Korean J. Chem. Eng., 37(1), 11-18 (2020)
DOI: 10.1007/s11814-019-0403-y

pISSN: 0256-1115
eISSN: 1975-7220

Anomaly detection in a hyper-compressor in low-density polyethylene manufacturing processes using WPCA-based principal component control limit

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(*Received 18 April 2019 • accepted 12 October 2019*)

Abstract−Low-Density Polyethylene (LDPE) was synthesized from ethylene at high-temperature and pressure condition. Hyper-compressor used to increase pressure up to 3,500 atm should be monitored and controlled delicately or it cannot guarantee stable operation of the process causing process shutdown (SD), which is directly related to product yield and process safety. This paper presents a data-based multivariate statistical monitoring method to detect anomalies in the hyper-compressor of a LDPE manufacturing process with weighted principal component analysis model (WPCA), which can consider both time-varying and time-invariant characteristic of data combining principal component analysis (PCA) and slow feature analysis (SFA). Operation data of the LDPE manufacturing process was gathered hourly for four years. WPCA-based principal component control limit (PCCL) was used as an index to determine anomaly and applied to five emergency shutdown (ESD) cases, respectively. As a result, all the five anomalies were detected by a PCCL, respectively, as a sign of SD. Moreover, it shows a better anomaly detection performance than the monitoring method using T^2 and squared prediction error (SPE) based on PCA, SFA, or WPCA.

Keywords: Fault Detection, Fault Isolation, Slow Feature Analysis, Principal Component Analysis

INTRODUCTION

The global polymer market is expected to grow due to applicability such as thermoplastics, thermosets, and elastomers. Polyethylene is one of the most widely used polymers worldwide. Low-density polyethylene (LDPE), along with linear low-density polyethylene (LLDPE), accounts for 60% of total plastics production and is used in reusable bags, trays, containers, and agricultural film [1]. This widespread use is the result of the broad range of possible molecular and structural properties of the various grades of LDPE and its copolymers.

Ethylene is a precursor of LDPE, which is compressed by hyper-compressor and is synthesized ranging at 140-330 °C and 1,000-3,500 atm. Even under the normal operating condition ethylene can undergo two further side reactions known as decomposition into methane and hydrogen. This reaction can be initiated by a point source of energy, by a flame, by sudden compression or a sudden excess of catalyst [2]. Then methane as a major product raises the pressure inside the reactor about four to six-times the initial pressure. It affects process safety as well as a yield reduction. Therefore, a stable process operation is essential.

One of the main obstacles to stable operation of the process is the process shutdowns (SDs), especially emergency shutdowns (ESDs). This is because a sudden stop of the process could damage the process equipment; therefore, it takes much time to restart the process. Most of the SDs occur in the hyper-compressor. Moreover, the hyper-compressor anomaly can be a sign of a more serious and dangerous situation, resulting in process SD or blackout rather than the decomposition of ethylene and yield loss.

To detect anomalies in the hyper-compressor, several methods have been applied. Time-frequency analysis method was applied to extract the features of the anomaly in the hyper-compressor [3], and classified the features as the condition of operation. This method is only applicable when the sampling frequency is high enough. However, in the LDPE manufacturing process, it is difficult to get data with high sampling frequency due to lack of storage capacity. Mathematical modeling of the single-stage compressors was also applied to detect anomalies [4]. However, on-site compressors are different from the proposed mathematical model, and it is impractical to obtain a mathematical model of the field compressor. Therefore, fault diagnosis based on operational data is essential.

To overcome such drawbacks, we applied multivariate statistical process monitoring analyses (MSPM) based on data-driven method. The widely used one is principal component analysis (PCA), which is a method of compressing high-dimensional inputs into a few orthonormal variables since process variables are highly correlated, process monitoring should be based on techniques which look at all the critical variables simultaneously. PCA has widely been applied in process monitoring to detect and diagnose process anomaly, including LDPE manufacturing process as well. Sharmin et al. developed a PCA-based fault detection model for autoclave reactors to predict the decomposition with reasonable detection time [2]. Sivalingam et al. used iterative PCA technique to confirm the selection of the model and predicted reactant decomposition based on overall heat balance around the autoclave reactor [5]. Kumar et al. used a PCA-based monitoring scheme to predict decomposition of reac-

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tants and loss of normal reaction in high-pressure LDPE reactors [6]. However, these papers cannot consider the time-varying feature of process data. That is, the normal operating condition of actual processes changes continuously and slowly, and thus the sensor value in the normal operation range also changes. PCA does not reflect the time-varying characteristic because it only analyzes at a single time. Furthermore, previous studies have mainly focused on decomposition reaction occurring in the reactor.

Several new methods have been developed to supplement the drawbacks of PCA. Dynamic PCA (DPCA) uses a time lag shift method to include the dynamic behavior of data in the PCA model [7]. Kernel PCA (KPCA) uses nonlinear kernel functions to satisfy the theoretical assumption of PCA [8], and recently KPCA was applied to a wastewater treatment process to detect process faults [9,10]. Sensitive PCA (SPCA) uses select index principal components (PCs), which represent the dominant variance of abnormal observation objectively [11]. Multiway PCA (MPCA) was developed and applied to detect faults in batch processes [12]. A principal component based method that weighs each PCs to maximize the detection rate was proposed and applied to simulation data [13]. Recently, sparse probabilistic PCA was applied to obtain the sparse loading matrix that makes the PCs easier to interpret [14].

However, these methods were developed under the assumption that the normal operating condition is time-invariant. Therefore, when a PCA-based method is applied to monitor a nonstationary process in which normal conditions of process variables are time-varying, this time-variant characteristic should be considered.

To consider the time-varying and time-invariant characteristics of the data, weighted principal component analysis (WPCA) extracts useful information for time-variant processes [15] by combining PCA and slow feature analysis (SFA), which extracts slowly varying feature from process data. This representation could increase the accuracy of the model when the target process changes continuously and slowly over time.

Therefore, in this research, an anomaly detection model was developed using WPCA for the hyper-compressor in LDPE manufacturing process. This model was applied to the process operation data to detect if there was any prognostics on ESD based on ESD history, then the cause of ESD was diagnosed. The process operation data was collected every 1 hour from the LDPE manufacturing process for four years (July of 2012 to March of 2016). The data consisted of 55 process variables related to the hyper-compressor, booster compressor, and primary compressor. Using this data, a normal operation model was developed first (offline modeling). Then PCs and their normal operation regions based on WPCA were calculated, and PCs were monitored separately by principal component control limits (PCCL) to guarantee the sensitive detectability of the process faults [16]. The developed fault detection model is expected to increase the safety and productivity of the LDPE manufacturing process by predicting abnormalities and preventing SDs in advance.

METHOD

1. WPCA Algorithm and Monitoring Statistics

Because PCA cannot consider time-varying processes, a weighted criterion in dimension reduction methods was developed to extract feature information by Shanmao et al. [15]. Therefore, WPCA combines PCA and SFA to consider both the slowly varying features hidden in process data and the time-invariant features. WPCA can be performed by solving a constrained maximization problem with a joint objective function of PCA and SFA. For PCA, the objective function is defined as

$$J_1 = \max \mathbf{w}^T\mathbf{X}\mathbf{X}^T\mathbf{w}, \tag{1}$$

where $\mathbf{w}\in\Re^{d\times d}$ is a transformation matrix, and $\mathbf{X}\in\Re^{d\times n}$ (n is the number of samples and d is the number of variables) is a matrix of high-dimensional data.

Unlike PCA, SFA minimizes the variation of hidden features. The optimization equation is as follows:

$$\min \Delta y_j(t) = \min \langle \dot{y}_j^2 \rangle_t \tag{2}$$

where $\dot{y}_j$ is the jth first-order derivative of y and y is a d-dimensional slow feature. $\langle\,.\,\rangle_t$ is the sample mean of all the available time. y satisfies the following constraints:

$$\langle y_j \rangle_t = 0 \tag{3}$$

$$\langle y_j^2 \rangle_t = 1 \tag{4}$$

$$\langle y_i y_j \rangle_t = 0 \tag{5}$$

Let $y_j = \mathbf{w}_j^T\mathbf{x}$ and $\dot{y}_j = \mathbf{w}_j^T\dot{\mathbf{x}}$. Eq. (2) can be represented as

$$J_2 = \min \mathbf{w}^T\Delta\mathbf{X}\Delta\mathbf{X}^T\mathbf{w}, \tag{6}$$

where $\Delta\mathbf{X}=[\Delta\mathbf{x}_1\ \Delta\mathbf{x}_2\ \cdots\ \Delta\mathbf{x}_d]$ and $\Delta\mathbf{x}(t)=\mathbf{x}(t)-\mathbf{x}(t-1)$ [17,18]. Objective functions J_1 and J_2 have a similar structure. Therefore, by integrating the two objective functions, both characteristics of PCA and SFA can be considered simultaneously. After integrating the functions, WPCA can be performed by finding $\mathbf{w}$ satisfying the following objective function:

$$\begin{aligned} J &= \max \alpha\mathbf{w}^T\mathbf{X}\mathbf{X}^T\mathbf{w} - (1-\alpha)\mathbf{w}^T\Delta\mathbf{X}\Delta\mathbf{X}^T\mathbf{w} \\ &= \max \mathbf{w}^T(\alpha\mathbf{X}\mathbf{X}^T - (1-\alpha)\Delta\mathbf{X}\Delta\mathbf{X}^T)\mathbf{w} \qquad \text{s.t. } \mathbf{w}^T\mathbf{w}=1, \\ &= \max \mathbf{w}^T\mathbf{X}'\mathbf{w} \end{aligned} \tag{7}$$

where $\mathbf{X}'=\alpha\mathbf{X}\mathbf{X}^T-(1-\alpha)(\Delta\mathbf{X}\Delta\mathbf{X}^T)$, and α is a weighting factor that is to weight PCA or SFA ($0\le\alpha\le1$). To guarantee the detectability of WPCA, α must be chosen appropriately because it specifies the relative influences of PCA and SFA.

The optimal solution of Eq. (7) corresponds to the optimal transformation vector and eigenvalues as follows:

$$\mathbf{X}'\mathbf{P} = \lambda\mathbf{P}, \tag{8}$$

where $\mathbf{P}=[\mathbf{p}_1\ \mathbf{p}_2\ \cdots\ \mathbf{p}_d]$ is optimal transformation vectors, also called a loading vector. Since WPCA aims to extract low-dimensional linear features, we used a certain number of PCs which explain most of their variances. Therefore, the loading vector becomes $\mathbf{P}_{new}=[\mathbf{p}_1\ \mathbf{p}_2\ \cdots\ \mathbf{p}_q]$, where $q\ll d$. Then PCs can be calculated as

$$\mathbf{t} = \mathbf{P}_{new}^T\mathbf{x}. \tag{9}$$

Like PCA, Hotelling's T^2 and squared prediction error (SPE) are used as the monitoring statistics in WPCA-based process monitoring method [19]. T^2 represents the distance between the current

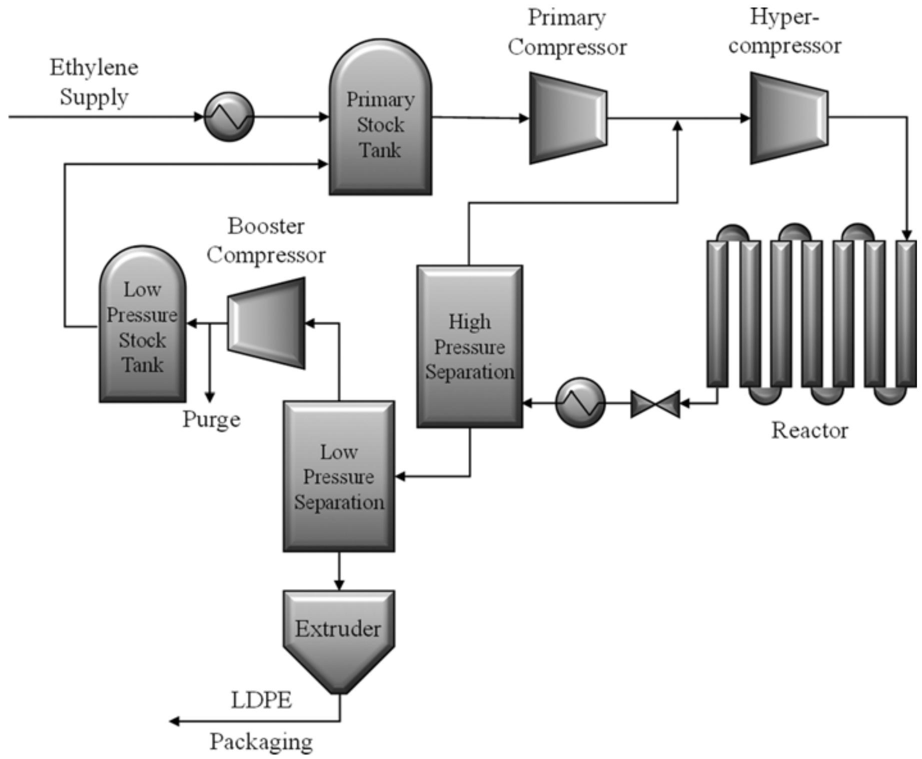

Fig. 1. Diagram of LDPE manufacturing process.

value of a variable and its average in the PC subspace, considering the variance of the data as follows:

$$T^2 = \sum_{i=1}^{q} \frac{t_i^2}{\sigma_i^2}, \tag{10}$$

where t_i is the score on i-th PC, and σ_i is the standard deviation of scores on the i-th PC. The score on i-th PC is obtained from WPCA. SPE represents the error between the process data and the WPCA model in the residual space as follows:

$$SPE=(\mathbf{x}-\mathbf{P}_{new}\mathbf{t})^T(\mathbf{x}-\mathbf{P}_{new}\mathbf{t}) \tag{11}$$

Strictly speaking, the given process data have non-Gaussian distribution, therefore the control limits of T^2 and SPE are calculated using kernel density estimation (KDE) method. When T^2 or SPE exceeds the control limits, it is considered as an alarm. KDE can be performed as follows:

$$f(x) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right), \tag{12}$$

where f is density function, n is the number of samples, h is smoothing parameter, x_i is an observed value and K is kernel function. We used Gaussian kernel function in this paper.

Because T^2 is a summation that represents the variation and error of PCs as a single statistic, it is not easy to detect with T^2 that which PCs exceeded the control limit. Therefore, we used PCCL rather than T^2 and SPE to guarantee more sensitive monitoring. The control limits of each PC are obtained by setting upper and lower control limit (UCL and LCL) for each i-th PC based on the KDE as given in Eq. (12). A fault can be detected by setting appropriate control limits based on normal data [16]. We used KDE to calculate UCLs and LCLs of PCs for the same reason mentioned above.

When an anomaly is detected in a PC, we could identify variables that might have caused the anomaly by using the column of the loading vector which was used to calculate the PC. Each column of the loading vector matches the relative effect of each variable to the corresponding PC. For example, if an anomaly is detected in PC1 and the absolute value of the coefficient that corresponds to variable 1 is large, then the variable 1 may have the most contribution to the anomaly.

2. Process Description

LDPE is manufactured through four steps: compression, reaction, extruding and packing (Fig. 1). In the first step, the raw material (ethylene) is passed through two compressors (primary compressor and hyper-compressor) to reach reaction pressure. In this step, an initiator and a modifier are injected, ethylene is compressed to 250 bar in the primary compressor, and the pressure is increased to maximum 3,200 bar by hyper-compressor. Then ethylene polymerizes into polyethylene in the reactor.

The hyper-compressor has two stages, each of which consists of four cylinders (Fig. 2). The branched feed stream flows into the first stages (1AS, 1AN, 1BS, and 1BN) of the hyper-compressor and then is cooled down in each cooler. The compressed stream in the first stages is compressed again in the second stages (2AS, 2AN, 2BS, and 2BN).

3. Process Data and Shutdown History

Operation measurements of the LDPE manufacturing plant were collected hourly for four years (July of 2012 to March of 2016; a total of 32,759 points). The data consist of 55 variables that are related

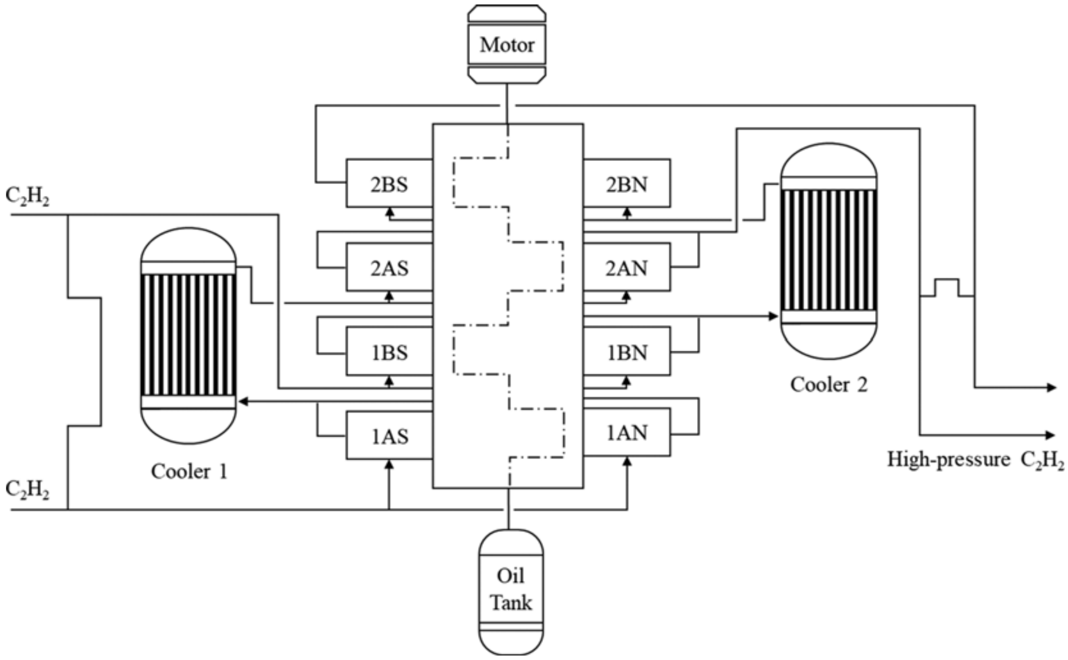

Fig. 2. Diagram of a hyper-compressor in LDPE manufacturing process.

Table 1. 55 Monitoring variables of the LDPE production process

Equipment	No.	Description
Hyper compressor	1-4	Cylinder suction temperature
	5-11	Cylinder discharge temperature
	12, 13	Cylinder suction pressure
	14-16	Cylinder discharge pressure
	17-23	Hyper frame bearing temperature
	24-27	Frame bearing temperature
	28	Frame oil tank pressure
	29	Frame oil leak gas temperature
	30	Cooling oil flowrate
	31	Frame oil end pressure
	32	Cooling oil end pressure
Booster compressor	33, 34	Suction temperature
	35-40	Discharge temperature
	41-42	Discharge pressure
Primary compressor	43-46	Suction temperature
	47-50	Discharge temperature
	51	Suction pressure
	52, 53	Discharge pressure
	54	Frame oil pressure
Booster/Primary	55	Booster/primary frame oil tank temperature

to hyper-compressor, booster compressor, and primary compressor (Table 1). Variables of the booster and primary compressor were included because they could affect the operation of the hyper-compressor.

During the four years of the operation of LDPE manufacturing process, five ESDs (Table 2) occurred. ESD is a type of SD. When

Table 2. The history of the ESD that occurred in the hyper-compressor

# of ESD	Start time (samples)	End time (samples)
1	12-09-09 04:30 (1,684)	12-09-10 14:30 (1,720)
2	13-03-31 00:00 (6,552)	13-03-31 21:00 (6,574)
3	13-11-14 03:30 (12,028)	13-11-15 08:00 (12,057)
4	13-12-26 06:30 (13,039)	13-12-26 23:30 (13,057)
5	15-04-23 08:30 (24,633)	15-04-23 21:30 (24,647)

the process anomaly is too severe to shut down the process properly, ESDs occur. The developed fault detection model is aimed at prognosing ESD since unexpected SD of a plant has a greater impact on profitability and process safety. The prognostic of ESD is defined as a process fault that occurs within a week ahead of the ESD.

4. Data Pretreatment and Fault Detection Procedure

The normal operation model should be established by normal operation data. However, we cannot distinguish between the normal and abnormal operation in the total data but SD history. Moreover, even if the SDs are removed, the abnormal behavior of the process may be imposed in the total data. So, the normal operation data should be extracted from the total operation data. To extract the normal data from the total data, we applied Tukey's outlier isolation method that uses the interquartile range (IQR) [20]. IQR is the distance between the lower and upper quartile. The lower quartile Q_1 is the middle value between the lower extreme value and the median. The second quartile Q_2 is the median. The third quartile Q_3 is the middle value between the median and the upper extreme value. This method is more robust than the outlier isolation method using z-score because it uses not the mean but median. The method is performed as follows:

(1) Calculate IQR as Q_3-Q_1.

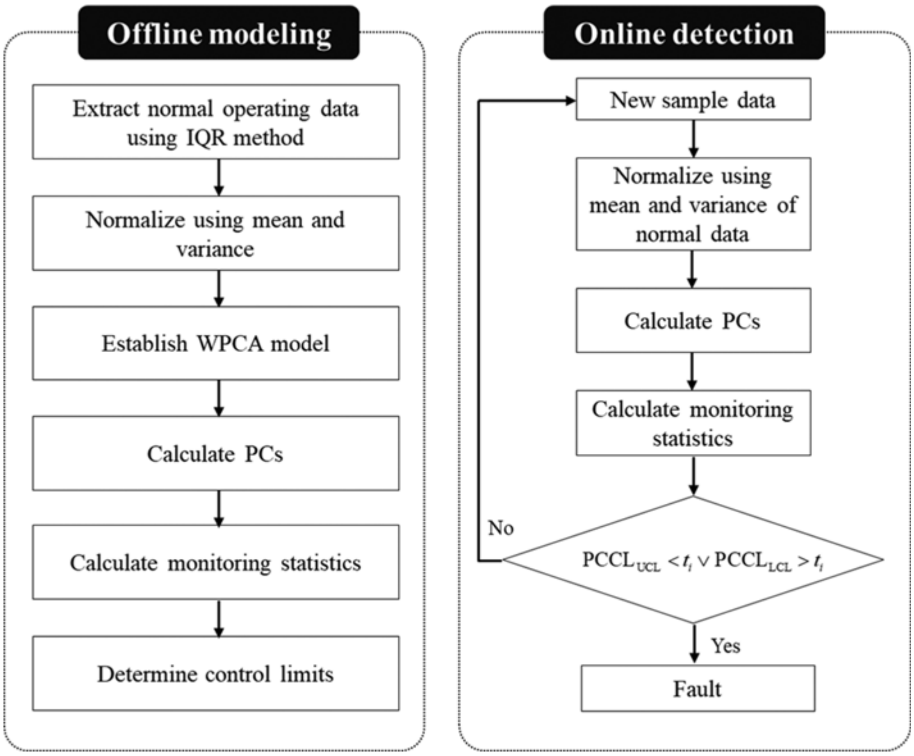

Fig. 3. Offline modeling and online detection procedure of using WPCA.

(2) Obtain fences using
Lower fences: $Q_1-(3.0\times IQR)$,
Upper fences: $Q_3+(3.0\times IQR)$.
(3) If a value violates the fences, remove the value.

The fault detection algorithm based on WPCA consists of offline modeling and online detection. We could establish the fault detection model through the offline modeling procedure and detect the process fault through the online detection procedure. In the offline modeling procedure (Fig. 3), the normal operating model was obtained by applying WPCA to the normal data extracted in the data pretreatment procedure. The confidence limits are determined using the KDE of T^2, SPE, and each PC in the normal operation model. In the online fault detection procedure (Fig. 3), the collected data is normalized using the mean and variance of the normal data, which were extracted by the data pretreatment. Then, by projecting the data onto the PC subspace, each PC can be calculated. We could identify the process fault if a PC exceeds the control limits obtained from the offline modeling procedure, otherwise perform the online detection procedure using a new sample data.

RESULTS

The fault detection model was established by applying WPCA to the 18,393 samples extracted from the total data using the IQR method. We used eight PCs as dominant PCs, which accounted for 80% of variances in the total variances. They were also used to calculate T^2 and SPE for a fair comparison and verifying the effectiveness of the proposed method. The control limits of PCs were set to 95%, and T^2 and SPE were also set to 95%. Then, the model was applied to determine whether it could detect five ESD by using PCCL. Initial analysis considered the effects of weighting factors α=[0.0 0.2 0.4 0.6 0.8 1.0] that adjusts the relative importance of

Table 3. ESD detection results using WPCA models with different weighting parameters α. O: successfully detection; X: detection failure

Monitoring method	α	ESD1	ESD2	ESD3	ESD4	ESD5	Detection rate (%)
T^2	0.0	O	X	X	O	O	60
	0.2	O	X	X	O	O	60
	0.4	X	X	X	X	X	0
	0.6	O	X	X	O	X	40
	0.8	O	X	X	O	X	40
	1.0	O	X	X	O	O	60
SPE	0.0	O	X	X	O	O	60
	0.2	O	X	X	O	O	60
	0.4	O	X	X	O	O	60
	0.6	O	X	X	O	O	60
	0.8	O	X	X	O	O	60
	1.0	O	X	X	O	O	60
PCCL	0.0	O	X	X	O	O	60
	0.2	O	X	O	O	O	80
	0.4	O	X	X	O	O	60
	0.6	**O**	**O**	**O**	**O**	**O**	**100**
	0.8	O	X	O	O	O	80
	1.0	O	X	X	O	O	60

PCA and SFA. When α=1.0 the model becomes the conventional PCA; the influence of SFA increases as α decreases. The proposed fault detection model shows better accuracy than the conventional PCA when SFA characteristic was added appropriately, not biased to either one of them. When the α is 0.6, the WPCA-based PCCL showed the best detection accuracy of 100%, whereas the conventional PCA and SFA approach with the T^2 or SPE statistic achieved only 60% detection rate, respectively (Table 3).

PCCL evaluates data more sensitively than T^2 and SPE because it monitors each PC. Therefore, the method identifies the process

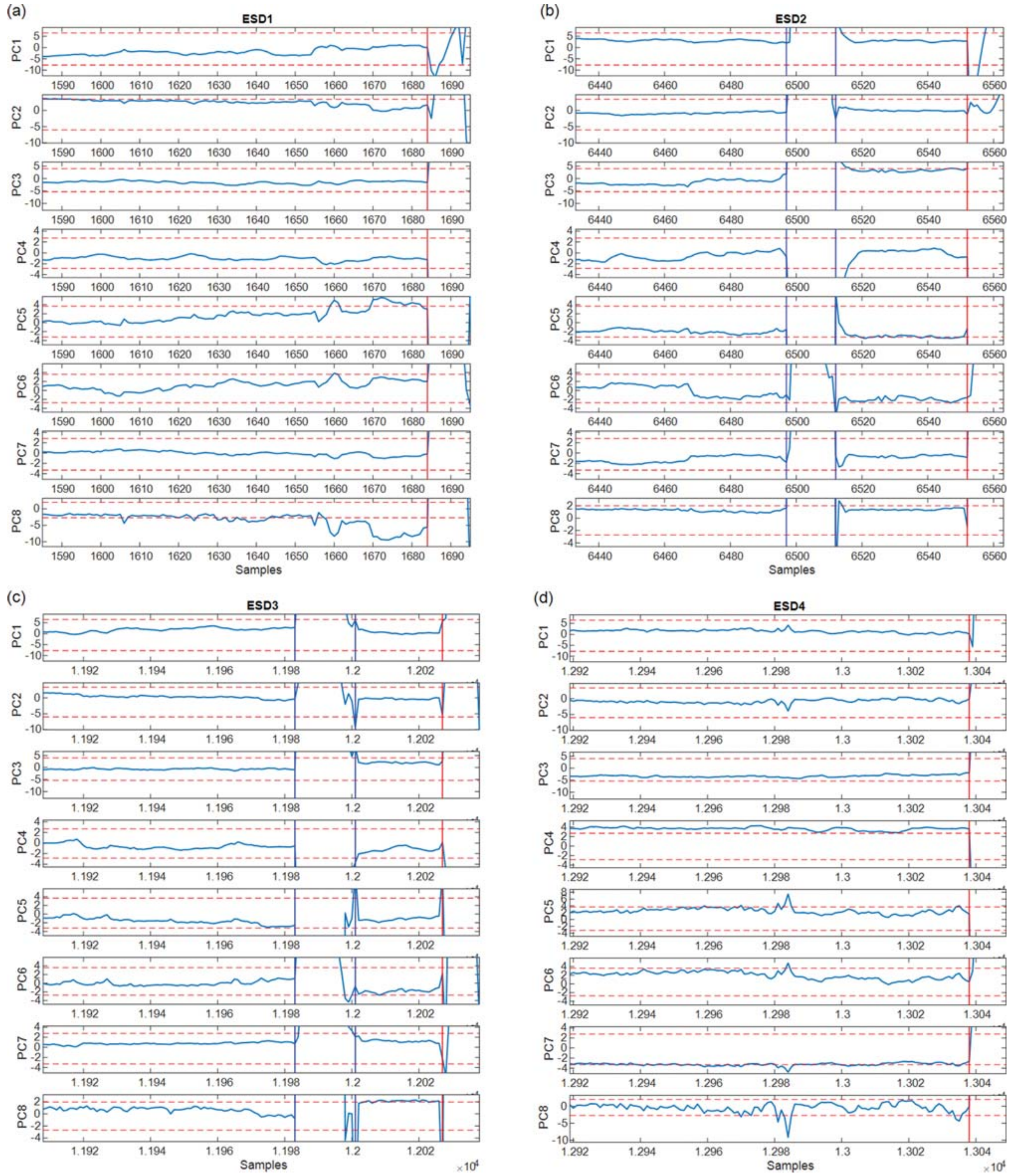

Fig. 4. PCCL monitoring charts of emergency first ESD case detected using WPCA when α=0.6. Vertical red solid line: ESD, vertical blue solid line: other SD, dashed red line: control limits of 95%. (a) first ESD. (b) second ESD. (c) third ESD. (d) fourth ESD. (e) fifth ESD.

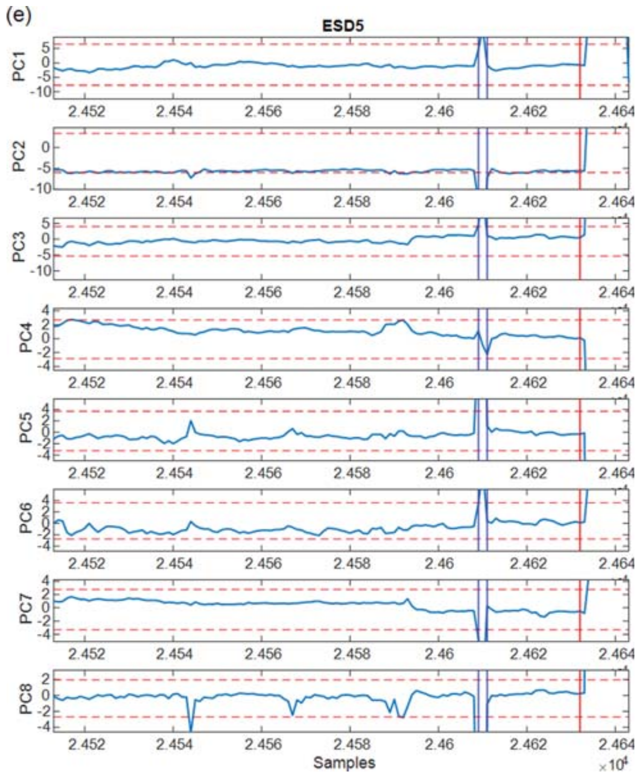

Fig. 4. Continued.

condition as faulty PCs of observation data that exceeds the control limits. In the first case of ESD, abnormal behavior was detected at the PC5 and 8 by the PCCL monitoring chart about 24 hours earlier before the ESD occurred (Fig. 4(a)). For the second ESD, The PC5 nearly exceeded the lower control limit after the SD (sample 6,497-6,512, Fig. 4(b)). This anomaly was not detected by conventional PCA and SFA-based method. An anomaly before the third

Table 4. PCs those have anomalies before the ESDs

	ESD 1	ESD 2	ESD 3	ESD 4	ESD 5
# of PCs	5, 8	5	8	5-8	2

ESD was also detected in the PC8 (Fig. 4(c)). The values of the PC8 nearly exceeded the upper control limit after the SD (sample 11,983-12,001). An anomaly that may cause the fourth ESD was found in the PC5-8 (Fig. 4(d)). These PCs 5, 6, and 8 showed peaks exceeded the control limits in sample 12987, which is 51 hours earlier than the ESD occurred. The PC7 was kept nearly exceeding the lower control limit after an SD (sample 12,679-12,701). This means that some variables of the process had abnormal values compared with the normal operating condition after the SD. An anomaly before the fifth ESD was detected in PC2 (Fig. 4(e)). The values in PC2 kept exceeding the lower control limit. This anomaly continued after the SD (sample 23,832-24,229).

The abnormal variables that may cause the anomalies can be identified using the projection vector because it is used to calculate PCs from the variables. Therefore, by finding the large values of each column of the loading vector, we could figure out which variables had a large effect on the PCs. In the five ESDs, the anomalies most frequently occurred in PC5 and 8 (Table 4). The fifth column of the loading vector, which was used to calculate PC5, showed that variable 18 (hyper frame bearing temperature of the hyper-compressor) and 45 (suction temperature of the primary compressor) were the most influential variables (Fig. 5). The eighth column of the loading vector showed that variable 35 and 38 (discharge temperature of the booster compressor) had a large effect on PC8. Therefore, those variables should be monitored more carefully than other variables.

CONCLUSION

The goal of this research was to detect the anomalies which may

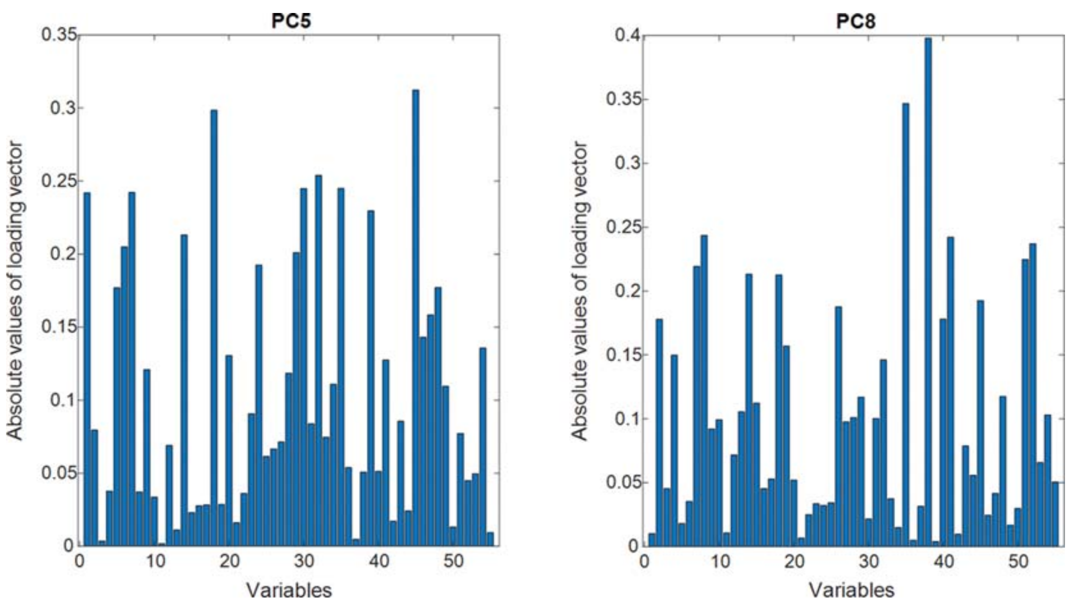

Fig. 5. Absolute values of loading vector for calculating PC5, and 8.

cause the ESD in advance by establishing a fault detection model of an LDPE manufacturing plant. The model was developed using plant operation data collected hourly for four years. The model considered 55 variables, including pressure and temperature of the first compressor, primary compressor, and hyper-compressors. The normal operation data were extracted from the operation data using the IQR method. Five ESD cases were analyzed using a WPCA-based PCCL model established using normal data. PCCL, which was used as monitoring statistics, showed better prediction accuracy than the T^2 and SPE statistics. The WPCA-based PCCL model with a weighting factor α of 0.6 showed the detection rate of 100%. The significance of this research is that we established a model to predict hyper-compressor faults and thereby increase the safety of process compared with the previous studies, which focused on reactor faults and the methods using PCA or SFA. Furthermore, it is expected to ensure the efficiency of replacing equipment, and productivity.

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