



# A particle filter driven dynamic Gaussian mixture model approach for complex process monitoring and fault diagnosis

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## ABSTRACT

Complex non-Gaussian processes may have dynamic operation scenario shifts so that the conventional monitoring methods become ill-suited. In this article, a new particle filter based dynamic Gaussian mixture model (DGMM) is developed by adopting particle filter re-sampling method to update the mixture model parameters in a dynamic fashion. Then the particle filtered Bayesian inference probability index is established for process fault detection. Furthermore, the particle filtered Bayesian inference contributions are decomposed among different process variables for fault diagnosis. The proposed DGMM monitoring approach is applied to the Tennessee Eastman Chemical process with dynamic mode changes and the results show its superiority to the dynamic principal component analysis (DPCA) and regular Gaussian mixture model (GMM) in terms of fault detection and diagnosis accuracy.

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## 1. Introduction

Industrial process monitoring is essential to safeguard process operation, ensure product quality and improve manufacturing profit [1–3]. Over the past two decades, multivariate statistical process monitoring (MSPM) methods have been widely applied to various kinds of industrial processes with some successes [4–13]. The most well-known MSPM techniques include principal component analysis (PCA) and partial least squares (PLS) [4,14,15]. To handle the process nonlinearity and dynamics, the kernel principal component analysis (KPCA) and dynamic principal component analysis (DPCA) are further developed in literature [16,17,21]. The monitoring statistics of PCA/PLS methods require the process data to follow multivariate Gaussian distribution approximately in order for their confidence limits to become valid. In practice, however, the normal process data often follow non-Gaussian distribution so that the traditional PCA/PLS monitoring approaches become inappropriate [18,19].

More recently, different types of non-Gaussian process monitoring techniques such as independent component analysis (ICA) and Gaussian mixture model (GMM) have been developed and applied to complex chemical process monitoring [20–26]. The ICA method takes into account the higher-order statistics in order to extract the non-Gaussian features from process data. The industrial

processes are often characterized by shifting operation conditions or strategies so that the data shows strong multimodality [27]. In such situations, the objective function of negentropy used in ICA does not necessarily capture the multi-Gaussianity in multimode process data. Though the GMM based monitoring approach can nicely handle the multi-Gaussianity, it assumes that the multiple operating conditions and their corresponding prior probabilities remain unchanged throughout the entire plant operation. The potential issue may arise when the collected training data are not representative of all the possible operation scenarios in the plant or the operation mode shifts have strong transient behavior.

To tackle this challenge, a new particle filter driven dynamic Gaussian mixture model (DGMM) approach is proposed to monitor complex non-Gaussian processes with dynamic operation scenario changes. The initial Gaussian mixture model is first estimated by the modified Expectation–Maximization (E–M) algorithm. Then the particle filter is adopted to dynamically update the mixture model parameters and the time-varying operation scenarios in processes. The particle filtered Bayesian inference statistics are then developed from the dynamic Gaussian mixture model method and used to detect the abnormal operation events in the processes. Furthermore, the particle filtered Bayesian inferential contributions are derived to diagnose the process faults and identify the faulty variables with abnormal behaviors. The utility of the present DGMM monitoring approach is demonstrated through the application example of Tennessee Eastman process (TEP) with operating scenario changes and the monitoring results are compared to those of DPCA and GMM methods.

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The organization of the paper is as follows. The regular Gaussian mixture model is briefly reviewed in Section 2. Then the particle filter based dynamic Gaussian mixture model along with the new DGMM based fault detection and diagnosis approach is developed in Section 3. In Section 4, the performance of the DGMM based monitoring approach is demonstrated through the Tennessee Eastman Chemical process example. The fault detection and diagnosis results of the proposed approach are compared to those of the DPCA and GMM methods. Conclusions are given in Section 5.

## 2. Preliminaries

The multiple operating modes in normal process can be characterized by different Gaussian components in GMM and the prior probability of each Gaussian component represents the possibility when the process runs at each particular operating condition. The probability density function of Gaussian mixture model is equivalent to the weighted sum of the density functions of all Gaussian components as given below

$$p(y|\Lambda) = \sum_{i=1}^K \beta_i g(y|\lambda_i) \quad (1)$$

where  $y$  is a  $l$ -dimensional measurement sample,  $\beta_i$  denotes the prior probability of the  $i$ th Gaussian component and  $g(y|\lambda_i)$  is the multivariate Gaussian density function of the  $i$ th component. For each component, the model parameters to be estimated are  $\beta_i$  and  $\lambda_i = \{\mu_i, \Sigma_i\}$ , the latter of which include the mean vector  $\mu_i$  and covariance matrix  $\Sigma_i$ . During the model learning, the following log-likelihood function is used as objective function to estimate the parameter values

$$\log L(y|\Lambda) = \sum_{j=1}^N \log \left( \sum_{i=1}^K \beta_i g(y_j|\lambda_i) \right) \quad (2)$$

where  $y_j$  is the  $j$ th training sample among the total  $N$  measurements.

The static Gaussian mixture model can be estimated by the modified E–M algorithm through the following iterative procedure:

- E-step: compute the posterior probability of the  $j$ th training sample  $y_j$  at the  $s$ th iteration

$$p^{(s)}(C_i|y_j) = \frac{\beta_i^{(s)} g(y_j|\lambda_i^{(s)})}{\sum_{l=1}^K \beta_l^{(s)} g(y_j|\lambda_l^{(s)})} \quad (3)$$

where  $C_i$  denotes the  $i$ th Gaussian component and the Gaussian density function  $g(y_j|\lambda_i^{(s)})$  is given by

$$g(y_j|\lambda_i^{(s)}) = \frac{1}{(2\pi)^{l/2} |\Sigma_i^{(s)}|^{1/2}} \exp \left[ -\frac{1}{2} (y_j - \mu_i^{(s)})^T (\Sigma_i^{(s)})^{-1} (y_j - \mu_i^{(s)}) \right]$$

- M-step: update the model parameters at the  $(s+1)$ th iteration

$$\mu_i^{(s+1)} = \frac{\sum_{j=1}^N p^{(s)}(C_i|y_j) y_j}{\sum_{j=1}^N p^{(s)}(C_i|y_j)} \quad (4)$$

$$\Sigma_i^{(s+1)} = \frac{\sum_{j=1}^N p^{(s)}(C_i|y_j) (y_j - \mu_i^{(s+1)}) (y_j - \mu_i^{(s+1)})^T}{\sum_{j=1}^N p^{(s)}(C_i|y_j)} \quad (5)$$

$$\beta_i^{(s+1)} = \frac{\sum_{j=1}^N p^{(s)}(C_i|y_j)}{N} \quad (6)$$

It should be noted that the initial parameter values can be selected through an initial guess based on user's prior knowledge or may

be estimated from the  $K$ -means algorithm. Through the iterative procedure in the EM algorithm, the final parameter values of different Gaussian components can converge to the actual values.

To overcome the drawback of traditional E–M algorithm, the minimum message length (MML) criterion is used as model selection index to search for the optimal number of Gaussian components [28].

## 3. Dynamic Gaussian mixture model based process monitoring method

### 3.1. Particle filter based dynamic Gaussian mixture model

Though GMM can be used to characterize the multiple operating conditions or steady states in processes, it assumes the fixed mixture model structure and parameter values throughout the entire operation. Therefore, the regular GMM lacks strong capability of handling dynamic mode changes such as new operating conditions in process and significantly transient behavior during mode shifts. However, as the operation scenario may change over time and the transient behavior can occur between different modes, the Gaussian components and the corresponding model parameters need to be updated dynamically so that the operating trajectory can be precisely captured.

Kalman filter, as a popular technique, can be used to estimate state transitions in linear dynamical systems [29]. Nevertheless, the conventional Kalman filter is based upon the assumption that the posterior density functions of state variables at each step are Gaussian approximately. In practice, the multiple operating modes usually lead to non-Gaussian states and thus the Kalman filter approach may not be appropriate for describing the dynamics of multi-mode operation. Particle filter is a sequential model estimation technique and suitable for dynamic processes with non-Gaussian state-space latent variables [30]. In this study, particle filter is adopted to re-evaluate the initial model parameters of Gaussian components and then update the mixture model for mode transitions and dynamic changes.

Let  $\{x_t^{(i)}, \omega_t^{(i)}\}_{i=1}^P$  be a random measure to determine the posterior density function  $p(x_t|y_t)$  as follows

$$p(x_{0:t}|y_{1:t}) = \sum_{i=1}^P \omega_t^{(i)} \delta(x_{0:t} - x_{0:t}^{(i)}) \quad (7)$$

where  $P$  is the number of the defined particle samples,  $x_t^{(i)}$  is a particle sample and  $\delta(\cdot)$  stands for the Dirac delta function. Moreover,  $x_{0:t} = \{x_j\}$  with  $j=0, 1, \dots, t$  represents the set of process state sequence up to the sampling time  $t$ ,  $y_{1:t} = \{y_j\}$  with  $j=1, 2, \dots, t$  denote the set of process measurements up to the sampling time  $t$ , and  $x_{0:t}^{(i)} = \{x_j^{(i)}\}$  with  $i=1, 2, \dots, P; j=1, 2, \dots, t$  are the set of particle samples up to the sampling time  $t$ . Suppose that the particle samples  $x_t^{(i)}$  ( $1 \leq i \leq P$ ) are drawn from an importance density  $q(x_t|x_{t-1}^{(i)}, y_t)$  [31]. It can be selected by minimizing the variance of the particle weights so that the importance density equals the prior probability as

$$q(x_t|x_{t-1}^{(i)}, y_t) = p(x_t|x_{t-1}^{(i)})$$

Meanwhile, the measurement samples  $y_t$  come from the estimated Gaussian mixture density function  $P(y_t|\Lambda) = \sum_{i=1}^K \beta_i g(y_t|\lambda_i)$ . The corresponding weights of the particle samples is recursively updated as follows

$$\omega_t^{(i)} = \omega_{t-1}^{(i)} \frac{p(y_t|x_t^{(i)})p(x_t^{(i)}|x_{t-1}^{(i)})}{q(x_t^{(i)}|x_{t-1}^{(i)}, y_{1:t})} \quad (8)$$

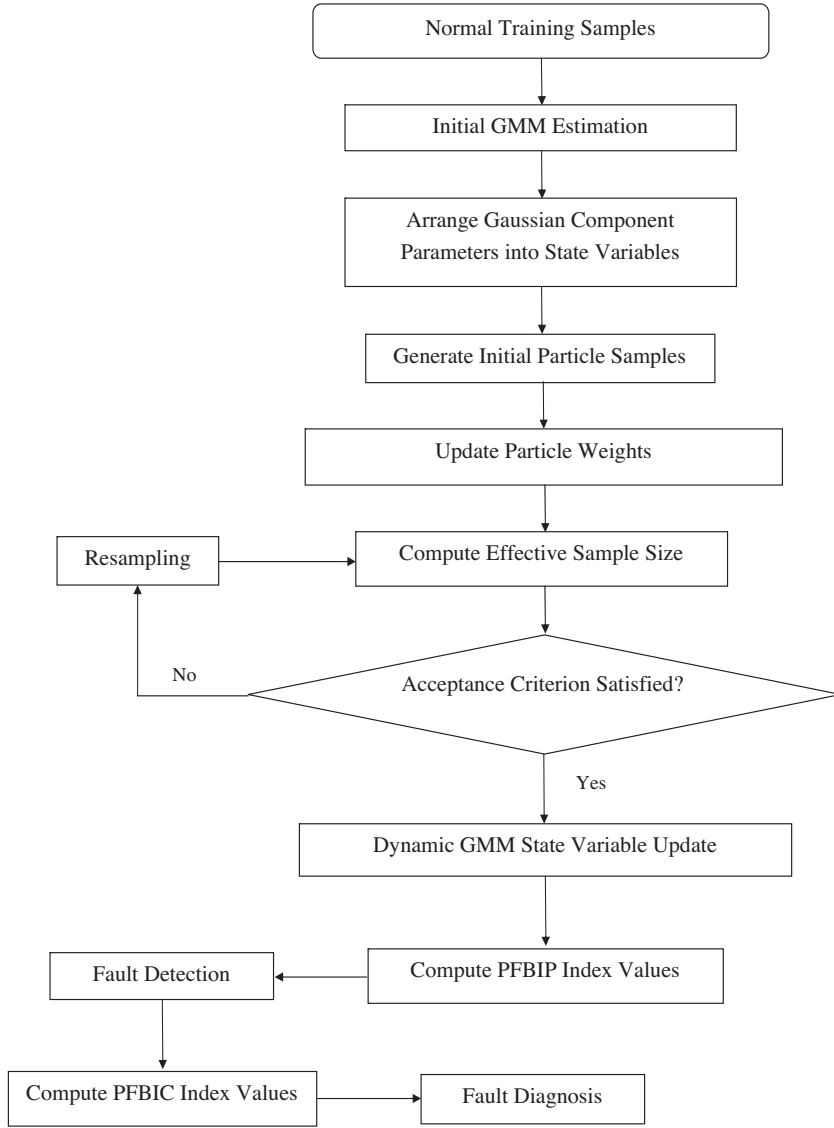


Fig. 1. Flow diagram of particle filter driven dynamic Gaussian mixture model based fault detection and diagnosis approach.

Since the importance density normally depends on the current instead of the past measurements, then we have

$$q(x_t^{(i)} | x_{t-1}^{(i)}, y_{1:t}) = q(x_t^{(i)} | x_{t-1}^{(i)}, y_t) = p(x_t^{(i)} | x_{t-1}^{(i)})$$

Thus Eq. (8) can be approximated as

$$\omega_t^{(i)} = \omega_{t-1}^{(i)} p(y_t | x_t^{(i)}) \quad (9)$$

Here the likelihood  $p(y_t | x_t^{(i)})$  can be estimated from the observations and the generated particle samples. The obtained weights are then normalized as

$$\bar{\omega}_t^{(i)} = \frac{\omega_{t-1}^{(i)}}{\sum_{i=1}^P \omega_{t-1}^{(i)}} \quad (10)$$

The posterior filtered density is approximated as

$$p(x_t | y_{1:t}) = \sum_{i=1}^P \bar{\omega}_t^{(i)} \delta(x_t - x_t^{(i)}) \quad (11)$$

To measure the degeneracy of particle filter, the effective sample size  $\hat{N}_{eff}$  is estimated from the following [30]

$$\hat{N}_{eff} = \frac{1}{\sum_{i=1}^P (\bar{\omega}_t^{(i)})^2} \quad (12)$$

If the estimated  $\hat{N}_{eff}$  value is below a pre-defined threshold value  $N_T$ , then the re-sampling procedure is carried out. Otherwise, the samples are accepted with the probability

$$p_a = \min \left\{ 1, \frac{\bar{\omega}_t^{(i)}}{N_T} \right\} \quad (13)$$

Typically the threshold value is set to  $N_T = P/2$  and the weights of accepted samples are updated to

$$\hat{\omega}_t^{(i)} = \min \left\{ 1, \frac{\bar{\omega}_t^{(i)}}{N_T} \right\} \quad (14)$$

For a non-Gaussian dynamic system, the corresponding state space model is written as

$$x_t = f_t(x_{t-1}, \omega_{t-1}) + \epsilon_t \quad (15)$$

and

$$y_t = L_t x_t + \theta_t \quad (16)$$

where  $f_t$  is a nonlinear function,  $L_t$  denotes the state matrix, and  $\epsilon_t$  and  $\theta_t$  represent the independently and identically distributed process and measurement noise sequences. It is noted that the explicit function of  $f_t$  is not needed in the numerical computations of DGMM method. The state variable can be updated from particle filter as

$$\hat{x}_t = \sum_{i=1}^P \tilde{\omega}_t^{(i)} x_t^{(i)} \quad (17)$$

and the state covariance is computed from

$$P_t^x = \sum_{i=1}^P \tilde{\omega}_t^{(i)} (x_t^{(i)} - \hat{x}_t)(x_t^{(i)} - \hat{x}_t)^T \quad (18)$$

For the Gaussian mixture model, the estimated means, covariances and prior probabilities of the  $j$ th Gaussian components are set as state variables. The covariance matrix is first converted into vector form as

$$\sigma_{t,j}^i = [\Sigma_{t,j}^i(1,1) \Sigma_{t,j}^i(2,1) \dots \Sigma_{t,j}^i(l,1) \Sigma_{t,j}^i(2,2) \dots \Sigma_{t,j}^i(l,2) \dots \Sigma_{t,j}^i(l,l)]^T \quad (19)$$

where the  $\Sigma_{t,j}^i$  is the estimated  $l \times l$  covariance matrix of the  $j$ th Gaussian component corresponding to the  $i$ th particle and  $\sigma_{t,j}^i$  is the unfolded covariance vector. As the covariance matrix is symmetric, only the lower diagonal entries are needed. Then the state variable can be further expressed as

$$\hat{x}_{t,j} = [\mu_{t,j}^T \quad \sigma_{t,j}^T \quad \beta_{t,j}]^T \quad (20)$$

where  $\mu_{t,j}^i$  and  $\beta_{t,j}$  are the estimated mean vector and prior probability of the  $j$ th Gaussian component corresponding to the  $i$ th particle. The updated Gaussian components can be merged or split using the MML criterion so that the number of components is optimized [28].

The step-by-step procedure of DGMM method is summarized below:

- (i) Estimate the Gaussian mixture model with the modified E–M algorithm from Eqs. (3)–(6).
- (ii) Generate initial particle samples from the specified importance density function as in Eq. (11).
- (iii) Update and normalize the particle weights according to Eqs. (9) and (10).
- (iv) Compute the effective sample size from Eq. (12) and conduct re-sampling until the acceptance criterion is satisfied.
- (v) Convert the covariance matrix of each Gaussian component into vector form and further combine it with the corresponding mean vector and prior probability into a state vector as in Eqs. (19) and (20).
- (vi) Update all the states according to Eqs. (17) and (18) and further merge or split the Gaussian components until the component number is optimized. Then convert the particle filtered covariance vector back into matrix form.

### 3.2. Fault detection and diagnosis using dynamic Gaussian mixture model

With the particle filtered Gaussian components, the Bayesian inference based monitoring statistic can be computed and compared against the pre-specified confidence level for fault detection.

The particle filtered Bayesian inference probability (PFBIP) index is defined as follows

$$\text{PFBIP} = \sum_{i=1}^{\tilde{K}} P(\tilde{C}_i | y_T) P_M^{(i)}(y_T) \quad (21)$$

with

$$P(\tilde{C}_i | y_T) = \frac{\beta_{T,i} g(y_T | \tilde{\mu}_i, \tilde{\Sigma}_i)}{\sum_{j=1}^{\tilde{K}} \beta_{T,j} g(y_T | \tilde{\mu}_j, \tilde{\Sigma}_j)}$$

where  $y_T$  is the test sample,  $\tilde{K}$  is the updated number of Gaussian components after particle filter,  $P(\tilde{C}_i | y_T)$  represents the posterior probability of  $y_T$  within the  $i$ th particle filtered Gaussian component  $\tilde{C}_i$ ,  $g(y_T | \tilde{\mu}_i, \tilde{\Sigma}_i)$  denotes the multivariate Gaussian density function, and  $P_M^{(i)}(y_T)$  is the probability of the test sample  $y_T$  outside of the Mahalanobis-distance based ellipsoid under the pre-specified confidence level  $(1 - \alpha) \times 100\%$ , as computed from the following equation

$$P_M^{(i)}(y_T) = \Pr\{D_r((y, \tilde{C}_i) | y \in \tilde{C}_i) \leq D_r((y_T, \tilde{C}_i) | y_T \in \tilde{C}_i)\} \quad (22)$$

with

$$D_r((y, \tilde{C}_i) | y \in \tilde{C}_i) = (y - \tilde{\mu}_i)^T (\tilde{\Sigma}_i + \varepsilon I)^{-1} (y - \tilde{\mu}_i)$$

where  $D_r$  is the regularized Mahalanobis distance and follows a  $\chi^2$  distribution with  $l$  degrees of freedom while  $\varepsilon$  is a small number to remove the ill condition of particle filtered covariance matrix  $\tilde{\Sigma}_i$  (Mao and Jain, 1996; Yu and Qin, 2008). As long as the  $\varepsilon$  value is much smaller than all the diagonal variance entries of covariance matrix  $\tilde{\Sigma}_i$  and can eliminate the ill condition of  $\tilde{\Sigma}_i$ , the fine tuning of small  $\varepsilon$  value has no significant effect on the fault detection results.

In fault detection stage, the process is identified as faulty operation when the PFBIP index value is below the confidence level. Otherwise, the process operation is determined as normal. It should be emphasized that the proposed monitoring method is targeted at detecting abnormal operation events rather than isolating or classifying different types of process abnormalities such as biases, drifts, random variations, etc. For disturbances resulting in significant process upsets, they can be detected as faults in the proposed method.

To further diagnose the faulty variables after abnormal operation is alarmed, the regularized Mahalanobis distance metric can be decomposed as follows

$$\begin{aligned} D_r((y_T, \tilde{C}_i) | y_T \in \tilde{C}_i) &= (y_T - \tilde{\mu}_i)^T (\tilde{\Sigma}_i + \varepsilon I)^{-1/2} (y_T - \tilde{\mu}_i) \\ &= \sum_{j=1}^l \{s^{(j)} (\tilde{\Sigma}_i + \varepsilon I)^{-1/2} (y_T - \tilde{\mu}_i)\}^2 \end{aligned} \quad (23)$$

where  $s^{(j)}$  denotes the  $j$ th unit vector. Thus the particle filtered Bayesian inference contribution (PFBIC) index can be defined as

$$\text{PFBIC} = \sum_{i=1}^{\tilde{K}} \{P(\tilde{C}_i | y_T) \{s^{(j)} (\tilde{\Sigma}_i + \varepsilon I)^{-1/2} (y_T - \tilde{\mu}_i)\}^2\} \quad (24)$$

which is used to diagnose the leading faulty variables from the contribution plots. In practice, the above contribution index can be normalized so that the sum of all variable contributions equals one.

The detailed procedure of the dynamic Gaussian mixture model driven process monitoring and fault diagnosis approach is summarized below and the algorithm flow diagram is shown in Fig. 1:

- (i) Estimate the initial Gaussian mixture model via modified E–M algorithm from normal training samples.
- (ii) With the training and monitored samples, generate particles through re-sampling until the acceptance condition is met.
- (iii) Dynamically update the Gaussian mixture components including the means, covariances and prior probabilities as well as the number of components through particle filter.
- (iv) Compute the particle filtered Bayesian inference probability index values of monitoring samples according to Eqs. (21) and (22) and detect the faulty operation.
- (v) Further decompose the distance metric and calculate the particle filtered Bayesian inference contribution index values of all the measurement variables according to Eq. (24).
- (vi) Plot the contribution charts and identify the faulty variables with the leading contributions.

#### 4. Application example

##### 4.1. Tennessee Eastman Chemical process

In this study, the Tennessee Eastman Chemical process [32] is used to evaluate the effectiveness of the proposed DGMM based process monitoring and fault diagnosis approach and the results are compared to those of DPCA and regular GMM methods.

The process consists of five unit operations, which are a reactor, a vapor–liquid separator, a recycle compressor and a stripper. Chemical reactions occur in the reactor with two products and one by-product formed. The process includes 12 manipulated variables and 41 measurement variables, among which there are 19 composition variables sampled infrequently. Thus the total 22 continuous measurement variables are selected as monitored variables and the sampling interval for data collection is set to 3 min. The monitored process variables are listed in Table 1. During the normal operation, the process may run at one of the six modes as summarized in Table 2. The process flow diagram of the Tennessee Eastman Chemical process is shown in Fig. 2.

**Table 1**

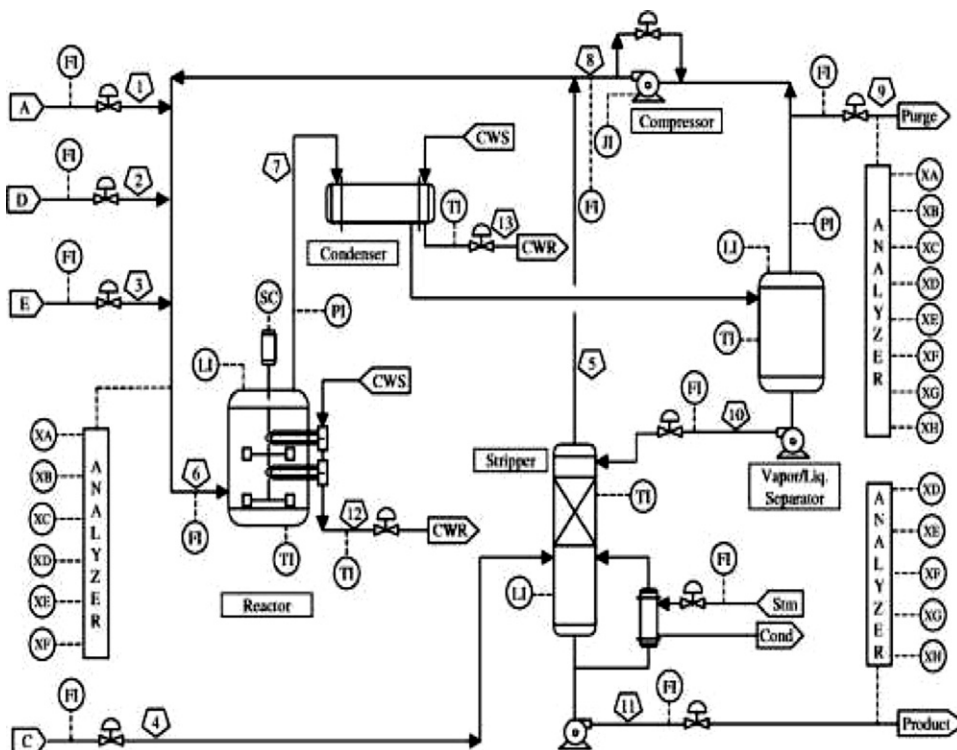
Monitored variables in the Tennessee Eastman Chemical process.

Variable no.	Monitored variables
1	A feed rate
2	D feed rate
3	E feed rate
4	A + C feed rate
5	Recycle flow rate
6	Reactor feed rate
7	Reactor pressure
8	Reactor level
9	Reactor temperature
10	Purge rate
11	Separator temperature
12	Separator level
13	Separator pressure
14	Separator underflow
15	Stripper level
16	Stripper pressure
17	Stripper underflow
18	Stripper temperature
19	Steam flow rate
20	Compressor work
21	Reactor coolant temperature
22	Condenser coolant temperature

**Table 2**

Six operating modes in the Tennessee Eastman Chemical process.

Mode	G/H mass ratio	Production rate (stream 11)
1	50/50	7038 kg/h G and 7038 kg/h H
2	10/90	1408 kg/h G and 12,669 kg/h H
3	90/10	10,000 kg/h G and 1111 kg/h H
4	50/50	Maximum
5	10/90	Maximum
6	90/10	Maximum



**Fig. 2.** Process flow diagram of the Tennessee Eastman Chemical process.

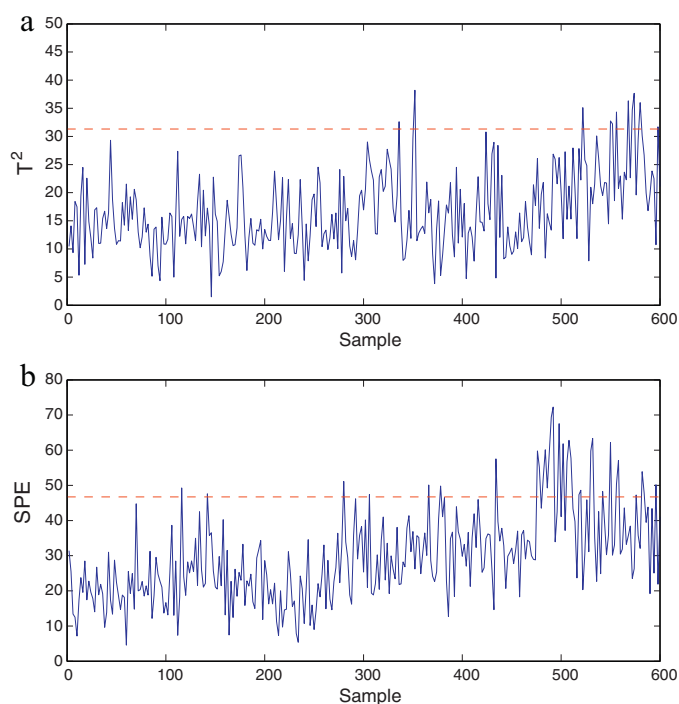
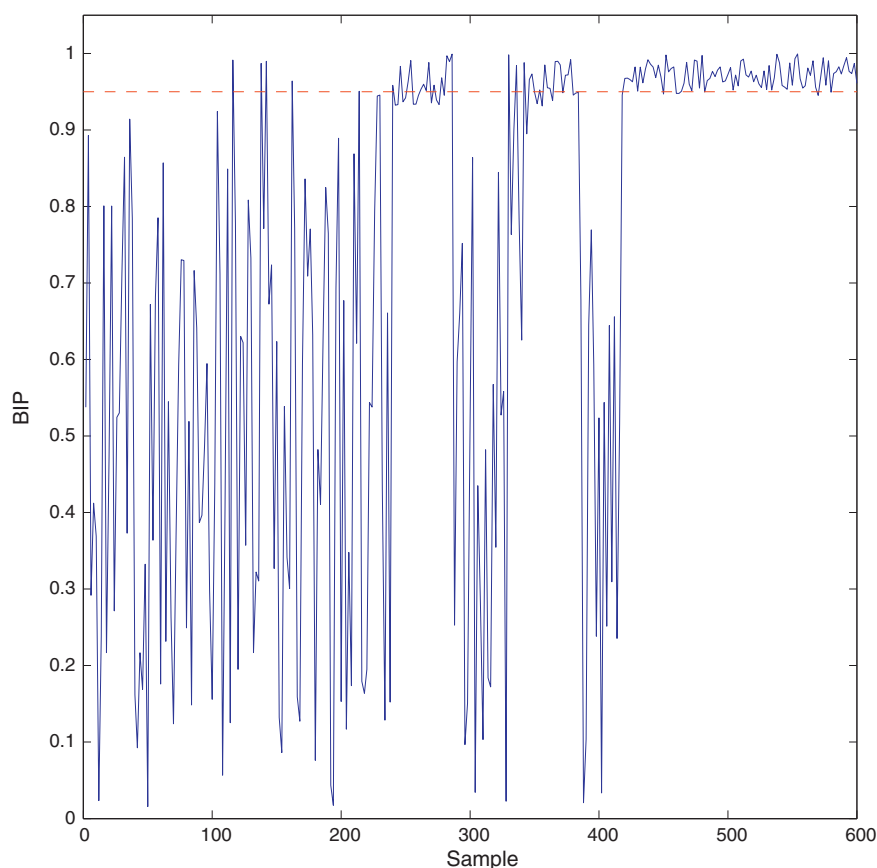


**Table 3**

Two test cases in the Tennessee Eastman Chemical process.

Case no.	Test scenario
1	1st–200th samples: Mode 1 or 3 201st–400th samples: Mode 3 or 5 401st–600th samples: Mode 5 with slow drifting error in reaction kinetics
2	1st–200th samples: Mode 3 or 6 201st–400th samples: Mode 1 401st–600th samples: Mode 4 with variations on condenser coolant temperature

During the training period, the process is operated under one of the first three modes and total 500 samples are collected. Then two test scenarios are designed to examine the performance of DGMM monitoring approach. In the first test case, the entire operation period consists of three stages. During the first stage, the process is operated under either Mode 1 or 3. Then in the second stage, it runs at either Mode 3 or 5. In the last stage, the process is at Modes 5 with a slow drifting error in reaction kinetics. Each stage has 200 test samples and so there are total 600 samples collected as the test set. The second test scenario includes four stages. The process operation is under Mode 3 or 6 for the first stage. Then it is followed by normal Mode 1 during the second stage. In the third stage, the operation is shifted to Mode 4 along with increased variations on condenser coolant temperature. Each of the above three stages also contains 200 samples. The designs of two test cases are summarized in Table 3. The three monitoring methods, DPCA, GMM and dynamic GMM, are applied to both test cases for fault detection and diagnosis.

**Fig. 3.** Fault detection results of the DPCA method in the first test case of the Tennessee Eastman Chemical process.**Fig. 4.** Fault detection results of the GMM method in the first test case of the Tennessee Eastman Chemical process.

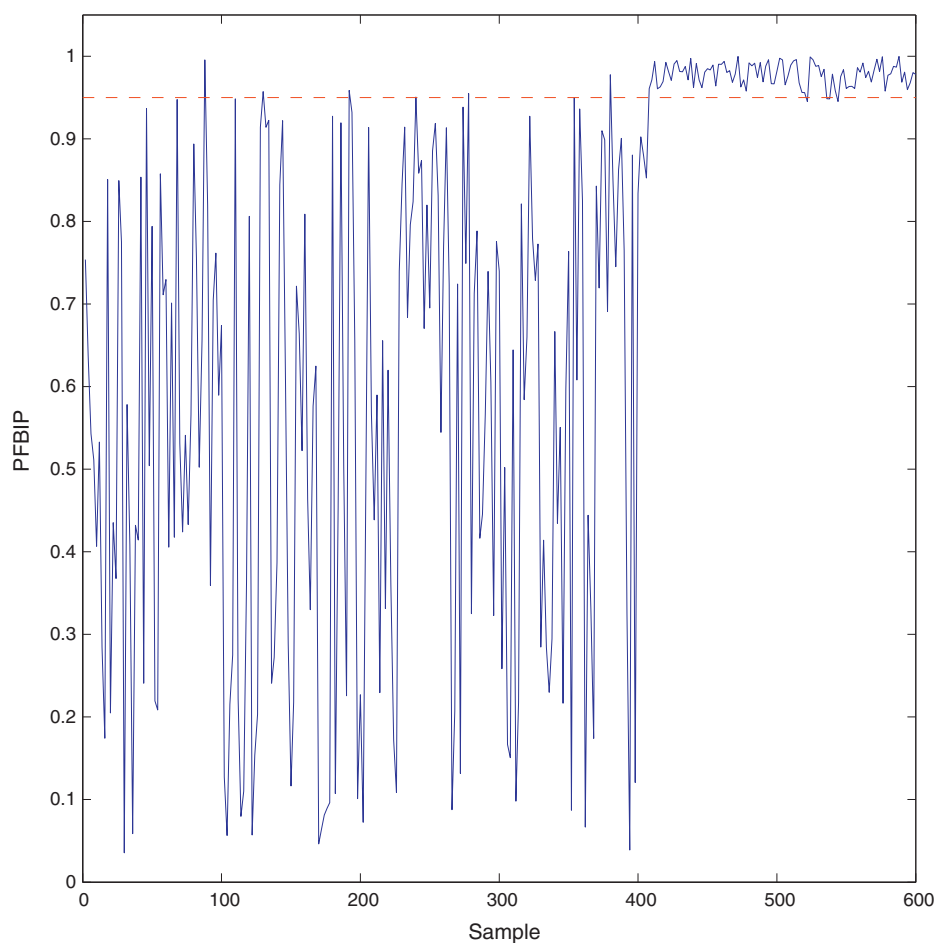


Fig. 5. Fault detection results of the DGMM method in the first test case of the Tennessee Eastman Chemical process.

#### 4.2. Process monitoring and fault diagnosis results

In the first test case, the fault detection results of DPCA, GMM and DGMM are shown in Figs. 3–5, respectively. It can be readily observed that both  $T^2$  and SPE indexes of DPCA have very low sensitivity to process fault. The fault alarms are triggered at small percentage of faulty samples in  $T^2$  and SPE plots. The fault detection rates of DPCA listed in Table 4 are as low as 9% and 28% for  $T^2$  and SPE, respectively. On the other hand, the performance of DPCA method in terms of false alarm rate is much more desirable. The false alarm rates of  $T^2$  and SPE are 0.5% and 1.5%, respectively. The main reason that the DPCA approach fails detecting the process faults is because the single PCA model combining multiple operating modes may significantly expand the ellipsoid of normal data. Thus many faulty samples may fall into the distorted normal operation region identified by DPCA and its fault sensitivity can be dramatically degraded. As a comparison, the regular GMM approach has better performance than DPCA particularly on fault detection. Majority of the faulty samples can be captured by the BIP index and the corresponding fault detection rate is 87%. Different from DPCA method, however, the GMM approach encounters

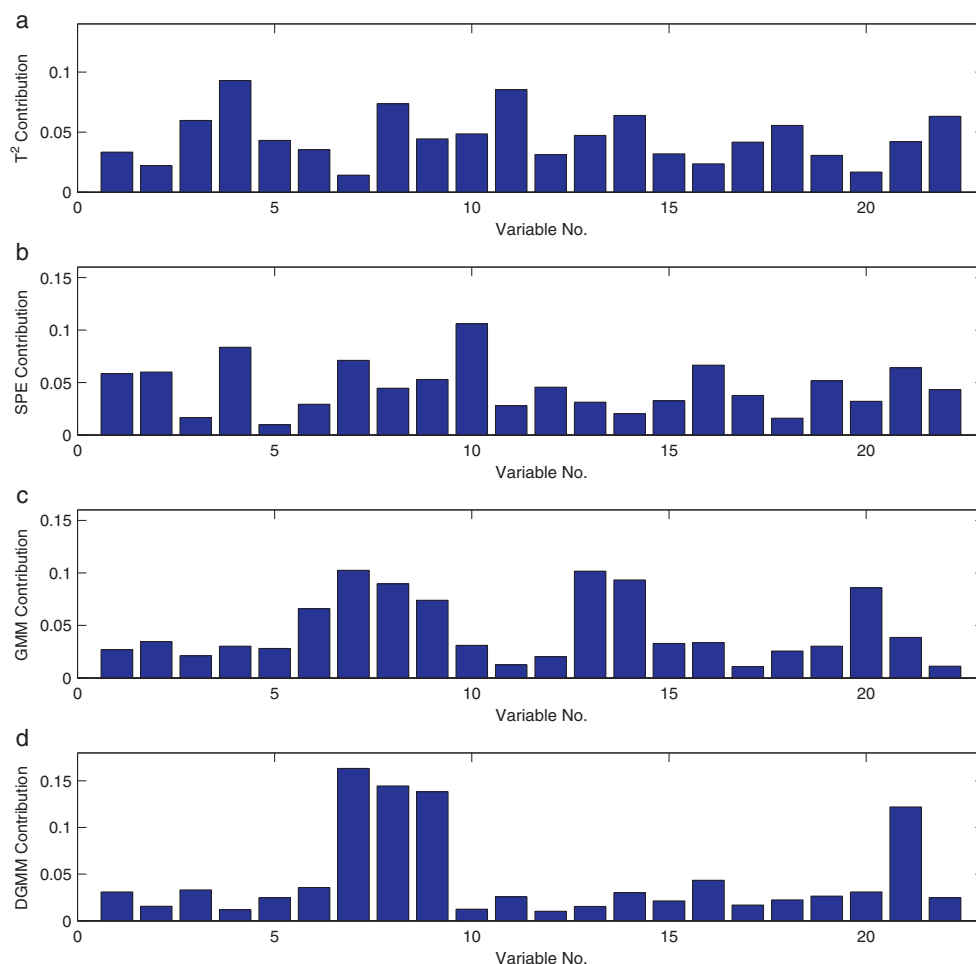
more significant challenge on controlling false alarms as its false alarm rate is 16.5%. The issue of regular GMM lies in the fact that it does not update the Gaussian mixture components after the initial estimate. For any new operating conditions like Mode 5 in this test case, regular GMM method may accidentally treat it as abnormal even though there is no fault occurrence. Therefore, significantly percentage of normal points from Mode 5 during the test period of 201st–400th samples are picked out as faulty ones incorrectly. In contrast, the DGMM approach has the best performance on both fault detection and false alarm rates. Total 94.5% of faulty samples are accurately detected while as low as 3% of normal samples are triggered with false alarms during the normal operation period. The fault is rapidly detected by DGMM method with a short delay of only five sampling periods. Compared to regular GMM, the DGMM method has the capability of dynamically updating Gaussian components and thus the new Mode 5 can be adaptively added to the mixture model so that the fault detection accuracy is significantly improved.

With the detected faulty samples from different methods, the fault diagnosis is further conducted to isolate the leading variables on the faulty operation. The DPCA, GMM and DGMM based

**Table 4**

Comparison of fault detection results among DPCA, GMM and DGMM methods (D1: fault detection rate; D2: false alarm rate).

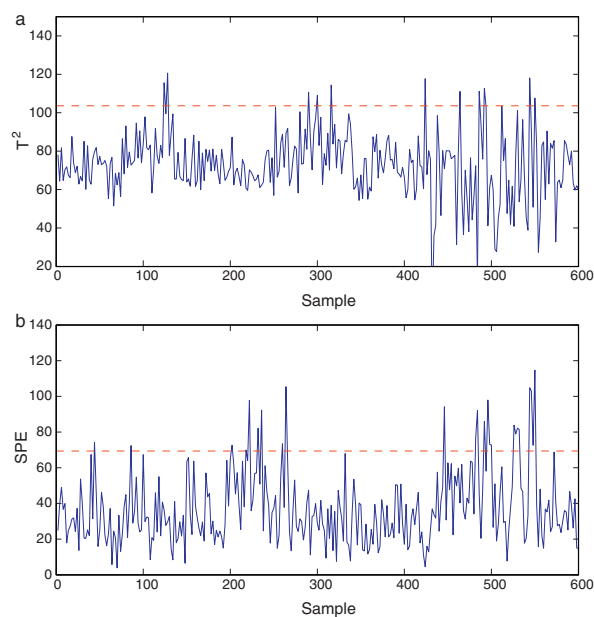
	DPCA $T^2$		DPCA SPE		GMM		DGMM	
	D1	D2	D1	D2	D1	D2	D1	D2
Case 1	9%	0.5%	28%	1.5%	87%	16.5%	94.5%	3%
Case 2	6%	5%	15%	9%	77%	22.5%	93%	5.5%



**Fig. 6.** Comparison of fault diagnosis results of the (a) DPCA  $T^2$ , (b) DPCA SPE, (c) GMM and (d) DGMM methods in the first test case of the Tennessee Eastman Chemical process.

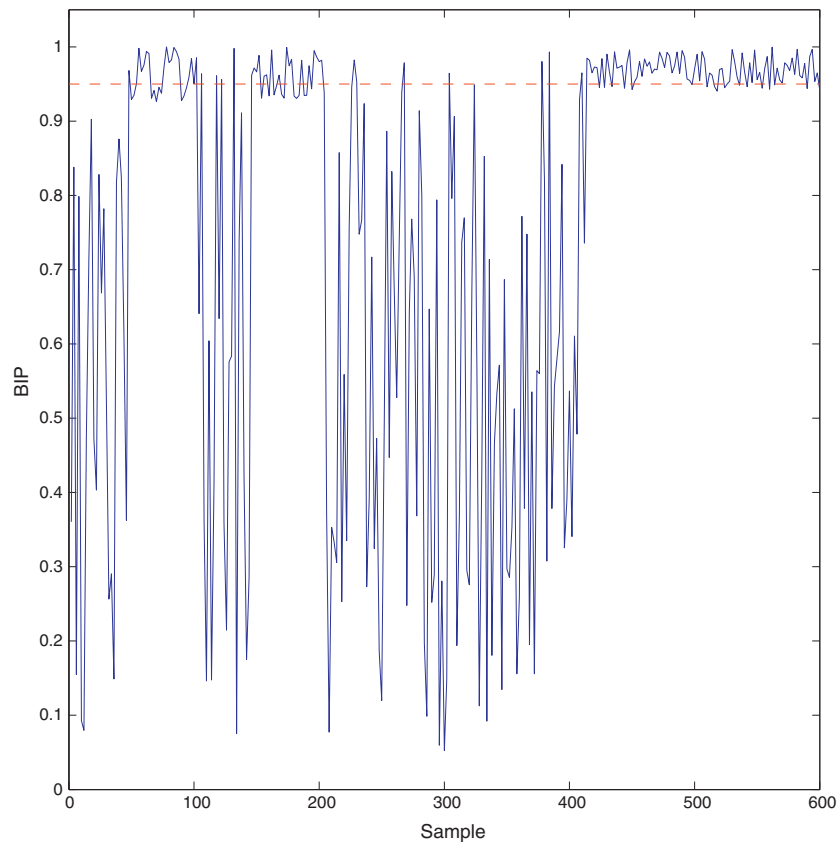
contribution plots are shown in Fig. 6(a), (b), (c) and (d), respectively. When the slow drift error on reaction kinetics occurs, the reactor temperature, pressure and level drift away from the steady-state values. Subsequently, the reactor cooling water temperature responds to control the reactor temperature. The DGMM based PFBIC plot in Fig. 6(d) successfully isolate the leading variables including reactor temperature, pressure, level and coolant temperature with the largest contributions. In contrast, the  $T^2$  and SPE contribution plots of DPCA method point to the wrong variables, which indicates the failure of DPCA method on fault diagnosis of multi-mode dynamic processes. Though the GMM based contribution plot shows relatively large contributions on some of the faulty variables including reactor pressure, temperature and level, several other variable like separator pressure, underflow and compressor work have comparable magnitudes of contributions so that those normal variables can hardly be isolated from the faulty ones.

For the second test case, the fault detection results shown in Figs. 7–9 further validate the superiority of the presented DGMM approach over the DPCA and GMM methods. The  $T^2$  and SPE indexes of DPCA method fail on vast majority of faulty samples with fairly low fault detection rates of 6% and 15%, respectively. The GMM method has much higher fault detection rate than those of DPCA. Due to the new operating Modes 4 and 6, however, neither the 77% fault detection rate nor the 22.5% false alarm rate of DGMM method is satisfactory. With the dynamic model updating feature, the particle filter driven DGMM approach results in both high fault

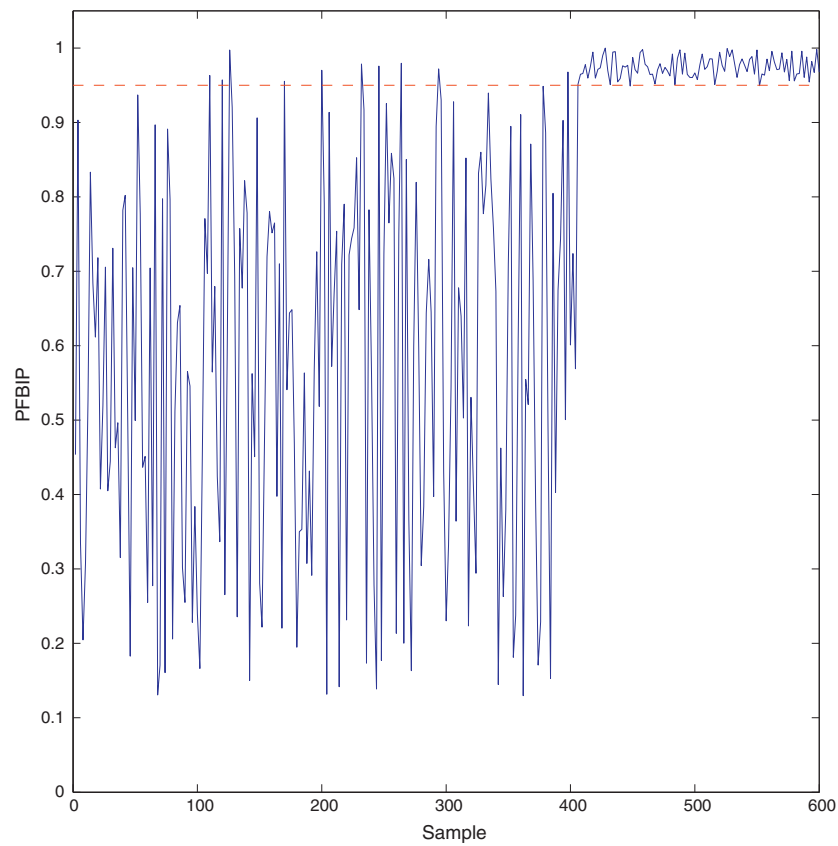


**Fig. 7.** Fault detection results of the DPCA method in the second test case of the Tennessee Eastman Chemical process.

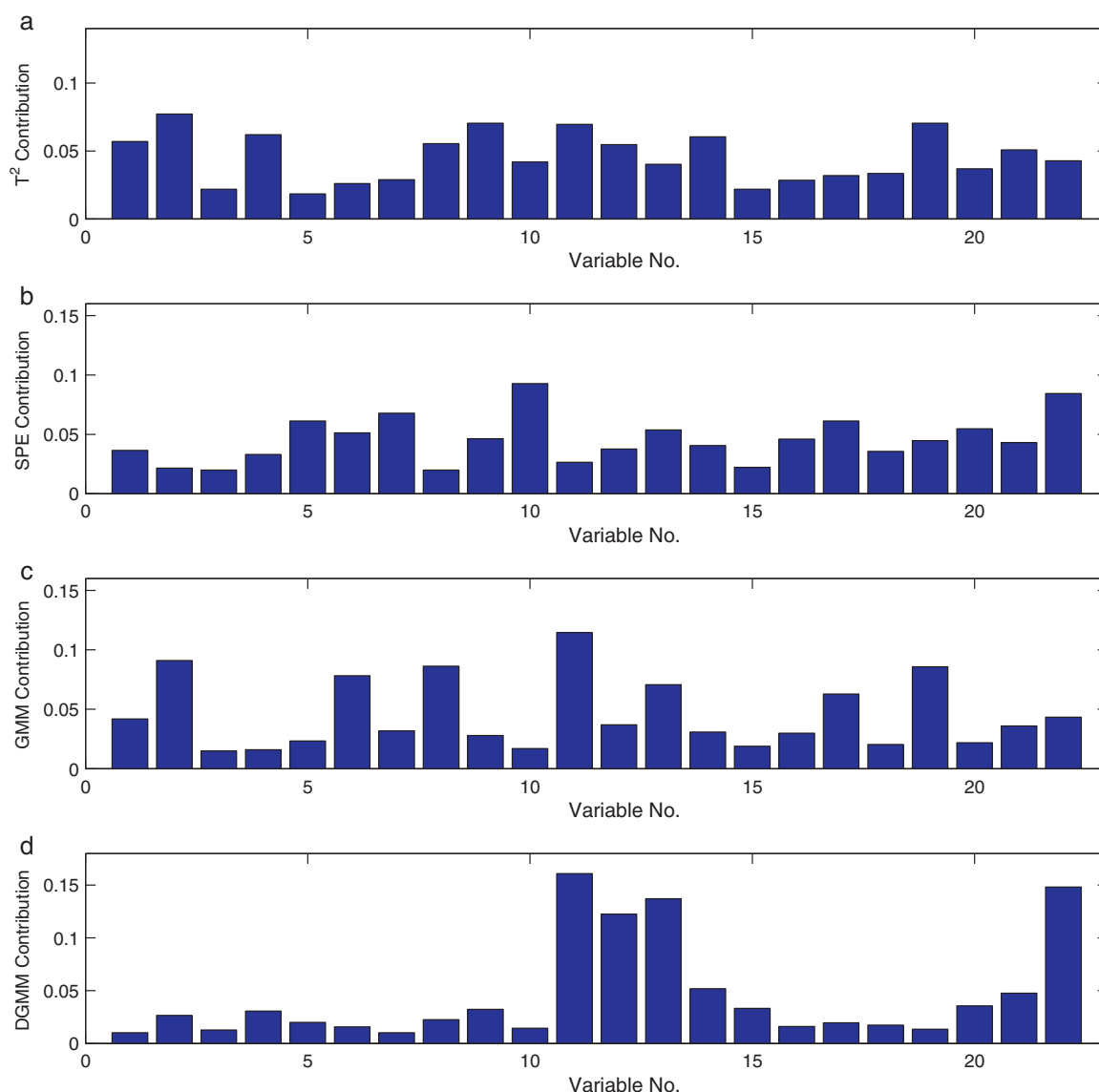




**Fig. 8.** Fault detection results of the GMM method in the second test case of the Tennessee Eastman Chemical process.



**Fig. 9.** Fault detection results of the DGMM method in the second test case of the Tennessee Eastman Chemical process.



**Fig. 10.** Comparison of fault diagnosis results of the (a) DPCA  $T^2$ , (b) DPCA SPE, (c) GMM and (d) DGMM methods in the second test case of the Tennessee Eastman Chemical process.

detection and low false alarm rates. There are as few as 7% faulty samples undetected and the fault detection is delayed by only four sampling periods. Meanwhile, the false alarms are triggered on only 5.5% of normal points. The fault diagnosis results are further compared among different methods. When the increased variations occur on the condenser cooling water temperature, the condenser coolant temperature immediately follows the fluctuations. Further, the increased variations the downstream separator temperature, pressure and level take place. The contribution plot of DGMM approach clearly points out the above four major variables with significantly larger contributions than the other variables. The DPCA based contribution charts are unable to capture the faulty variables as observed in Fig. 10(a) and (b). Though the GMM contribution plot shows the largest contribution on separator temperature, the other faulty variables are missed without clear isolation from the normal variables. For dynamically changing operation scenario, both the fault detection and diagnosis results of regular GMM method may suffer from the assumption of static combinations of operating modes.

## 5. Conclusions

In this article, a new dynamic Gaussian mixture model based fault detection and diagnosis approach is proposed for complex non-Gaussian processes with time-varying operation scenario shifts. The particle filter technique is adopted to update the mixture model parameters and thus account for the dynamic mode trajectory. Then the particle filtered Bayesian inference probability index and contribution metric are developed to detect abnormal operation events and diagnose major faulty variables.

The particle filter driven DGMM approach is applied to the Tennessee Eastman Chemical process with new operating modes and the monitoring results are compared to those of DPCA and GMM methods. The superior performance of DGMM approach in terms of fault detection rate, false alarm rate and faulty variable diagnosis demonstrates that it can effectively handle non-Gaussian process with dynamically switching operation scenarios and transient behaviors. Due to its unique capabilities,

the DGMM monitoring approach can be potentially applied to a wide range of industrial operations. Future study can be focused on the isolation and classification of different types of process faults and disturbances under dynamically shifting operation modes.

## References

- [1] I. Yélamos, G. Escudero, M. Graells, L. Puigjaner, Performance assessment of a novel fault diagnosis system based on support vector machines, *Comput. Chem. Eng.* 33 (2009) 244–255.
- [2] J. Thambirajah, L. Benabbas, M. Bauer, N.F. Thornhill, Cause-and-effect analysis in chemical processes utilizing XML, plant connectivity and quantitative process history, *Comput. Chem. Eng.* 33 (2009) 503–512.
- [3] J. Yu, S.J. Qin, Variance component analysis based fault diagnosis of multi-layer overlay lithography processes, *IIE Trans.* 41 (2009) 764–775.
- [4] P. Nomikos, J.F. MacGregor, Monitoring of batch processes using multi-way principal component analysis, *AIChE J.* 40 (1994) 1361–1375.
- [5] T. Kourti, J.F. MacGregor, Process analysis, monitoring and diagnosis, using multivariate projection methods, *Chemom. Intell. Lab. Syst.* 28 (1995) 3–21.
- [6] B.R. Bakshi, Multiscale PCA with application to multivariate statistical process monitoring, *AIChE J.* 44 (7) (1998) 1596–1610.
- [7] L.H. Chiang, E.L. Russell, R.D. Braatz, *Fault Detection and Diagnosis in Industrial Systems*, Advanced Textbooks in Control and Signal Processing, Springer-Verlag, London, Great Britain, 2001.
- [8] C. Ündey, A. Çinar, Statistical monitoring of multistage, multiphase batch processes, *IEEE Control Syst. Mag.* 10 (2002) 40–52.
- [9] B. Lennox, K. Kipling, J. Glassey, G. Montague, M. Willis, H. Hiden, Automated production support for the bioprocess industry, *Biotechnol. Prog.* 18 (2002) 269–275.
- [10] S.J. Qin, Statistical process monitoring: basics and beyond, *J. Chemom.* 17 (2003) 480–502.
- [11] V. Venkatasubramanian, R. Rengaswamy, K. Yin, S.N. Kavuri, A review of process fault detection and diagnosis: Part I: Quantitative model-based methods, *Comput. Chem. Eng.* 27 (2003) 293–311.
- [12] N.F. Thornhill, A. Horch, Advances and new directions in plant-wide disturbance detection and diagnosis, *Control Eng. Pract.* 15 (2007) 1196–1206.
- [13] J. Yu, Nonlinear bioprocess monitoring using multiway kernel localized Fisher discriminant analysis, *Ind. Eng. Chem. Res.* 50 (2011) 3390–3402.
- [14] M.J. Piovoso, K.A. Kosanovich, Applications of multivariate statistical methods to process monitoring and controller design, *Int. J. Cont.* 59 (1994) 743–765.
- [15] J.F. MacGregor, T. Kourti, Statistical process control of multivariate processes, *Control Eng. Pract.* 3 (3) (1995) 403–414.
- [16] W. Ku, R.H. Storer, C. Georgakis, Disturbance detection and isolation by dynamic principal component analysis, *Chemom. Intell. Lab. Syst.* 30 (1995) 179.
- [17] R.J. Treasure, U. Kruger, J.E. Cooper, Dynamic multivariate statistical process control using subspace identification, *J. Proc. Cont.* 14 (2004) 279–292.
- [18] Y. Zhang, Y. Zhang, Fault detection of non-Gaussian processes based on modified independent component analysis, *Chem. Eng. Sci.* 65 (2010) 4630–4639.
- [19] J. Yu, Localized Fisher discriminant analysis based complex chemical process monitoring, *AIChE J.* 57 (2011) 1817–1828.
- [20] M. Kano, S. Tanaka, S. Hasebe, I. Hashimoto, H. Ohno, Monitoring independent components for fault detection, *AIChE J.* 49 (4) (2003) 969–976.
- [21] J.M. Lee, C.K. Yoo, I.B. Lee, Statistical process monitoring with independent component analysis, *J. Proc. Cont.* 14 (2004) 467–485.
- [22] C.K. Yoo, J.M. Lee, P.A. Vanrolleghem, I.B. Lee, On-line monitoring of batch processes using multiway independent component analysis, *Chemom. Intell. Lab. Syst.* 71 (2004) 151–163.
- [23] J. Yu, S.J. Qin, Multimode process monitoring with Bayesian inference-based finite Gaussian mixture models, *AIChE J.* 54 (2008) 1811–1829.
- [24] Y. Yao, T. Chen, F. Gao, Multivariate statistical monitoring of two-dimensional dynamic batch processes utilizing non-Gaussian information, *J. Proc. Cont.* 20 (2010) 1188–1197.
- [25] J. Lee, B. Kang, S. Kang, Integrating independent component analysis and local outlier factor for plant-wide process monitoring, *J. Proc. Cont.* 21 (2011) 1011–1021.
- [26] J. Yu, A nonlinear kernel Gaussian mixture model based inferential monitoring approach for fault detection and diagnosis of chemical processes, *Chem. Eng. Sci.* 68 (2012) 506–519.
- [27] J. Yu, S.J. Qin, Multiway Gaussian mixture model based multiphase batch process monitoring, *Ind. Eng. Chem. Res.* 48 (2009) 8585–8594.
- [28] M.A.F. Figueiredo, A.K. Jain, Unsupervised learning of finite mixture models, *IEEE Trans. Pattern Anal. Mach. Intell.* 24 (2002) 381–396.
- [29] A.C. Harvey, *Forecasting, Structural Time Series Models and the Kalman Filter*, Cambridge University Press, Cambridge, UK, 1990.
- [30] M.S. Arulampalam, S. Maskell, N. Gordon, T. Clapp, A tutorial on particle filters for online nonlinear/non-Gaussian Bayesian tracking, *IEEE Trans. Signal Process.* 50 (2002) 174–188.
- [31] A. Doucet, J.F.G. de Freitas, N.J. Gordon, *Sequential Monte Carlo Methods in Practice*, Springer-Verlag, New York, NY, 2001.
- [32] J.J. Downs, E.F. Vogel, Plant-wide industrial process control problem, *Comput. Chem. Eng.* 17 (1993) 245–255.