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Faulty Sensor Detection and Reconstruction for a PVC Making Process*

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Abstract Based on principal component analysis, this paper presents an application of faulty sensor detection and reconstruction in a batch process, polyvinylchloride (PVC) making process. To deal with inconsistency in process data, it is proposed to use the dynamic time warping technique to make the historical data synchronized first, then build a consistent multi-way principal component analysis model. Fault detection is carried out based on squared prediction error statistical control plot. By defining principal component subspace, residual subspace and sensor validity index, faulty sensor can be reconstructed and identified along the fault direction. Finally, application results are illustrated in detail by use of the real data of an industrial PVC making process.
Keywords multi-way principal component analysis, dynamic time warping, faulty sensor detection, faulty sensor reconstruction

1 INTRODUCTION

Chemical process is usually very complex. A large amount of measurements such as temperature, flowrate and pressure need to be monitored accurately. How to control and monitor such process efficiently is always an important issue and many researchers have paid extensive attention. Batch process, popular in chemical process, is very difficult to build model due to its complexity. Therefore, in recent years, statistical process control and fault diagnosis have been playing an important role in batch processes. Since the amount of information collected by distributed control system is abundant, this makes statistical process control become realizable.

Principal component analysis (PCA) is a typical statistical process control method and has been widely used in many areas. Some control charts such as M-Shewhart, M-CUSUM, M-EWMA have been shown very effective in detecting abnormalities in multivariate industrial equipments[1,2]. Contribution plot based fault identification methods have been proposed[3,4]. This approach uses a simple criterion when a fault is intrinsically related to the sensor measurement. Dunia *et al.* defined a sensor validity index (SVI) to identify sensor faults and proposed a unified geometric approach to process and sensor fault identification and reconstruction[5]. Fault detectability, reconstructability and identifiability were defined by Duina *et al.*[6]. Qin and Duina also defined the variance of reconstruction error (VRE) to select principal components (PCs) in PCA models[7]. In the reconstruction of faulty data, the minimal PCs can be obtained when the VRE reaches the minimum. Moreover, Duina and Qin defined various fault vector directions to distinguish different sensor faults, then fault identification and reconstruction can be completed based on the fault vector directions using PCA[8]. These methods have been shown effective for fault detection and reconstruction in chemical processes.

This paper presents some application results on faulty sensor detection and reconstruction in a polyvinylchloride (PVC) making process in a chemical plant in China. Multi-way principal component analysis (MPCA) and dynamic time warping (DTW) methods will be adopted. PVC making process is a very typical chemical batch process[9,10]. Owing to its complexity, monitoring and fault diagnosis are difficult for this process. Although many statistical methods for monitoring and fault diagnosis in batch process have been proposed, some practical problems remain to be resolved before the practical application. Multi-way PCA is a special kind of PCA method to decompose 3-D data into 2-D[11,12]. DTW, that has been widely used in phonetic recognition, also has the ability to reconcile inconsistent data[13]. In the PVC making process, inconsistent data always exist, since the chemical reaction time of each batch is usually different. In this paper, based on MPCA and DTW methods, a process statistical model for the PVC making process is built first, then some statis-

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tical indexes are calculated. They are projected onto the statistic model respectively, and faults can be detected based on PCA. Based on SVI, faulty sensor can be identified[8]. By defining the principal component subspace (PCS), residual subspace (RS) and fault direction, faulty data will be projected onto the two subspaces, and faulty sensors will be reconstructed along fault direction. After faulty sensor is replaced by the reconstructed sensor, the influences of faulty sensor will disappear, and the process will run normally again. These strategies are illustrated based on the real data from a PVC making process.

2 PVC BATCH POLYMERIZATION PROCESS

PVC is produced on a large scale by Shell in its plant in Liaoning province, China. The PVC polymerization process is shown in Fig. 1. Due to its inconsistency, traditional MPCA for fault detection and diagnosis has many problems. This paper combines DTW and MPCA technique to overcome these problems and makes PVC making process monitoring and fault diagnosis realizable.

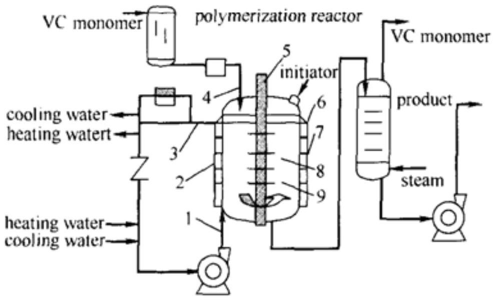


Figure 1 Flow diagram of the PVC polymerization process

Figure 1 shows the process flow diagram of PVC making process. The kernel is the polymerization reactor. The vinylchloride(VC) monomer is polymerized in aqueous suspension in the reactor. At different stage of reaction, the phases of product are different. There are three phases including water phase, liquid VC phase, and solid PVC phase. Firstly, water, VC, suspension of stabilizers and initiator are added into the reactor through different inlets. Then these materials are stirred so that suspension of VC droplets in water is obtained.

In the polymerization process, it is important that the temperature at different reaction stage in the reactor must be controlled to certain extent. Several temperature monitoring measurements are installed. In the 9 monitored variables, temperature variables occupy 5 (see Table 1). At the beginning of reaction, the heating water is pumped into the jacket of reactor to heat the reactor content to the set temperature(57℃). The heating continues until the polymerization reaction generates sufficient heat by itself. PVC is insoluble in water and only weakly soluble in VC, so it will precipitate quickly, forming a solid PVC phase inside the VC monomer droplets. The polymerization takes place in the PVC phase and in the monomer phase.

During the polymerization, the temperature in reactor will increase. A lot of heat has to be withdrawn from the process since the polymerization reaction is highly exothermic. The cooling water will be pumped into the jacket to make temperature decrease. The excess of heat is withdrawn by the cooling jacket surrounding the reactor, and by condensing monomer vapor to liquid in a condenser on top of the reactor. When the temperature is lower than set point, the heating water is pumped. This process is repeated. After a period of polymerization, the monomer phase is nolonger present and all remaining VC is present in the gas phase or in the polymer phase. The polymerization continues and VC is absorbed from the gas phase, resulting in a decreasing pressure. The polymerization is finally stopped by adding a killing agent.

In this process, some key variable parameters are measured accurately by distributed control system. Fig. 1 shows the location of the variables, and they are also listed in Table 1.

3 FAULTY SENSOR DETECTION AND RECONSTRUCTION

The proposed procedure of faulty sensor detection and reconstruction for PVC production is showed in Fig. 2.

Table 1 Polymerization reactor variables

Variable No.	Sensor No.	Variable name	Unit
1	TIC-P101	temperature of the reactor	℃
2	TIC-P102	temperature of the reactor jacket inlet	℃
3	TI-P107	temperature of water inlet	℃
4	TI-P108	temperature of baffle outlet	℃
5	TI-P109	temperature of the reactor Jacket outlet	℃
6	PIC-P102	pressure of the reactor	MPa
7	FIC-P101	flow rate of baffle water	$m^3 \cdot h^{-1}$
8	FIC-P102	flow rate of jacket water	$m^3 \cdot h^{-1}$
9	JI-P101	stirring power	kW

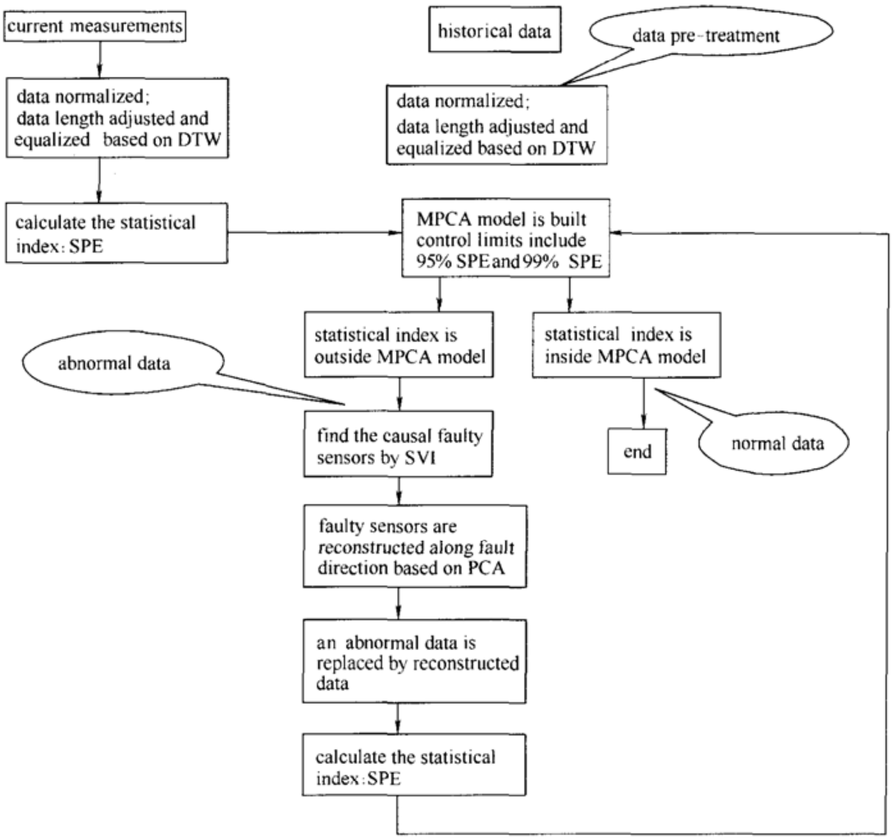


Figure 2 Procedure of faulty sensor detection and reconstruction

In Fig. 2, the historical normal data are used to set up the MPCA model. Data pre-treatment includes scaling and synchronization, where the DTW is introduced to synchronize batch trajectories that may have different data length. The pre-treated data are used to build MPCA model. By projecting the current data onto the MPCA model, faults can be detected. Based on the SVI, the faulty sensor can be isolated from normal sensors. Along the fault direction, the faulty sensor can be reconstructed according to other normal sensor data. Then the faulty sensor data is replaced by the reconstructed data, and are mapped onto MPCA model again. In the end, there is no fault in the process, which illustrates the reconstruction is successful. This procedure will be explained in detail below.

3.1 Synchronization of batch trajectories based on DTW

DTW is a dynamic-programming-based technique, and has been used in the area of speech recognition for the recognition of isolated and connected words[14–16]. Two modes can be reconciled by DTW and similarly two trajectories can be synchronized based on DTW[17,18].

Consider two trajectories of $\boldsymbol{T}$ and $\boldsymbol{R}$, their durations are not same. $\boldsymbol{T}$ is a $t \times n$ matrix, and $\boldsymbol{R}$ is a $r \times n$ matrix. t is the number of observations of $\boldsymbol{T}$, and r is the number of observations of $\boldsymbol{R}$, n is the number of measured variables. DTW can extract the features in the two trajectories and extend or compress some of them, and it is based on the distance between two trajectories[19].

There are different definitions of distance between two trajectories. The local distance is

$$\begin{aligned} &d[i(k), j(k)] = \{\boldsymbol{T}[i(k), :] - \boldsymbol{R}[j(k), :]\}\cdot \\ &\boldsymbol{W}\{T[i(k), :] - \boldsymbol{R}[j(k), :)]\}^T, \\ &k = 1, \cdots, K \end{aligned} \tag{1}$$

where $\boldsymbol{W}$ is a positive definite weighting matrix that reflects the relative importance of each measured variables. $i(k)$ and $j(k)$ are two indexes in the new common frame of the observations $\boldsymbol{T}$ and $\boldsymbol{R}$, respectively. k is the time index in the new frame. The normalized total distance is

$$D^*(\boldsymbol{t}, \boldsymbol{r}) = \frac{1}{\sum\limits_{1}^{k} N(k)} \min_{\mathrm{F}} \left\{ \sum_{k=1}^{K} d[i(k), j(k)] w(k) \right\} \tag{2}$$

where $w(k)$ is a nonnegative weighting function for $d[i(k), j(k)]$; $N(k)$ is the standard factor of $w(k)$[17].

Based on the minimal distance in Eq. (2), the optimal path F^* can be obtained

$$F^* = \arg\min_{\mathrm{F}}[D^*(\boldsymbol{t}, \boldsymbol{r})] \tag{3}$$

Based on the optimal path, synchronization of trajectories can be completed. DTW provides a new way to synchronization of trajectories, to make batch trajectories be consistent and provide reliable data for faulty sensor detection and reconstruction in batch processes.

3.2 Fault detection based on MPCA using DTW

Since batch process data are of three dimensions in batch process, conventional PCA can not be applied directly to such processes[12]. To this end, one has proposed multi-way PCA, which can decompose a 3-D array into a 2-D matrix, and the translated 2-D data can be modeled by the conventional PCA method[2,4,11,20].

PCA is an effective data analysis tool. The original data matrix, $\boldsymbol{X}$, can be discomposed as a sum of the products of scores and loadings for each column in the model (T_p and P_p) and the array of residual errors $\boldsymbol{E}$

$$\boldsymbol{X} = T_1 \otimes P_1 + T_2 \otimes P_2 + \cdots + T_p \otimes P_p + \boldsymbol{E} \tag{4}$$

where $\otimes$ denotes the Kronecker product, p is the number of principal component. $\boldsymbol{X}$ is composed of score vectors, loading matrices and residual matrix $\boldsymbol{E}$. In other words, the measurement space can be decomposed into principal subspace and residual subspace.

Due to the characteristic of batch process, some process trajectories have distinct time duration from batch to batch. Not only modeling but also diagnosing batch process need consistent data trajectories based on MPCA. For this purpose, a new approach that can make some data from different batches to be consistent based on DTW firstly, then build MPCA model based on these new consistent batch trajectories, make new batch trajectories to be disposed based on DTW and project them onto the MPCA model for monitoring and fault diagnosis.

Some data come from an industrial real PVC making processes is used for modeling and fault diagnosis based on MPCA. If I batches of normal data are used for model, it is firstly necessary to make all data have the same duration based on DTW. An important thing is how to choose a reference trajectory and then make others to match it. Usually the average trajectory will be a reasonable choice. But all the raw data are not of the same duration and it is impossible to get the average. Normal method is to select one trajectory from the I batches of data freely, and synchronize other I-1 batches to this particular one using DTW. As a result, I batches will have the same duration. Then the average of I trajectories is defined to be the reference trajectory. The whole procedure will be repeated to make every trajectory be synchronized with the reference one.

MPCA model should be built that includes 95% SPE limit and 99% SPE limit[1,11]. Usually they are called statistic control limits, and these indexes can be used for fault detection. The SPE of the model captures what is not explained by the calibration model, thus it provides better understanding of unanticipated changes in the process. MPCA model can be built only if the duration of all batches is equal. Therefore, consistent MPCA model is built after using DTW to synchronize all batch trajectories.

By projecting new batch data onto a MPCA model, fault will be detected. The detailed applications are shown in Section 4.

3.3 Faulty sensor reconstruction based on PCA

According to Eq. (4), $\boldsymbol{X}$ can be decomposed into two parts:

$$\boldsymbol{X} = \boldsymbol{T}\boldsymbol{P}^{\mathrm{T}} + \boldsymbol{E} \tag{5}$$

where $\boldsymbol{T}$ is the principal component matrix, $\boldsymbol{P}$ is the loading matrix. Eq. (5) can be rewritten as

$$\boldsymbol{X} = \widehat{\boldsymbol{X}} + \widetilde{\boldsymbol{X}} \tag{6}$$

in which the projection on principal component subspace is

$$\widehat{\boldsymbol{X}} = \boldsymbol{P}\boldsymbol{P}^{\mathrm{T}}\boldsymbol{X} = \boldsymbol{C}\boldsymbol{X} \tag{7}$$

and the projection on residual subspace:

$$\widetilde{\boldsymbol{X}} = (\boldsymbol{I} - \boldsymbol{P}\boldsymbol{P}^{\mathrm{T}})\boldsymbol{X} = (\boldsymbol{I} - \boldsymbol{C})\boldsymbol{X} = \widetilde{\boldsymbol{C}}\boldsymbol{X} \tag{8}$$

Assuming that the new sample data are detected by squared prediction error (SPE) plot to be faulty, the faulty sensor can be isolated by applying the SVI. The SVI is defined for sensor fault identification as Refs. [5,6,8]:

$$\eta_i = \frac{SPE_i}{SPE}$$

where η_i is the SVI of reconstruction along fault direction i. If η_i is close to 0, variable i is just faulty variable. Otherwise η_i is close to 1.

Faulty sensor reconstruction is that the corrupted data are reconstructed along the direction of the fault. The reconstructed data are as close as to the normal data, and make the process return normal state from abnormal state[5-7].

Assuming that the normal data is $\boldsymbol{x}^n$, and the corrupted sample data is $\boldsymbol{x}$, the reconstructed data is $\boldsymbol{x}_i$. The corrupted data $\boldsymbol{x}$ is the sum of normal data $\boldsymbol{x}^n$ and the faulty data $\boldsymbol{x}_f$:

$$\boldsymbol{x} = \boldsymbol{x}^n + \boldsymbol{x}_f \tag{9}$$

$$\boldsymbol{x}_f = \beta \Xi_i \tag{10}$$

Here β is the magnitude of fault i, Ξ_i is the direction vector of fault i.

$$\Xi_i = [0, 0, \cdots, 1, \cdots, 0, 0]^{\mathrm{T}} \tag{11}$$

in which the ith element is 1, and others are 0. The reconstructed data is given by

$$\boldsymbol{x}_i = \boldsymbol{x} - \beta_i \Xi_i \tag{12}$$

If the reconstructed data is projected onto the MPCA model, the statistics of the process outputs will go back to normal statistical regions[5-7].

4 APPLICATION TO PVC MAKING PROCESS

4.1 Data pre-treatment

Data from different batches in the PVC making process (in a large Shell plant in Liaoning province, China) have different time durations. Usually the duration of one batch is about 4 h and 10 min. The sampling interval is 5 s, so the average data length is about 3000 for a batch. 50 normal batches are used for modeling, and their average length is just 3000.

Data scaling is carried out at first, *i.e.*, the data matrix for each batch is normalized, so that it has zero-mean, and unity variance[20]. One batch trajectory is shown in Fig. 3, where there are 10 variables in it. 9 variables are shown in Table 1, and the other one is the set temperature in the reactor, it is a constant (57℃) and is scaled to be 0.

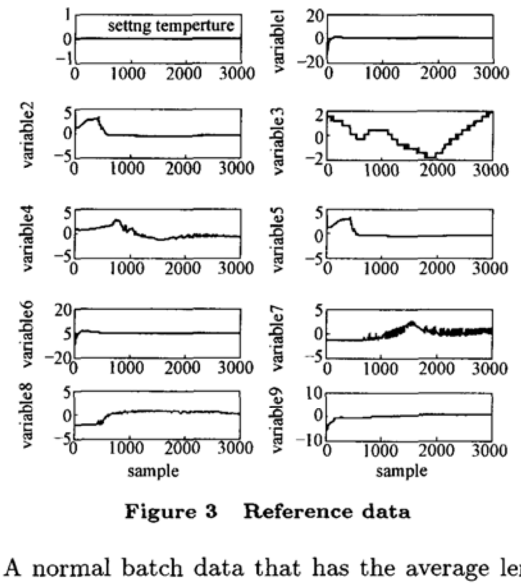


Figure 3 Reference data

A normal batch data that has the average length is defined as the selected data matrix, and its length is 3000. The other 49 batches are synchronized with the selected data matrix by the DTW technique. Synchronized data is denoted by $\boldsymbol{X}$ $(50 \times 3000 \times 9)$. Then the 50 batches trajectories are averaged, and the averaged trajectory is called the reference trajectory in DTW (see Fig. 3). 50 batches data are synchronized with the reference trajectory respectively. The consistent MPCA model can be built based on the 50 batches that have been synchronized to have the same duration. Faults can be detected based on the consistent MPCA model and faulty sensor can be reconstructed in the polymerization reaction process.

Now take one batch data as an example, it is shown in Fig. 4. Based on Section 3.1, the data matrix in Fig. 4 will be matched onto the reference trajectory with fixed length 3000 using DTW. The optimal path is shown in Fig. 5.

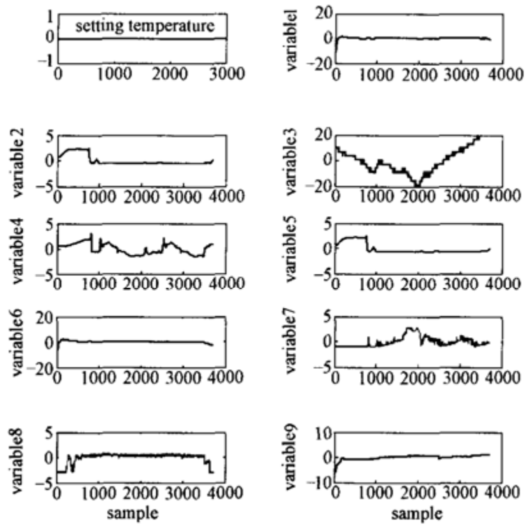


Figure 4 Original data

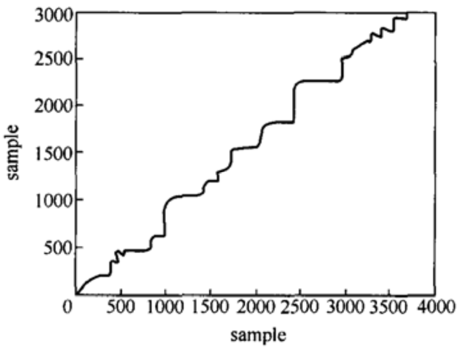


Figure 5 Optimal path

Figure 5 shows the optimal path of synchronization between two trajectories $(3704 \times 9$ and $3000 \times 9)$ based on DTW, which interprets the process of synchronization between two batches. As are shown in Figs. 3 and 4, two batch trajectories $(3704 \times 9$ and $3000 \times 9)$ are projected onto the common time index frame respectively, and the optimal path is obtained firstly in Fig. 5. This process is called symmetric DTW. Then the original trajectories (3704×9) in Fig. 4 will match the reference trajectories (3000×9) in Fig. 3. This process is called asymmetric DTW, and new trajectories (3000×9) in Fig. 6 are obtained, the new trajectories contain all important information in old one (3704×9).

50 batches data will be synchronized with reference trajectory respectively. Then MPCA model will

be built based on the 50 normal batches that have the same duration 3000.

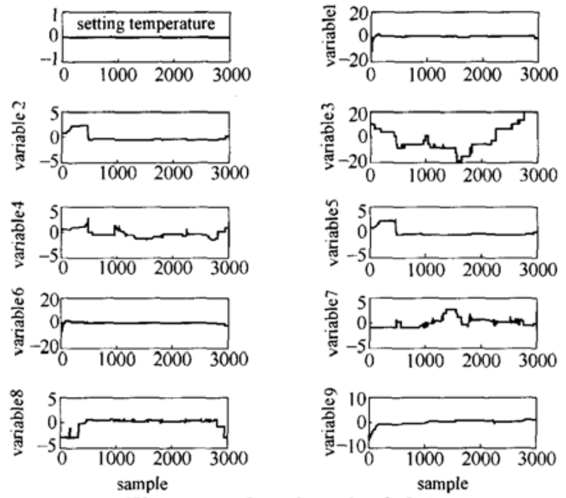


Figure 6 Synchronized data

4.2 Fault detection

Figure 7 shows a new batch data that has 9 variables (3049×9). It has been synchronized with reference trajectories. The SPE of this new batch is calculated and projected onto 99% SPE and 95%SPE model(see Fig. 8). This model is just the consistent MPCA model built in Section 4.1. It is obvious that data before 1500 are inside the control limits, but after 1500, some samples are outside the control limits. This illustrates that sensor faults occur after 1500.

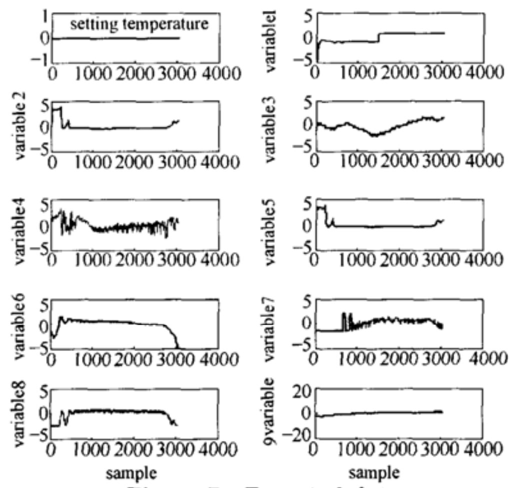


Figure 7 Detected data

4.3 Fault reconstruction

Now, we need to isolate the faulty sensors, the SVI will be used for fault identification. After fault occurs, all variables are reconstructed along their own fault directions as

$$\Xi_1 = [1,0,0,0,0,0,0,0,0]$$
$$\Xi_2 = [0,1,0,0,0,0,0,0,0]$$
$$\vdots$$
$$\Xi_9 = [0,0,0,0,0,0,0,0,1]$$

If the faulty sensor is reconstructed, the SPE in fault direction will decreases apparently. Thus, every sensor output is reconstructed along its fault direction, and all SVIs are calculated based on the reconstructed sensors. The sensor corresponding to the minimal SVI is just the faulty one. Fig. 9 shows the fault identification results. All SVIs are given at 1502 and 2000, respectively. The minimal SVI is obtained in sensor 1, and one's reconstruction along direction $\Xi_1 = [1,0,0,0,0,0,0,0,0]$. So sensor 1 is isolated to be faulty, *i.e.*, the sensor for temperature of the reactor (TIC-P101) is faulty. In Fig. 10, the SVI of reconstruction along sensor 1 direction is close to 1 before 1500, and close to 0 after 1500, this also shows that the fault is originated from sensor 1.

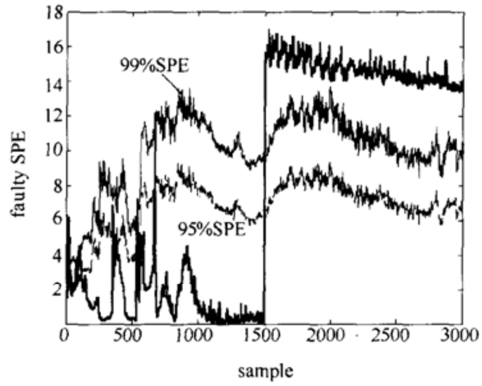


Figure 8 Fault detection based on SPE

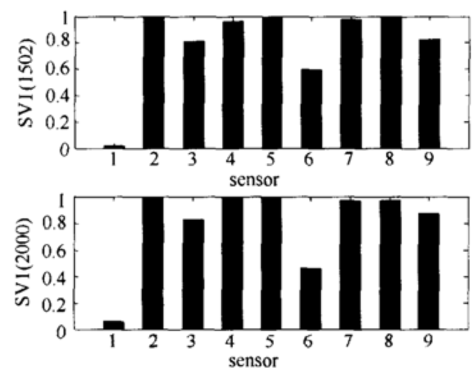


Figure 9 Fault identification based on SVI

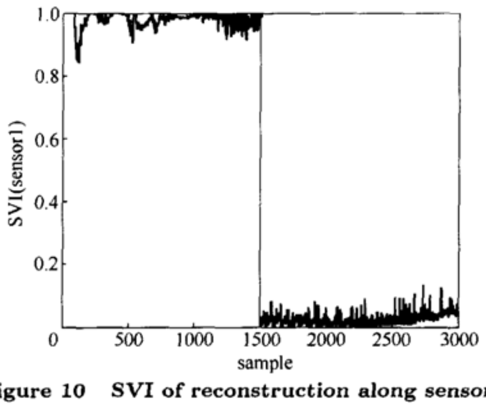
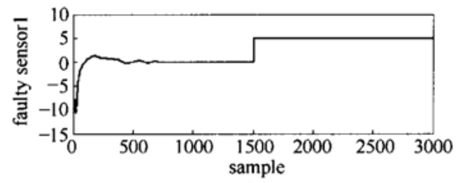
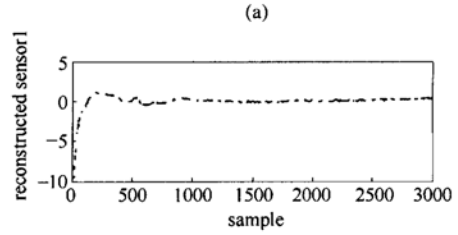


Figure 10 SVI of reconstruction along sensor 1

Figure 11 (a) shows the output of faulty sensor 1, and Fig. 11 (b) reconstructs sensor 1 output. After the faulty data is replaced by its reconstructed one, the SPE of reconstructed one will be inside 99% SPE and 95% SPE limits(see Fig. 12), which shows that the reconstruction is successful. Our next work will focus on fault identification for batch processes with non-stationary process noise and earlier identification of faulty sensors from the online data from the ongoing batch processes.



(a)



(b)

Figure 11 Faulty sensor1 reconstruction

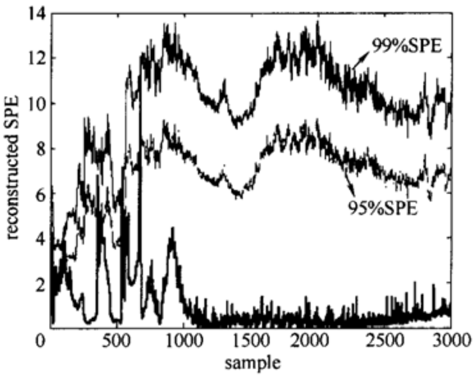


Figure 12 SPE after reconstruction

5 CONCLUSIONS

The results of application on faulty sensor detection and reconstruction for a PVC making process are presented in this paper, in which the DTW technique plays an important role to make the batch process data synchronized. Although DTW was originally proposed for speech recognition, it shows valid in the synchronization of batch trajectories. Fault detection is carried out based on consistent MPCA using DTW. By calculating the SVIs of sensor outputs, faulty sensor can be identified, the SPE of the reconstructed data will decrease significantly in fault direction. After faulty sensors are reconstructed along fault direction, the process will run normally again.

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