on [1], [2], and thus a satisfactory gold recovery is required in practice.

In GCLP, however, large-sized ore fines gradually sink and accumulate in the bottom of CSTRs, forming an ore-accumulation phenomenon, due to the gravitational setting function. The ore accumulation, hereinafter referred to as the slow time-varying feature (STVF), is a slow process of change in process feature that occurs over months because large-sized ore fines are a tiny minority of the total. STVF will not have much impact on GCLP in the short term, but it can seriously affect gold recovery after a period of accumulation because it gradually encroaches on the volumes of CSTRs and the residence time of ore pulp. This directly leads to a reduction of time for the chemical reaction between ores and leaching solution and then results in an increase of residual gold concentration in the ore (RGC-O). Hence, the plant will take some effective measures to treat STVF, i.e., accumulated ores will be pumped out from the bottom of CSTRs, ground into fine grains and then re-injected into CSTRs. However, due to the irregularity of STVF, it is very difficult for the plant to obtain useful information for guiding the treatment of STVF. Concretely, it is hard to determine when and how long STVF should be treated. A practical method for operators is to frequently or continuously treat it by virtue of experience. However, such operation has the disadvantages of wasting energy and leading to an overly small granularity of ore fines. Thus, a monitoring scheme that is capable of determining the occurrence of STVF is to be desired to guide operators in carrying out purposeful rather than blind treatment.

Affected by the variability of mineral resources, the initial gold concentration in the ore (IGC-O) is going to shift, which causes the multimode characteristic of GCLP. Thus, there is another change type in the process feature — change of working condition (COWC). Both STVF and COWC may cause the degradation of the soft-measuring model (SMM) of RGC-O. COWC is an abrupt change in the process feature, and it will cause SMM to be immediately unavailable. STVF is a gradual change in the process feature, which will lead to a gradual drift of model precision. In this case, SMM will be available in the short term, but it will no longer be applicable after a period of ore accumulation. Apparently, GCLP also faces an model correction problem derived from both COWC and STVF. Therefore, it is theoretically and practically significant to correct SMM while being able to recognize the type of change in the process feature.

However, GCLP affected by STVF and COWC has the following specificities: (1) a need to recognize STVF to guide the treatment of STVF; (2) both STVF and COWC have relatively low occurrence frequencies, so STVF treatment and model correction can be activated only after confirming that the process feature has changed; (3) STVF and COWC generally do not appear at the same time, so it is reasonable to respectively take countermeasures for them. Thus, according to the above specificities, a coping strategy should have the following characteristics and abilities: (1) recognizing and pre-judging the occurrence of STVF online to practically guide its treatment; (2) monitoring SMM performance online and activating countermeasures only when it does not meet accuracy requirements; and (3) recognizing the type of change in the process feature based on model performance monitoring and then implementing targeted countermeasures for STVF and COWC. Such a coping strategy is proposed in this study.

Firstly, an improved model-based principal component analysis (MBPCA) monitoring scheme is presented to monitor SMM performance and the process feature. In traditional MBPCA [7]–[10], the error between the actual process output and the estimated model's output is taken as input information to build a principal component analysis (PCA) model. The improved one in this study takes not only error information but also error change information as the input of PCA model. This monitoring scheme can achieve two functions: (1) SMM mismatch and changes in the process feature can be detected; and (2) feature information of STVF and COWC can be reflected in their statistics. Compared with traditional MBPCA, the improved one has the advantage of being able to detect STVF much earlier.

Secondly, a wavelet analysis (WA)-based feature extraction method and a support vector machine (SVM)-based process feature change recognition method are proposed to extract the main feature from the statistics and then recognize the type of change in the process feature. In [11], a state classifier was proposed to diagnose the type of change in the process feature according to the discrete Fourier transforms of the model performance index sequence. By referring to the basic thought in [11], this work presents a classifier used for recognizing the type of change in the process feature (hereinafter referred to as the type classifier). Such a type classifier is essentially a classification model, in which the characteristic variables that respectively characterize STVF and COWC are taken as the input and two types of change in the process feature (STVF and COWC) are taken as the output. Because STVF and COWC have entirely different features, their monitoring statistics can reflect their respective feature information. Thus, a WA-based feature extraction method can be introduced to extract the main feature of the statistical sequence that will be taken as the input information of the type classifier. SVM is a very efficient tool for classification, especially when the sample size is small, and it has been successfully applied to various classification tasks in chemistry [12]–[14]. Therefore, SVM is used for the training type classifier in this study.

Thirdly, an adaptive model correction strategy that combines case-based correction and just-in-time learning (JITL)-based correction is proposed for COWC. Not only STVF but also COWC can be online recognized using a type classifier, and then respective countermeasures for STVF and COWC should be implemented. For STVF, the STVF treating system can be turned on to treat it until the statistics return to their respective control limits. With the assistance of the proposed recognition approach, the blindness in treating STVF can be avoided. For COWC, an adaptive model correction approach is proposed to solve the problem of SMM degradation. This correction approach involves two model correction schemes, case-based correction and JITL-based correction, which work separately according to the level of similarity between the current working condition (WC) and historical WCs (also called historical cases). If the similarity reaches an appropriate threshold, then the models (including SMM and monitoring model) of the most similar case are directly switched to perform soft measurement and process monitoring under the current WC. Case-based correction is based on the idea of the case-based reasoning (CBR) methodology [15]–[17], and it can improve the utilization rate of historical information and avoid repetitive modeling for similar WCs. If there are no similar cases that have enough similarities to the current WC in the historical case base (HCB), there is always one case that is closest to the current WC. Then, this closest case is selected, and its process data that are most relevant to the data under the current WC are chosen by correlation-based JITL [18]. The chosen similar data, together with the existing data of the current WC, are utilized to reconstruct an SMM. Then, this reconstructed SMM can be updated with a moving window (MW) by incorporating new data of the current WC and discarding the borrowed data until all of the borrowed data are discarded. After that, the monitoring model under this new WC is also built. The combination of the SMM, monitoring model and process data is stored in the HCB as a new case, which achieves the update of HCB.

The remainder of this paper is organized as below. Section 2 gives a brief process description and mechanistic model of GCLP and the main theoretical methods used in this paper. In Section 3, the recognition of change in the process feature is presented. The adaptive model correction strategy is described in Section 4. The overall framework of the proposed coping strategy is discussed in Section 5. Finally, the study's conclusions are presented in Section 6.

II. PRELIMINARIES

A. BRIEF PROCESS DESCRIPTION AND MECHANISTIC MODEL OF GCLP

The procedure to extract gold from ores in this plant is mainly composed of floatation, washing and conditioning, gold cyanidation leaching, two-stage washing and gold recovery by zinc, of which gold leaching is the most crucial. In this study, a GCLP plant with four ideal pneumatic CSTRs is investigated. The simplified plant flowsheet of GCLP is shown in Fig. 1 [1]. For a detailed process description of GCLP, please refer to [1]–[3] and [5]; it will not be covered here.

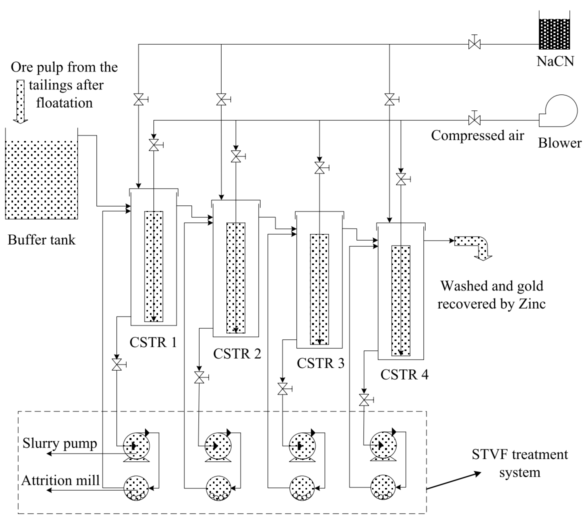

FIGURE 1. **Simplified plant flowsheet of GCLP.**

The mechanistic model presented in [4] and [6] is used to simulate the reality of GCLP, and the dynamical model for the ith CSTR is composed of the following mass conservation equations of gold in the ore, gold in the liquid and cyanide in the liquid [1]:

$$\frac{Qs_i}{Ms_i}(Cs_{i-1}-Cs_i)-r_{Au,i}=\frac{dCs_i}{dt}, \tag{1}$$

$$\frac{Ql_i}{Ml_i}(Cl_{i-1}-Cl_i)+\frac{Ms_i}{Ml_i}r_{Au,i}=\frac{dCl_i}{dt}, \tag{2}$$

$$\frac{Ql_i}{Ml_i}(Ccn_{i-1}-Ccn_i)+\frac{Qcn_i}{Ml_i}-r_{cn,i}=\frac{dCcn_i}{dt}, \tag{3}$$

with:

$$\begin{aligned} r_{Au,i} &= (1.13\times10^{-3}-4.37\times10^{-11}\bar{d}^{2.93}) \\ &\quad \times(Cs_i-Cs_\infty(\bar{d}))^{1.1}Ccn_i^{0.991}Co_i^{0.228}, \end{aligned} \tag{4}$$

$$r_{cn,i}=(\frac{1.69\times10^{-8}}{\bar{d}^{0.547}-6.40})Ccn_i^{2.91}, \tag{5}$$

$$Cs_\infty(\bar{d})=0.357(1-1.49e^{-1.76\times10^{-2}\bar{d}}), \tag{6}$$

where Qs_i, Ms_i, and Cs_i respectively represent the ore flow rate, ore hold-up and ore gold concentration in the ith CSTR; Ql_i, Ml_i, and Cl_i are the liquid flow rate, liquid hold-up and liquid gold concentration, respectively; Qcn_i and Ccn_i are the cyanide addition flow rate and the liquid cyanide concentration; $r_{Au,i}$ and $r_{cn,i}$ are the gold dissolution rate and the cyanide consumption rate; Co_i is the oxygen concentration in solution; and $\bar{d}$ is the average diameter of ore particles. The subscript i represents the corresponding variable in the ith CSTR. In addition, because of the negligible segregation and well-mixed reactants in the reactor assumption, the average residence time τ_i of the solid particles, liquid and ore pulp is given by [6]:

$$\tau_i=\frac{V_i}{\frac{Qs_i}{\rho s}+\frac{Ql_i}{\rho l}}\times1000, \tag{7}$$

with:

$$Ql_i=Qs_i\left(\frac{1}{Cw_i}-1\right), \tag{8}$$

where Cw_i is the weight concentration of solid in the pulp, V_i is the volume of the ith CSTR, and ρs and ρl are the solid and liquid densities, respectively. Then, Ms_i and Ml_i can be formulated as [3]:

$$Ms_i=Qs_i\times\tau_i, \tag{9}$$

$$Ml_i=Ql_i\times\tau_i. \tag{10}$$

The differential equations (1) to (3) with the kinetic reaction rate expressions given by (4) to (6) and the corresponding variable expressions given by (7) to (10) can be solved simultaneously by the ODE45 solver in MATLAB to obtain the final RGC-O and gold leaching rate.

The mechanistic model described above is applied to simulate the reality of GCLP, and the used model parameters are listed in Table 1.

TABLE 1. Parameters used in the mechanistic model.

Symbol	Quantitative value	Symbol	Quantitative value
Qs	2540 kg/h	Co	7 %
Ccn_0	0 mg/kg	V	70 m^3
Cl_0	0 mg/kg	ρs	2.8 g/cm^3
Cw	39 %	ρl	1.0 g/cm^3
$\bar{d}$	80 μm		

B. THEORETICAL METHODS USED IN THIS STUDY

1) MODEL-BASED PRINCIPAL COMPONENT ANALYSIS

PCA is a widely used multivariate statistical method for process monitoring [8], [19]. The detailed procedures of establishing a PCA model can be found in [8]; they will not be covered here. An MBPCA technique was presented by Wachs and Lewin [20] and has been widely used in process monitoring [7]–[10]. In this approach, model errors, **e**, between actual outputs and estimated outputs are calculated and subsequently used as input information to construct a PCA model, as is shown in Fig. 2(a). For a new observed data point $\mathbf{x}^{new}$, its associated T^2 and Q are compared with their respective control limits $T^2_{\lim}$ and $Q_{\lim}$ to determine if the criteria:

$$T^2 < T^2_{\lim}, \quad Q < Q_{\lim}, \tag{11}$$

is satisfied. If so, the system can be considered under the normal condition with $100(1-\alpha)\%$ confidence. Otherwise, some faults may occur in the process, and the monitoring system will alarm. For the detailed procedures of MBPCA, please refer to [8] and [9].

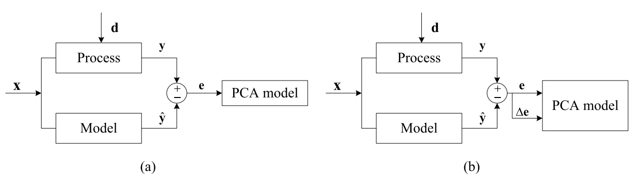

FIGURE 2. MBPCA monitoring scheme. (a) Traditional MBPCA. (b) Improved MBPCA.

2) WAVELET ANALYSIS THOERY

WA was developed by Grossmann and Morlet [21] during the 1980s and has already been an effective time-frequency signal processing tool [22]. WA can be considered as an extension of classic Fourier analysis, but it demonstrates the advantage of providing better time-frequency in contrast to Fourier analysis [23], [24]. Recently, WA has been widely used in feature extraction for pattern classification and recognition due to its function in decomposing a signal into components that appears at different scales (or resolutions) [25]–[27].

3) SUPPORT VECTOR MACHINE

SVM is known as a powerful classifier that has been applied to a large range of pattern recognition problems [12]. The aim of SVM is to split data into two groups by using an optimal hyperplane (classifier), which is defined by an orthogonal weight vector that has its vector length minimized with constraints [12], [13]. The effect is to leave the largest possible fraction of points of the same group on the same side and maximize the distance of either group from the hyperplane [12]. SVM has strong generalization capabilities to effectively avoid the over-fitting problem because it is based on the structural risk minimization principle from computational learning theory, which always converges to a global optimum [12], [14]. Please see [14] for more details of SVM.

4) CASE-BASED REASONING METHODOLOGY

CBR has received considerable attention with its ability to use historical data, such as cases or experiences, to predict a solution to the current problem [15]–[17]. The general principle of CBR is that similar problems have similar solutions [28]. In CBR, past experiences are stored as cases, each of which encloses the description of a source problem and its associated solution (source solution), and a new problem named the target problem can be solved by retrieving the most similar cases and relying on the source solutions [28].

5) CORRELATION-BASED JUST-IN-TIME LEARNING

Recently, JITL has attracted increasing attention in process modeling and soft sensor development of nonlinear systems [18], [29], [30]. The correlation-based JITL [18] is used to select the dataset that can most correctly describe the correlation fit for the current data sample for local modeling. In this approach, statistics of T^2 and Q are integrated into a comprehensive index for the dataset selection [31]:$J = \lambda T^2 + (1-\lambda)Q$, $0 \leq \lambda \leq 1$. For more details regarding correlation-based JITL, please refer to [18]; they will not be covered here.

III. PROCESS FEATURE CHANGE RECOGNITION

As outlined above, GCLP concurrently faces the challenges of STVF and COWC, which results in the need to determine and recognize their occurrence.

A. DETERMINATION OF CHANGE IN PROCESS FEATURE

1) THE IMPROVED MBPCA-BASED MONITORING

In this section, an improved MBPCA-based monitoring scheme will be proposed to monitor SMM performance and the process feature; refer to Fig. 2(b) for its basic schematic diagram. This approach can be primarily split into an offline training phase and online monitoring phase, as shown in Fig. 3.

Suppose that a dataset $\mathbf{Z} = \{\mathbf{X}, \mathbf{y}\} = \{\mathbf{x}_i, y_i\}_{i=1}^n$ is collected as the modeling database. When collecting modeling data, it is necessary to avoid modeling data being affected by STVF and COWC. Thus, the modeling data should be collected under a steady state after treating STVF, and meanwhile, the IGC-O should be offline measured once a day to make sure that there is no COWC occurring during data collection.

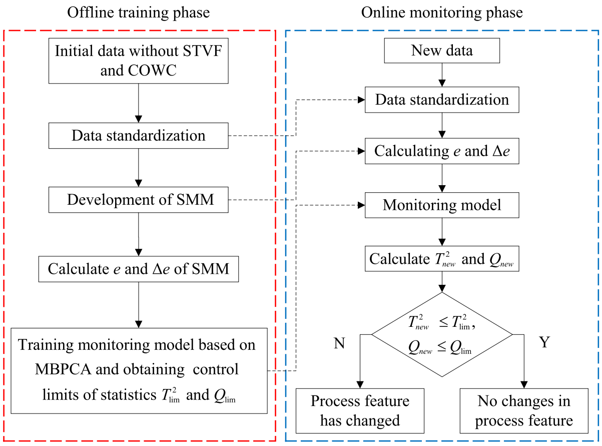

FIGURE 3. Improved MBPCA-based process monitoring scheme.

Note that the offline measurement of IGC-O can only be acceptable and necessary in collecting modeling data for initial modeling work to ensure that the modeling data are not affected by COWC. It is difficult to realize frequent offline measurement for IGC-O in actual normal production because there are other important process variables (RGC-O, for instance) that need to be measured offline. Moreover, it is also unnecessary to frequently measure IGC-O because decision-makers care about RGC-O value but not IGC-O value. Normally, RGC-O is only measured three times a day due to the complexity of offline measurement. Thus, the offline measurement of IGC-O will not play an important role and would only increase the field burden.

After SMM $f(\cdot)$ is developed and put into use, the estimated outputs $\hat{y}_i$ can be obtained according to the input variables $\mathbf{x}_i$. The errors between actual outputs y_i and estimated outputs $\hat{y}_i$, and the change information of errors can be obtained:

$$e_i = y_i - \hat{y}_i, \tag{12}$$

$$\Delta e_i = e_i - e_{i-1}. \tag{13}$$

Then, a PCA model F_{PCA} that takes e_i and Δe_i as input is constructed, and the control limits $T^2_{\lim}$ and $Q_{\lim}$ under normal conditions are respectively calculated.

For the newly observed data $D_i^{new} = (\mathbf{x}_i^{new}, y_i^{new})$, we have

$$\hat{y}_i^{new} = f(\mathbf{x}_i^{new}), \tag{14}$$

$$e_i^{new} = y_i^{new} - \hat{y}_i^{new}, \tag{15}$$

$$\Delta e_i^{new} = e_i^{new} - e_{i-1}^{new}. \tag{16}$$

Then, $(e_i^{new}, \Delta e_i^{new})$ is fed to F_{PCA} to calculate their respective statistics, T_i^2 and Q_i. If T_i^2 and Q_i are smaller than their respective control limits $T^2_{\lim}$ and $Q_{\lim}$, then SMM is considered to be working under normal conditions and the current process feature has not changed; otherwise, once model degradation is detected, it is indicated that some changes in the process feature may have occurred in GCLP.

2) SIMULATION STUDIES OF IMPROVED MBPCA-BASED MONITORING

The SMM of GCLP is developed based on PLS regression [32], where the flow rates of added cyanide, Qcn_i, are taken as input variables and RGC-O, Cs_r, is taken as an output variable. The number of modeling data is set to 10. STVF is an ongoing process, and it is simulated by gradually reducing the volumes of CSTRs linearly to simplify problems. COWC is simulated by abruptly changing the IGC-O. The MBPCA-based monitoring model is developed to evaluate SMM performance and monitor the process feature. The Q statistic is used as a performance evaluation index in this study. The simulation results of modeling and process monitoring under normal conditions (without STVF and COWC), with STVF and with COWC are shown in Fig. 4.

Under normal conditions, SMM has accurate soft measurement performance in tracking the actual value, and both model error and Q statistic have stable distributions below their respective control limits. During STVF, the measurement accuracy of SMM can be acceptable in the short term, but model error will be larger and larger with accumulation of STVF until SMM does not meet the precision requirement, which leads to a similar change in Q statistic. However, we can see that Q statistic alarms much earlier than model error, which provides an opportunity to anticipate the occurrence of STVF in advance and to deal with STVF before it affects model availability. When COWC occurs (600-750 mg/kg), if SMM under a WC of 600 is continually used for a new WC of 750, then model error will suddenly increase and result in model mismatch, which causes Q statistic to abruptly go beyond its control limit. Therefore, the simulation results have indicated that changes in the process feature can be determined with process monitoring when STVF and COWC occur, which is consistent with our previous theoretical analysis.

The difference between improved MBPCA monitoring and a traditional one is the introduction of model error change information, $\Delta\mathbf{e}$. Next, the advantages of introducing $\Delta\mathbf{e}$ into MBPCA will be illustrated in detail through simulation experiments.

Firstly, when traditional MBPCA is applied to the monitoring task in this study, because the input to PCA model has only one variable (model error, $\mathbf{e}$), the principal component of input variable is the model error, and there is no residual information that is used to calculate Q statistic. That is to say, only the T^2 statistic can be calculated by applying traditional MBPCA. Thus, the introduction of $\Delta\mathbf{e}$ can firstly solve the problem that the Q statistic cannot be calculated.

Secondly, from Fig. 4, it is indicated that $\Delta\mathbf{e}$ has an abrupt pulse signal when COWC occurs, which makes COWC very unique due to the identical and stable trends of $\Delta\mathbf{e}$ under normal conditions and STVF. Therefore, it seems that the introduction of $\Delta\mathbf{e}$ is able to increase the difference of feature information between COWC and STVF. However, it is obviously infeasible to recognize STVF and COWC only with $\Delta\mathbf{e}$ due to the identical trends of $\Delta\mathbf{e}$ under normal conditions

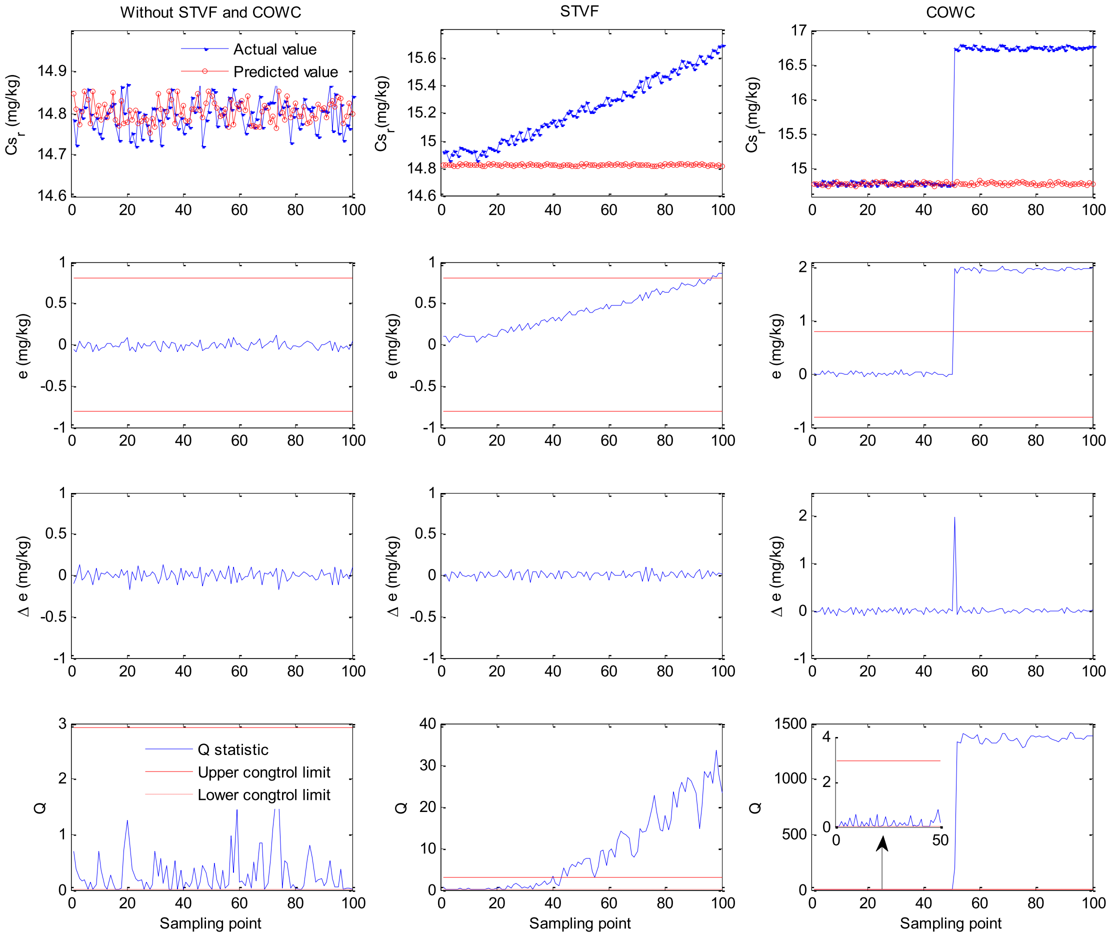

FIGURE 4. Simulation results of modeling and process monitoring under normal conditions, STVF and COWC.

and STVF. Traditional MBPCA and improved MBPCA are respectively used to monitor SMM performance and the process feature when STVF occurs; see Fig. 5 for simulation results, by which the following conclusions can be given: (1) MBPCA can detect STVF earlier than model error, which proves the importance and necessity of using MBPCA in process monitoring; and (2) Q statistic of improved MBPCA achieves the best performance in detecting STVF as soon as possible, which not only indicates the superiority of improved MBPCA but also proves the rationality in selecting Q statistic as the performance evaluation index.

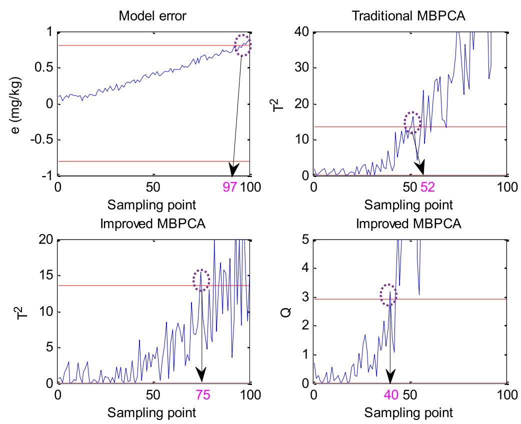

FIGURE 5. Simulation results of traditional MBPCA and improved MBPCA monitoring when STVF occurs.

B. TYPE RECOGNITION OF CHANGE IN THE PROCESS FEATURE

1) WA-BASED FEATURE EXTRACTION AND DEVELOPMENT OF AN SVM-BASED TYPE CLASSIFIER

As described above, the proposed MBPCA-based monitoring is applied to monitor SMM, and the changes in process feature can be detected. STVF and COWC have entirely different change features in Q statistic, and they can be effectively distinguished and recognized according to such obvious difference in the change feature of Q statistic. An effective method is to train a type classifier by taking these unique features in the change trend of Q statistic as input information. The type recognition by type classifier can be split into an offline training phase and online recognition phase. The following two steps are carried out to fulfill the offline training task of the type classifier. In the first stage, modeling data for development of the type classifier are obtained. However, note that the type classifier is unavailable during the offline training phase and that the type of change in the process feature cannot be recognized by the type classifier, so an MBPCA-based monitoring system is needed to assist in distinguishing STVF and COWC. Once the monitoring system alarms, which indicates that the process feature has changed, then a statistical sequence S_{eq} that contains L_{seq} continuous statistical data points before the over-limit point (including the over-limit point) is captured, and then the main feature of S_{eq} is extracted using WA, as shown in Fig. 6. Meanwhile, field operators will artificially observe the change trends of statistics to determine which change in the process feature caused the current alarm of the monitoring system. If the statistic gradually deviates from the normal state until it exceeds its control limit, then the current change in the process feature is caused by STVF; if the statistic abruptly jumps out of its control limit, then it is COWC causing the current change in the process feature. The captured statistic sequences in both cases of STVF and COWC are taken as input variables, and type tags of 0 (COWC) and 1 (STVF) are taken as output variables. After obtaining adequate modeling data, the second step of training the type classifier with the SVM training algorithm is then implemented. Then, the type classifier will be used to online recognize STVF and COWC. The schematic diagram of the type recognition of the change in the process feature is shown in Fig. 7.

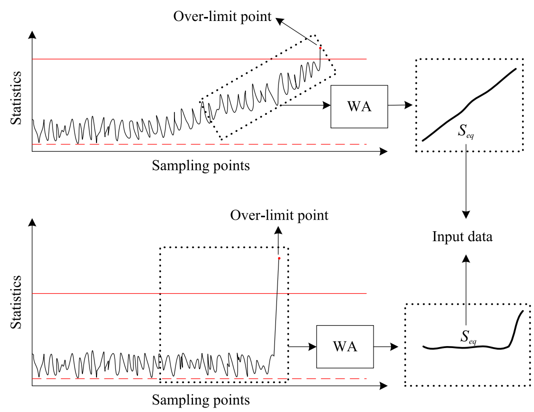

FIGURE 6. Schematic diagram of acquisition of modeling data for the type classifier.

2) SIMULATION STUDIES OF DEVELOPING AN SVM-BASED TYPE CLASSIFIER

When developing a type classifier, there are three parameters to be determined, including the length of the captured Q statistic sequence L_{seq}, kernel function of SVM and sample number in the training dataset N_{train}.

Determination of L_{seq}. In simulation experiments, a training set that includes 9 samples (4 for STVF and 5 for COWC) is utilized to train the type classifier, and a testing set that contains 31 samples (16 for STVF and 15 for COWC) is used to test it when L_{seq} equals 5, 8, 9 and 10. The accuracies of type classifiers with different values of L_{seq} are shown in Table 2, which indicates that the classification accuracy of the type classifier increases to 100% with the increase of L_{seq}. Thus, $L_{seq} = 10$ is selected in this study.

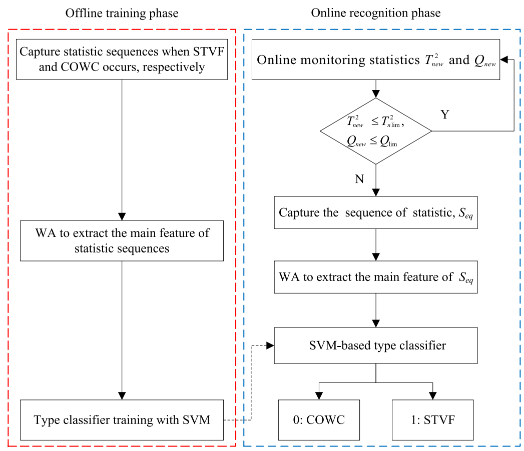

FIGURE 7. Schematic diagram of type recognition of changes in the process feature.

TABLE 2. Accuracies of type classifiers with different values of L_{seq}.

L_{seq}	Accuracy in training set	Accuracy in testing set
5	66.67%	58.06%
8	66.67%	58.06%
9	100%	96.77%
10	100%	100%

Selection of the kernel function. Three types of commonly used kernel functions, including linear, polynomial, and RBF kernels [20], are attempted to develop an SVM-based type classifier. The sample sizes for training are the same as in the determination of L_{seq}. For the simulation results of comparing the accuracies of type classifiers with different kernel functions, please refer to Table 3, which indicates that a linear kernel function is the best choice.

TABLE 3. Accuracies of type classifiers with different kernels.

Kernel	Accuracy in training set	Accuracy in testing set
Linear	100%	100%
Polynomial	100%	93.54%
RBF	100%	96.77%

Determination of N_{train}. Due to the complexity of data collection for training of the type classifier, the amount of modeling data should be as small as possible to shorten the offline training phase. Therefore, we try to reduce the number of samples in the training set. However, the number of samples in the testing set is still 31 to effectively verify the validity of type classifier. The simulation results of comparing the accuracies of type classifiers with different values of N_{train} are listed in Table 4, which gives the optimum sample size of $N_{train} = 3$.

TABLE 4. Accuracies of Type Classifiers With Different Values of N_{train}.

N_{train}	STVF	COWC	Accuracy in training set	Accuracy in testing set
9	4	5	100%	100%
7	3	4	100%	100%
5	2	3	100%	100%
3	1	2	100%	100%
2	1	1	100%	96.77%

IV. ADAPTIVE SMM CORRECTION STRATEGY

Either way, after recognizing STVF and COWC, the respective countermeasures in correcting SMM for STVF and COWC will be carried out, as shown in Fig. 8. For STVF, the STVF treating system can be enabled to eliminate its effect on the process until the statistics return to their respective control limits. Once the STVF is gone, the accuracy of SMM is naturally restored. For COWC, an adaptive model correction approach that combines case-based correction and JITL-based correction is proposed in this study.

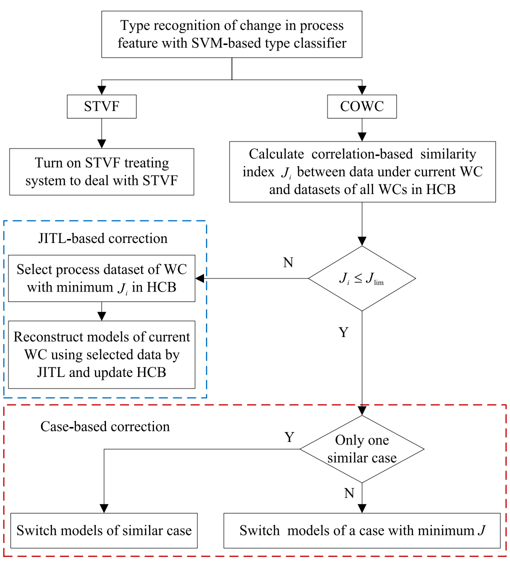

FIGURE 8. Respective countermeasures in correcting SMM for STVF and COWC.

A. ADAPTIVE MODEL CORRECTION APPROACH FOR COWC

The proposed adaptive model correction approach mainly consists of the following two parts: (1) case-based correction; and (2) JITL-based correction, as shown in Fig. 8. The central difference between the two correction approaches is whether there are any cases in the HCB that are sufficiently similar to the current WC.

Although GCLP is characterized by multiple WCs, the number of WCs that can be encountered is always limited. According to field experience, there is a high probability that the WCs that are the same or sufficiently similar to the historical WCs will occur in the production process. In this case, the process data, SMM and monitoring model of historical WCs can therefore be effectively reused, and thus the frequency of remodeling can be greatly reduced to lighten the burden of calculation when COWC occurs. In this approach, each WC is defined as a case, and an HCB is essential for fulfilling case-based correction. A HCB mainly contains historical process data, SMM and process monitoring model under various WCs. In this study, there is no such HCB at first, and it is constructed from scratch and is constantly being updated with the emergence of new WCs.

Assume that the current HCB has Nc historical cases:

$$HCB = \left\{ \begin{array}{c} (Z_1, \quad f_1, \quad F_{PCA,1}) \\ (Z_2, \quad f_2, \quad F_{PCA,2}) \\ \cdot \quad \cdot \quad \cdot \\ \cdot \quad \cdot \quad \cdot \\ \cdot \quad \cdot \quad \cdot \\ (Z_{Nc}, \quad f_{Nc}, \quad F_{PCA,Nc}) \end{array} \right\}, \tag{17}$$

and $D_c = (\mathbf{x}_c, y_c)$ is a data point of the current WC that has just changed from the last WC, i.e., D_c is a data point whose statistics have exceeded the control limits — the over-limit point. The correlation-based similarity index J_i between the current WC and the historical WCs in the HCB is represented by the correlativity between their process data [24]:

$$J_i = \lambda T^2_{c,i} + (1 - \lambda) Q_{c,i}, \quad 0 \le \lambda \le 1, \tag{18}$$

where $T^2_{c,i}$ and $Q_{c,i}$ represent the T^2 statistic and Q statistic when D_c is fed to the SMM and monitoring model of the ith case ($i = 1, 2, \cdots, Nc$), as is briefly described as follows:

$$D_c = (\mathbf{x}_c, y_c) \to f_i \Rightarrow (e_{c,i}, \Delta e_{c,i}) \to F_{PCA,i} \Rightarrow (T^2_{c,i}, Q_{c,i}). \tag{19}$$

If there is only one case in the HCB that satisfies the criteria $J_j \le J_{lim}$, then the models of the jth case will directly be used for soft measurement and SMM performance monitoring under the current WC. If more than one case (Ns, for instance) satisfies the criteria, then the J values of these cases that satisfy the criteria, $J_k (k = 1, 2, \cdots, Ns)$, will be compared to select a case with a minimum value of J, and the SMM and monitoring model of this case will be utilized in the current WC. The two situations described above are obviously subject to case-based correction.

However, if there is no case in the HCB that satisfies the criteria $J_i \le J_{lim}$, then a case whose process dataset has the maximum similarity with D_c will be selected, and correlation-based JITL will be used to chose the data most similar to D_c in the dataset of this case. The chosen data will be borrowed to reconstruct the SMM of the current WC, and the SMM will be updated with an MW (with a size of L_{MW} data points) by incorporating new data of the current WC and discarding the borrowed data until all the borrowed data are discarded. After a period of data collection, a combination of process data, SMM and monitoring model under the current WC is taken as a new case to update the HCB. A schematic diagram of JITL-based correction is shown in Fig. 9.

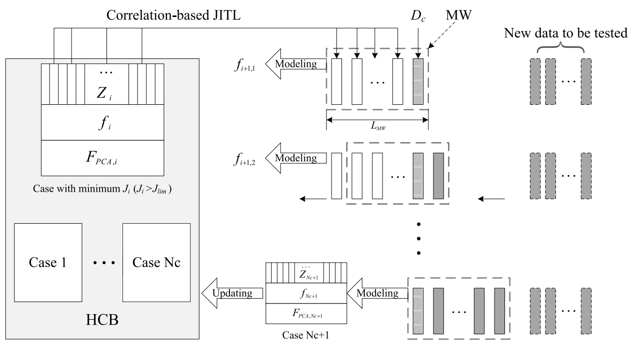

FIGURE 9. Schematic diagram of JITL-based correction.

B. SIMULATION STUDIES OF COUNTERMEASURES IN CORRECTING SMM FOR COWC

Actually, there are two types of situations for COWC. The first is that RGC-O, Cs_r, does not exceed a threshold of 15 mg/kg when WC changes, i.e., Cs_r still meets the production requirements. In such a situation, the field operators will not adjust their operating conditions. However, the second is that $Cs_r > 15$, which means that Cs_r no longer meets the production requirements. Thus, field operators will adjust their operating conditions to reduce Cs_r until it falls below the production index of 15 mg/kg. In this study, a data-driven control scheme named data-driven optimal iterative learning control (DDOILC) [33] will be used as a controller to simulate the operating condition adjustment in the field. Then, the simulation results of case-based correction and JITL-based correction will be illustrated.

Firstly, case-based correction will be implemented when there are cases that are sufficiently similar to the current WC in the HCB ($J < J_{\text{lim}}$). The simulation results of case-based correction are shown in Fig. 10 and Fig. 11 depending on

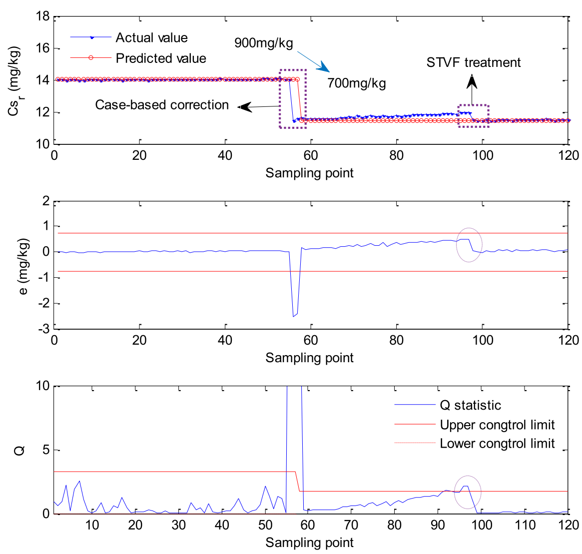

FIGURE 10. Simulation results of case-based correction under COWC with $Cs_r > 15$.

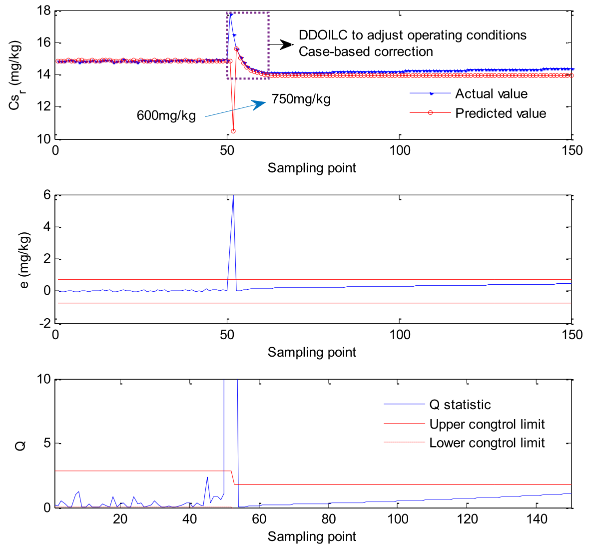

FIGURE 11. Simulation results of case-based correction under COWC with $Cs_r < 15$.

the type of COWC. As shown in Fig. 10, Cs_r changes from approximately 14.8 mg/kg to 17.8 mg/kg when COWC with $Cs_r > 15$ occurs (IGC-O: 600 to 750 mg/kg), and DDOILC will intervene to adjust the operating conditions until Cs_r meets the production requirements. Meanwhile, a sufficiently similar case selected from the HCB is applied to the current WC of 750 mg/kg. The simulation result indicates that both the model error and Q statistic return to their control limits after case-based correction. Due to the switch of monitoring model, the control limit of Q statistic has also changed. However, because of STVF, model error and Q statistic are still going to drift gradually until STVF is detected, and then STVF treatment system will be used to treat it. In Fig. 11, both model error and Q statistic exceed their control limits due to COWC with $Cs_r < 15$ (IGC-O: 900 to 700 mg/kg), but Cs_r changes from approximately 14.8 to 12.2 mg/kg. Thus, there is no adjustment of operating conditions in the field, and only case-based correction is needed for the SMM. The simulation results in Fig. 11 verify the validity of the case-based correction strategy. Similarly, model error and Q statistic will still drift away due to STVF, so the field operators turns on STVF treatment system to eliminate its effects when it is detected, as is shown in Fig. 11. Moreover, we can also see that model error is still below its control limit when STVF is detected (the Q statistic exceeds its control limit), so the simulation results demonstrate the feasibility of detecting STVF in advance and dealing with it before it affects SMM performance.

Secondly, if there are no cases that are sufficiently similar to the current WC in the HCB ($J > J_{\text{lim}}$), then JITL-based correction will be utilized. This study first takes COWC from 600 to 750 mg/kg as an example and then carries out JITL-based corrections by respectively borrowing data from various WCs, such as 600, 650, 680 and 700 mg/kg based on correlation-based JITL, in which the MW size is defined

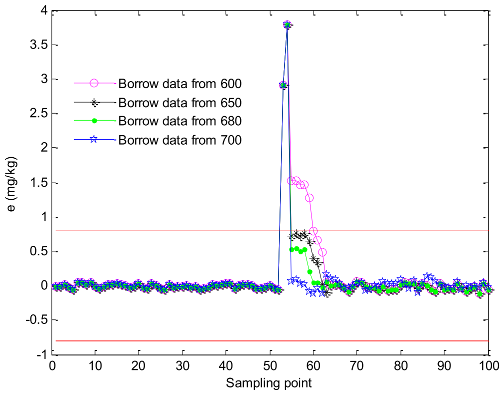

FIGURE 12. Simulation results of JITL-based correction by borrowing data from various WCs.

as $L_{MW} = 10$. These simulation results are compared and plotted in Fig. 12, which reveals that the best modeling effect can be obtained by borrowing process data under a WC of 700 mg/kg. Therefore, it is not feasible to reconstruct the SMM by borrowing data from any one of the WCs in the HCB, and it is necessary to select a WC whose dataset has the greatest correlation to the existing data under the current WC. Similarly, the simulation results of JITL-based correction under two types of COWC are respectively shown in Fig. 13 and Fig. 14. As shown in Fig. 13, Cs_r changes from approximately 14.2 to 16.9 mg/kg when COWC (IGC-O: 750 to 900 mg/kg) occurs, which activates the DDOILC adjustment and JITL-based correction simultaneously. The model error and Q statistic return back to their control limits after JITL-based correction. In this situation, the monitoring model of the current new WC also needs to be reestablished. When the MW is filled with process data under the current new WC, the SMM and monitoring model

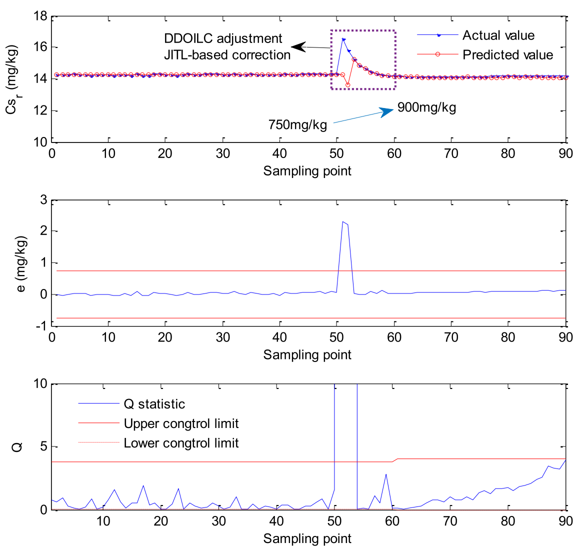

FIGURE 13. Simulation results of JITL-based correction under COWC with $Cs_r > 15$.

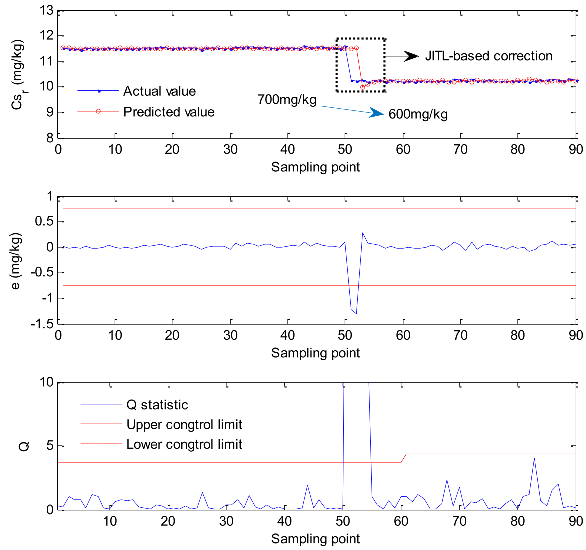

FIGURE 14. Simulation results of JITL-based correction under COWC with $Cs_r < 15$.

of this new WC will be developed and applied to the following soft measurement and process monitoring. The analysis for simulations in Fig. 14 is similar to that in Fig. 11 except for the different model correction approach, and it will not be described in detail here.

Finally, comparative simulations are implemented to verify the advantages of proposed model correction strategy. Compared with other situations, such as no correction (S-1), remodeling by waiting for 10 sets of data under new WC (S-2), and traditional MW correction by borrowing data from last WC until the borrowed data are all discarded with the collection of data under new WC (S-3), two simulation experiments (please refer to the simulation conditions shown in Fig. 11 and Fig. 13) are carried out. The simulation results shown in Fig. 15 indicate the advantages of case-based correction and JITL-based correction when COWC occurs.

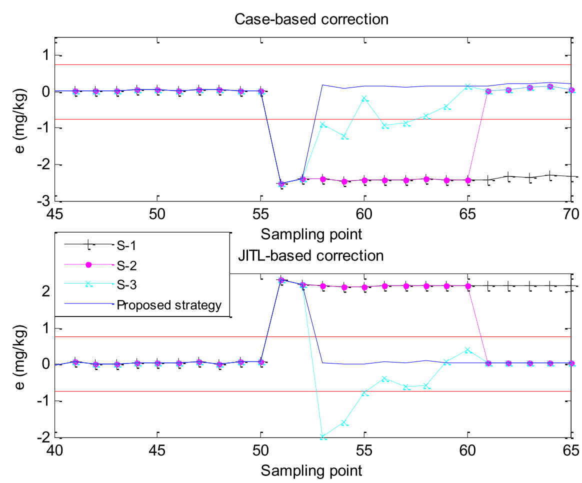

FIGURE 15. Comparative simulation results of proposed model correction strategy with other methods when COWC occurs.

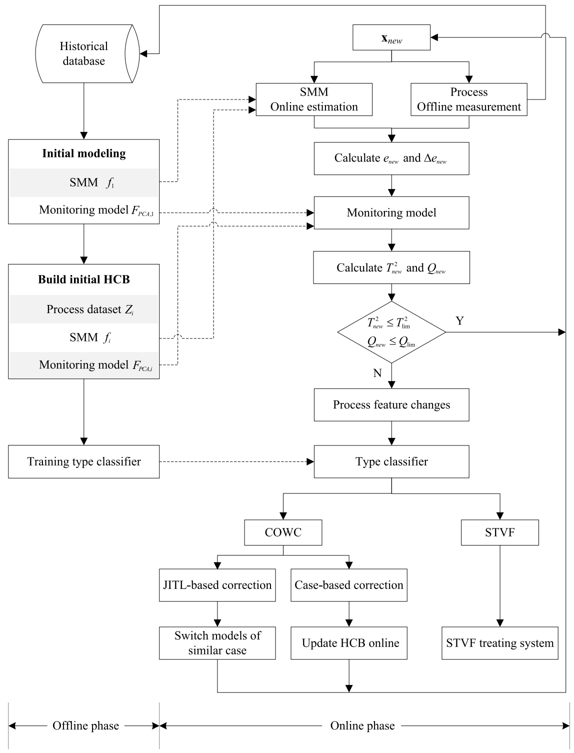

FIGURE 16. Schematic diagram of the overall framework of the proposed coping strategy.

V. OVERALL FRAMEWORK OF THE PROPOSED COPING STRATEGY FOR GCLP

Either the recognition of changes in the process feature or the adaptive SMM correction approach belong to an overall strategic framework proposed in this study, as is shown in Fig. 16. The overall strategic framework is mainly divided into an offline phase and online phase, which will be described in detail below.

A. OFFLINE PHASE

In the offline phase, there are three main modules: the initial modeling, building initial HCB and training type classifier. The first and third modules have been described in detail in the previous sections, and they will not be covered here.

It is assumed that there are no historical data and models in the initial phase to form an HCB and that an initial HCB is constructed from scratch during the offline phase. An initial SMM, f_1, and an initial MBPCA-based monitoring model, $F_{PCA,1}$, should be developed and applied to the current WC (defined as WC-1) at the beginning of the coping strategy. The combination of process data, f_1, and $F_{PCA,1}$ under WC-1 is defined as Case 1. Once the change in the process feature is detected, with the assistance of MBPCA-based monitoring, the type of process change is offline recognized by artificially observing the change trends in statistics. The STVF treatment system can be activated to treat STVF. However, if COWC occurs (from WC-1 to WC-2), and there must be no similar case in the HCB at this time, JITL-based correction is the only method to use. Then, the process data under WC-1 that are most relevant to the current data under WC-2 are selected to reconstruct the SMM, f_2, which will be continually updated by an MW method until the MW is fully filled with process data under WC-2. After that, a monitoring model, $F_{PCA,2}$, is also constructed to monitor the current SMM performance and process feature. The SMM f_2 and monitoring model $F_{PCA,2}$, together with the process data under WC-2, are defined as Case 2. Thus far, there have been two cases in the HCB. The difference between the constructions of Case 2 and the following Case 3 is that the similarity between WC-1 and WC-3 should be evaluated to determine whether a case-based correction method is available. If WC-3 is sufficiently similar to WC-1, then a case-based correction is utilized, and the models of WC-1 can be used in WC-3 while waiting for the arrival of a new WC, i.e., WC-3 is not defined as a new WC. If not, JITL-based correction can be activated, and a combination of the SMM, monitoring model and process data under WC-3 is defined as Case 3. The following construction of cases in the initial HCB can be completed by repeating the above steps in constructing Case 3. In this manner, the initial HCB can be built during the offline phase.

B. ONLINE PHASE

After building an initial HCB and a type classifier, the online phase is activated. The steps for the online phase are illustrated as follows:

Step 1: When a new offline measurement $(\mathbf{x}_{new}, y)$ is obtained, it is first stored in the historical database, and then the responding model estimate $\hat{y}$ is calculated to further obtain $(e_{new}, \Delta e_{new})$.

Step 2: $(e_{new}, \Delta e_{new})$ is fed to the monitoring model to calculate T^2_{new} and Q_{new}.

Step 3: If $T^2_{new} \le T^2_{\lim}$, $Q_{new} \le Q_{\lim}$, go to **Step 7**; otherwise, go to **Step 4**.

Step 4: Utilize the type classifier to recognize the change type in the process feature. If STVF, go to **Step 5**. If COWC, go to **Step 6**.

*Step 5:*The STVT treatment system is utilized to eliminate its effects.

Step 6: The adaptive model correction strategy for COWC is applied, go to **Step 7**.

Step 7: Utilize the current SMM for online estimation until the next offline measurement arrives, and then go to **Step 1**.

C. OVERALL SIMULATION STUDY OF THE ONLINE PHASE

The previous simulation studies have individually verified the effectiveness of various parts of the proposed coping strategy. In this section, an overall simulation study of the online phase in a simulated GCLP is performed, and the simulation results are shown in Fig. 17 and Fig. 18, which proves the effectiveness of the proposed coping strategy.

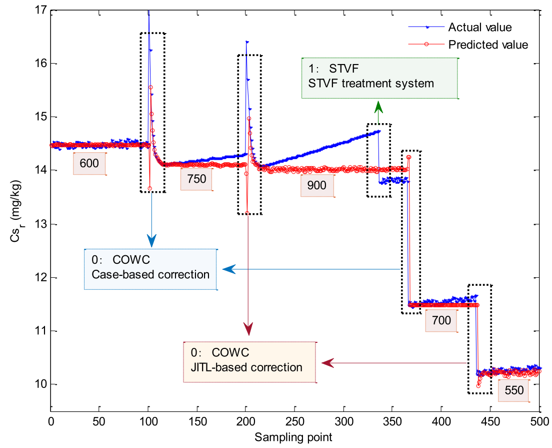

FIGURE 17. Overall simulation results of RGC-O for the proposed coping strategy.

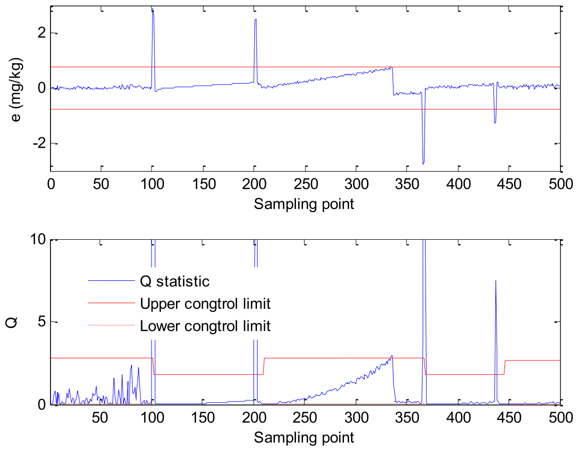

FIGURE 18. Overall simulation results of SMM error and *Q* statistic for the proposed coping strategy.

VI. CONCLUSION

In this study, a coping strategy that involves a type recognition approach of changes in the process feature and an adaptive model correction approach is proposed, not only to solve the problem of model correction for COWC but also to guide the field operators to deal with STVF at the theoretical and practical levels. Firstly, the SMM performance and process feature are monitored with an improved MBPCA-based monitoring to confirm whether the process feature has changed. Secondly, an SVM-based type classifier is developed to online recognize the type of change in the process feature. Such a type recognition strategy has two main roles: the first is to determine the occurrence of STVF and then provide guidance in treating STVF for field operators; the second is to recognize COWC and carry out an adaptive model correction strategy. Then, effective countermeasures for STVF and COWC are respectively implemented. For STVF, the STVF treatment system in the field can be enabled to eliminate its negative effects. For COWC, an adaptive model correction strategy that is composed of case-based correction and JITL-based correction is proposed. Lastly, simulation studies are performed in a simulated GCLP to verify the validity of proposed coping strategy.

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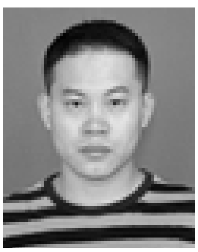

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