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Polymer Extrusion Process Monitoring Using Nonlinear Dynamic Model-based PCA

Xueqin Liu, Kang Li, Marion McAfee, Jing Deng

Abstract— **Polymer extrusion is one of the final forming stages in the production of many polymeric products in a variety of applications. It is also an intermediate processing step in injection moulded, blown film, thermo-formed, and blow moulded products. However, polymer extrusion is a complex process which is difficult to set up, monitor, and control. As a consequence, high levels of off- specification products and long down-times are the problems facing the plastics industry. This paper proposes a new method for fault detection of the polymer extrusion processes, where the nonlinear finite impulse response (NFIR) model and principal component analysis (PCA) are integrated to form a nonlinear dynamic model-based PCA monitoring scheme. Here the NFIR model is used to capture the nonlinearity and dynamics of the extrusion process. The residuals resulting from the difference between the model predicted outputs and process outputs are then analyzed by PCA to detect process faults. The experimental results confirm the efficacy of the proposed model-based PCA approach for fault detection of polymer extrusion processes.**

Keywords
Principal component analysis; nonlinear dynamic model; polymer extrusion process.

I. Introduction

Extrusion has been used widely as a major method of processing polymer materials for a few decades. However, polymer extrusion is a complex process which is difficult to set up, monitor, and control. As a consequence, high levels of off- specification products and long down-times are the problems facing the plastics industry. Thus the close monitoring of the system performance to provide early detection of significant process changes or disturbances, is recognized by the industry to be of increasing strategic importance. Various fault detection methods have been developed based on the first principles, the identified causal models [1] or the multivariate statistical process control including principal component analysis (PCA) [2] and independent component analysis [3].

It was reported that PCA had been successfully applied to a continuous polymer film production line [4], [5]. However, the conventional PCA is a linear method, it may not be able to describe the nonlinear and dynamic characteristics of the extrusion processes properly as they are complex in nature and nonlinear relationship exists between the process variables. To cope with this problem, extended versions of PCA for describing system nonlinear or dynamic behavior have been developed. For nonlinear process monitoring, nonlinear extensions of PCA have been investigated which include principal curves [6], [7], multi-layer auto-associative neural networks (ANNs) [8], [9], and the kernel function approach [10], [11]. For dynamic process monitoring, linear dynamic PCA (DPCA) was first proposed by augmenting matrix with time-lagged variables [12]. More recently, subspace identification for a state space model was proposed [13] which mainly deals with the linear dynamic system. Again, an attempt has been made to apply the time-lagged data extension with Kernel PCA for handling nonlinearity and dynamics. However, this combination could be computationally expensive due to the augmented data matrix [14]. Recently, Rotem *et. al* [15] presented a model-based PCA approach, where the system nonlinear and dynamic behavior are described by first-principle models. Unfortunately, it is often difficult to obtain such models to describe the complex thermodynamic behavior in the polymer extrusion process. To overcome this problem, this paper proposes a new method for monitoring of the nonlinear dynamic polymer extrusion processes, where the nonlinear finite impulse response (NFIR) model based on the Fast Recursive Algorithm (FRA) and the PCA are integrated to form a nonlinear dynamic model-based PCA monitoring scheme. Different from the DPCA, which makes use of all the potential time-lagged variables, the FRA determines and selects the most important and relevant nonlinear dynamic terms from the potential ones to construct the NFIR model. Here the NFIR model, which is a nonlinear extension of FIR [16], is employed to capture the nonlinear and dynamic behavior of the extrusion process. The residuals resulting from the difference between the model predicted outputs and process outputs are analyzed by PCA to detect process faults. The effectiveness of the proposed model-based PCA approach was demonstrated by the monitoring results for data recorded from a polymer extrusion process.

The paper is organized as follows. The PCA and the dynamic PCA methods are briefly described in Section II. This is followed by the proposed nonlinear dynamic model-based PCA for process monitoring in Section III. The experimental polymer extrusion process and data generation are described in Section IV. Section V then presents the monitoring results of an application study to a polymer extrusion process. A concluding summary is given in Section VI.

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X. Liu, K. Li and J. Deng is with the School of Electronics, Electrical Engineering and Computer Science, Queen's University Belfast, Belfast, BT9 5AH, U.K. k.li@qub.ac.uk

M. McAfee is with the Department of Mechanical and Electronic Engineering, Institute of Technology Sligo, Sligo, Ireland. McAfee.Marion@itsligo.ie

II. PCA AND DYNAMIC PCA

This section provides the description of the PCA and the dynamic PCA for process monitoring.

Suppose a data matrix $\mathbf{X} \in \mathbb{R}^{N\times m}$ consists of N samples and m variables, the PCA decomposition allows the construction of two statistics for a sample vector $\mathbf{x} \in \mathbb{R}^m$, a Hotelling's T^2 statistic and a Q statistic:

$$T^2 = \mathbf{x}^T\mathbf{P}\Lambda^{-1}\mathbf{P}^T\mathbf{x} = \mathbf{t}^T\Lambda^{-1}\mathbf{t}, Q = \mathbf{x}^T\left[\mathbf{I}-\mathbf{P}\mathbf{P}^T\right]\mathbf{x} \quad (1)$$

for which confidence limits can be calculated based on [2], Λ is a diagonal matrix consisting of r eigenvalue of covariance matrix of scaled $\mathbf{X}$. $\mathbf{t} = \mathbf{x}^T\mathbf{P}$ is a score vector, and $\mathbf{P} \in \mathbb{R}^{m\times r}$ ($r \le m$ is the number of retained PCs) is a loading matrix.

Dynamic PCA proposed by [12] arranges the process variables to form an autogressive (AR) structure:

$$\underline{\mathbf{X}} = [\mathbf{X}_0, \mathbf{X}_{-1}, \cdots \mathbf{X}_{-d}] \in \mathbb{R}^{(N-d)\times(d+1)m} \quad (2)$$

where $\underline{\mathbf{X}}$ is an augmented set of variables, representing an AR model structure of order d and the subscript $0, 1, d$ refer to the backshifts. The PCA is then applied to $\underline{\mathbf{X}}$ and the corresponding T^2 and Q statistics can be constructed. The above method could be computationally expensive due to the augmented variables. Moreover, the dynamic PCA model is obtained under the assumption that the recorded variables are linear, therefore, it may not be suitable to model the nonlinear dynamics efficiently. To tackle this problem, a new model-based PCA method is proposed to account for both the nonlinear and dynamic behaviors of the extrusion process. If the model is accurate, the residual between the measured values and the model predicted values will be relatively insensitive to the variations caused by the nonlinearity or dynamics of the normal operating conditions [15], [16]. Consequently, PCA is more sensitive to process variation caused by the process faults, such as the disturbance of the material variations. In the following section, a new model-based PCA monitoring scheme will be introduced in more detail.

III. NONLINEAR DYNAMIC MODEL-BASED PCA FOR PROCESS MONITORING

The proposed model-based PCA involves a nonlinear dynamic modelling approach to identify a non-linear finite impulse response model to capture the underlying relationship between the process input and output variables. The residuals resulting from the difference between the model predicted outputs and process outputs are analyzed by PCA to detect process faults.

A. Nonlinear Dynamic Model Based On Fast Recursive Algorithm

Assuming a general nonlinear dynamic MISO system can be formulated as

$$y(t) = f(u_1(t-1), \cdots, u_1(t-d_{u_1}), \cdots, u_p(t-1), \cdots, u_p(t-d_{u_p}) \quad (3)$$

where y and u_i ($i = 1, \cdots, p,\ p \le m$) are the system output and input variables respectively. p is the number of input variables. d_{u_i} is the time delay for the process inputs u_i. By using a polynomial function, Eq. (3) can be approximated by a linear-in-the-parameter model:

$$\mathbf{y} = \sum_{i=1}^{M} \theta_i\phi_i(\mathbf{u}) + \mathbf{e} \quad (4)$$

where $\phi_i(.)$, $(i = 1, \cdots, M)$ are all candidate model terms, $\mathbf{u} = [\mathbf{u}_1, \cdots, \mathbf{u}_p]^T$, $u_i^T = [u_i(t-1), \cdots, u_i(t-d_{u_i})]$ is the model input vector, and $\mathbf{e}$ is the model residual.

If N data samples $\{y, \mathbf{u}\}^N$ are used for model training, then Eq. (4) can be written in the form

$$\mathbf{y} = \Phi\Theta + \mathbf{e} \quad (5)$$

where $\Phi = [\phi_1, \ldots, \phi_M] \in \mathbb{R}^{(N-d)\times M}$ is the regression matrix, $\phi_i = [\phi_i(u(d-d_{u_i}+1)), \cdots, \phi_i(u(N-d_{u_i}))]^T$; $\mathbf{y} = [y(d+1), \ldots, y(N)]^T \in \mathbb{R}^{N-d}$, d is the maximum delay among d_{u_i}. $\Theta = [\theta_1, \cdots, \theta_M] \in \mathbb{R}^M$, and $\mathbf{e} = [e(d+1), \cdots, e(N)]^T \in \mathbb{R}^{N-d}$.

In Eq.(5), Θ can be estimated using least-squares by minimizing the loss function

$$J(\Theta) = \mathbf{e}^T\mathbf{e} \quad (6)$$

The corresponding solution is given by $\widehat{\Theta} = (\Phi^T\Phi)^{-1}\Phi^T\mathbf{y}$.

Due to the noise and correlation between regressors, the matrix $(\Phi^T\Phi)^{-1}\Phi^T$ is always ill-conditioned, which may lead to inaccurate calculation of the model coefficients. Therefore, a subset selection technique such as the Fast Recursive Algrithm [17] is applied in order to determine the most important and relevant terms of all potential ones with respect to the available data [18].

Fast Recursive Algorithm

The FRA employs a residual matrix $\mathbf{R}_k$ defined as:

$$\mathbf{R}_k \triangleq I - \Phi_k(\Phi_k^T\Phi_k)^{-1}\Phi_k^T \qquad \mathbf{R}_0 \triangleq I \quad (7)$$

where $\Phi_k = [\phi_1, \cdots, \phi_k]$, and $k = 1, \cdots, M$. According to [17] and [19], $\mathbf{R}_k$ can be updated recursively:

$$\mathbf{R}_{k+1} = \mathbf{R}_k - \frac{\mathbf{R}_k\phi_{k+1}\phi_{k+1}^T\mathbf{R}_k^T}{\phi_{k+1}^T\mathbf{R}_k\phi_{k+1}},\ k = 0, 1, \cdots, M-1 \quad (8)$$

Now, the cost function in (6) can be rewritten as: $J(\Theta, \Phi_k) = tr(\mathbf{y}^T\mathbf{R}_k\mathbf{y})$.

In a forward stepwise stage, the nonlinear model terms are selected one at a time. Thus, suppose at the kth step, one more term ϕ_j, $\ k+1 \leqslant j \leqslant M$ from the candidate term pool is to be selected. The net contribution of ϕ_j to the cost function can be calculated as

$$\Delta J_{k+1}(\Theta, \Phi_k, \phi_j) = \frac{\|\ (\mathbf{y}^{(k)})^T\phi_j^{(k)}\ \|^2}{\|\ \phi_j^{(k)}\ \|^2} \quad (9)$$

where $\phi_j^{(k)} \triangleq \mathbf{R}_k\phi_j$, $\mathbf{y}^{(k)} \triangleq \mathbf{R}_k\mathbf{y}$.

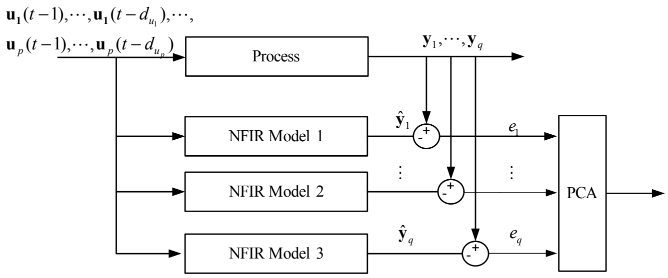


Fig. 1: Nonlinear dynamic model-based PCA

By defining an auxiliary matrix $\mathbf{A} \in \mathbb{R}^{k\times M}$ and $\mathbf{a}_u \in \mathbb{R}^{M\times q}$ with elements

$$a_{i,j} \triangleq \begin{cases} 0, & 1 \le j < i \\ (\phi_i^{(i-1)})^T \phi_j^{(i-1)}, & i \le j \le M \end{cases} \tag{10}$$

$$\mathbf{a}_{i,u} \triangleq \begin{cases} (\phi_i^{(i-1)})^T \mathbf{y}^{(k)}, & 1 \le i \le k \\ (\phi_i^{(k)})^T \mathbf{y}^{(k)}, & k < i \le M \end{cases} \tag{11}$$

the cost function can be updated recursively:

$$\Delta J_{k+1}(\Theta, \Phi_k, \phi_j) = \frac{\| \mathbf{a}_{j,u} \|^2}{a_{j,j}} \tag{12}$$

The model term that provides the largest contribution to (12) is then selected, and this procedure continues until some criterion (e.g., Akaike's information criterion [20]) is met or until a pre-set maximum number of model terms are selected. After a satisfactory model with M terms has been constructed, the model coefficients are then computed recursively from

$$\hat{\theta}_j = \left(\mathbf{a}_{j,u}^T - \sum_{i=j+1}^{M} \hat{\theta}_i a_{j,i} \right) / a_{j,j}, \quad j = k, k-1, \cdots, 1. \tag{13}$$

B. Nonlinear Dynamic Model-Based PCA Monitoring Scheme

Having discussed the nonlinear dynamic modelling approach based on the FRA, the model-based PCA monitoring scheme, as shown in Fig. 1, will be introduced in detail, where the nonlinear models are employed to predict process outputs. The residuals between the system outputs and predicted outputs are used to construct the PCA model. The following summarizes the construction procedure of the proposed model-based PCA and its application to the process monitoring:

1) Process dynamic data including the input and output variables are recorded for nonlinear dynamic modelling;
2) The nonlinear modelling approach based on the FRA is applied to obtain the NFIR models to describe the nonlinear dynamic relationship between the system input and output variables;
3) The residual resulting from the difference between the model outputs and process outputs is calculated as $\mathbf{e}_i = \mathbf{y}_i - \hat{\mathbf{y}}_i$ ($i = 1, \cdots, q$, q is the number of output variables).
4) The residual matrix $\mathbf{E} = [\mathbf{e}_1, \cdots, \mathbf{e}_q]$ is constructed and scaled;
5) Compute the PCA model for the scaled residual matrix $\mathbf{E}$;
6) Construct the T^2 and the Q statistics, and calculate the confidence limit as discussed in [21].
7) For a centered new data sample $\mathbf{z}$ during the on-line monitoring procedure, the scaled residual $\mathbf{e}_z$ between the actual process output and the model predicted ouput is calculated;
8) Calculate the constructed T^2 and Q statistics by:

$$T^2 = \mathbf{e}_z^T \mathbf{P} \Lambda \mathbf{P}^T \mathbf{e}_z \qquad Q = \mathbf{e}_z^T \left[\mathbf{I} - \mathbf{P}\mathbf{P}^T \right] \mathbf{e}_z, \tag{14}$$

9) Check whether T^2 or Q exceeds the corresponding control limit; if so, the hypothesis that the soft sensor is violated is accepted, otherwise the soft sensor is reliable.

It is clear that the effectiveness of the proposed model-based PCA method relies on the sensitivity of the system model to the different types of process faults. For instance, if process fault only affects the process output, then it is important that the model-based PCA should be insensitive to the process outputs. Therefore, if the NARX (nonlinear autoregressive with exogenous input) structure is employed, which relies on the past values of the process outputs, then the generated residuals couldn't reflect the influence of the process fault on the the process output. Consequently its monitoring ability can be compromised. However, with the NFIR structure, which only makes use of the past values of the process inputs, the predicted outputs are not affected by the process faults. As a result, the model residuals are capable of reflecting the deviation of process outputs from those obtained without process faults. Based on the above discussion, the NFIR model is preferred over the NARX model to be incorporated by PCA.

IV. Experimental Polymer Extrusion Process

There are two types of extrusion processes in the polymer industry: continuous and discontinuous. According to the number of screws used in the extruder, there are single-screw, twin-screw and multi-screw extruders. Of these single screw continuous extruders are the most commonly used in polymer industry. The conventional single screw extrusion process has a standard setup including a barrel which is heated by a number of electrical heaters, a rotating screw, and an extrusion die for the final product [22]. Typical temperature and pressure sensors are installed along the barrel and the die to provide continuous data for the process. For process operation, the polymer materials are fed into the barrel through the hopper by gravity, and then they are conveyed and melted along the flights of the screw and finally pushed out through the die to achieve a desired form.

Different types of faults may occur in a polymer extrusion process, such as (i) incoming material variations in terms of size, physical properties and compositions; (ii) process upsets; (iii) equipment faults; (iv) the operator errors.

Fig. 2: The laboratory extruder with a in-line-rheometer die

TABLE I: Description Of The Recorded Process Variables

Number	Description	Variable	Unit	Note
1	Screw speed	N	rpm	Input
2	Barrel zone 1 temperature	T_1	^{o}C	
3	Barrel zone 2 temperature	T_2	^{o}C	
4	Barrel zone 3 temperature	T_3	^{o}C	
5	Barrel pressure	P_b	MPa	Output
6	Die pressure 2	P_2	MPa	
7	Viscosity	η	Pas	

Figure 2 depicts the experimental single screw extruder (Killion KTS-100) used in this paper. An in-line-rheometer die is especially instrumented in the experiment for the calculation of the melt viscosity. The analyzed variables are given in Table I. For obtaining some information-rich data sets of process inputs, the screw speed, N, and the temperature settings at the three heating zones, T_1, T_2, T_3, were excited using a Pseudo-Random Signal applied in a 'random walk' algorithm respectively. That is the signal excited by a Gaussian sequence and the period of input change was also defined by a Gaussian sequence where the mean and standard deviation were defined on the basis of measured pressure and viscosity response time to step changes in the inputs. Thus a wide operating range was covered in the sequences while consecutive input changes were within practical operating limits [23].

Two low-density polyethylene (LDPE) materials were used in this work, one is LD159AC (LDPE(A)) and the other is DOW352E (LDPE(B)). All signals were acquired at 1Hz using a 16-bit DAQ card through a SC-2345 connector box. At first, 6000 process data samples of LDPE(A) were collected under the above conditions and used as fault free reference samples. These samples were divided into two data sets where the first 2000 samples was used for model identification using the FRA, and the remained 4000 samples for test purpose. A third data set of 4000 samples was collected under the same conditions as above with a different material LDPE(B), which is used as a faulty data set. The generated screw speed, barrel pressure and the viscosity signals under normal conditions are illustrated in Fig. 3.

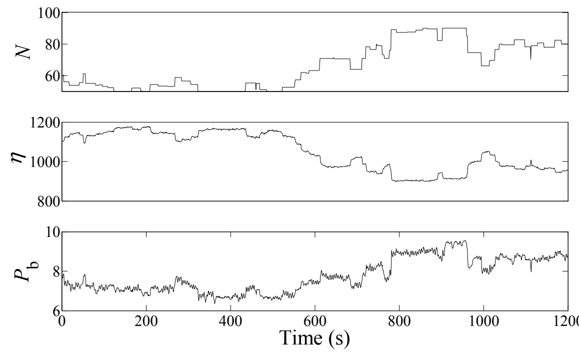


Fig. 3: Generated signals under normal conditions

V. APPLICATION OF MODEL-BASED PCA TO POLYMER EXTRUSION PROCESS

The description of the polymer extrusion line used in this application study was explained in Section IV. This section discusses the proposed monitoring approach involved in the NFIR model identification for process outputs using the FRA, followed by the PCA applied to the generated residuals.

To build the system model, the screw speed N, and the barrel set temperatures T_1, T_2, T_3, are employed as the process inputs to predict the three outputs, including the barrel pressure P_b, the die pressure P_2, and the viscosity η. As mentioned above, the different model structure employed by model-based PCA has distinct sensitivity to the process faults. To illustrate this point, both NARX and NFIR models are used to predict the process outputs. The three process outputs are generated using the FRA based on the LDPE(A) fault free data with a time series of system variables as below. The NFIR model is given as:

$$\begin{aligned} \mathbf{P}_b(t) &= -2.7 + 10^{-4}\mathbf{N}(t-1)\eta(t-1) \quad (15)\\ \mathbf{P}_2(t) &= 2.2 + 10^{-4}\mathbf{N}(t-1)\eta(t-1)\\ \eta(t) &= 202.5 - 0.06\mathbf{T_3}(t-1) - 0.05\mathbf{N}(t-1)\mathbf{T}_3(t-5)\\ &\quad +0.03\mathbf{N}(t-1)\mathbf{T}_3(t-8) \end{aligned}$$

The NARX model has the form of

$$\begin{aligned} \mathbf{P}_b(t) &= -0.2 + 0.6\mathbf{P}_b(t-1) + 3\times 10^{-5}\mathbf{N}(t-1)\eta(t-1) \quad (16)\\ \mathbf{P}_2(t) &= 0.3 + 0.4\mathbf{P}_b(t-1) + 3\times 10^{-5}\mathbf{N}(t-1)\eta(t-1)\\ \eta(t) &= 364.8 + 10^{-4}\eta(t-1) - 0.01\eta(t-1)^2\\ &\quad +0.04\mathbf{N}(t-1)\mathbf{T}_3(t-24) \end{aligned}$$

The error residuals of the above NFIR model has zero mean and variance of 0.04, which can be approximated by a normal distribution. Its performance on the unseen validation data of LDPE(A) including the measured barrel pressure, the melt pressure in the die, and the viscosity is shown in Fig. 4. It shows that the predicted values of the unseen data based on the NFIR model match the measured values very well. For comparison, the NARX model performance on the same data is also illustrated in Fig 4.

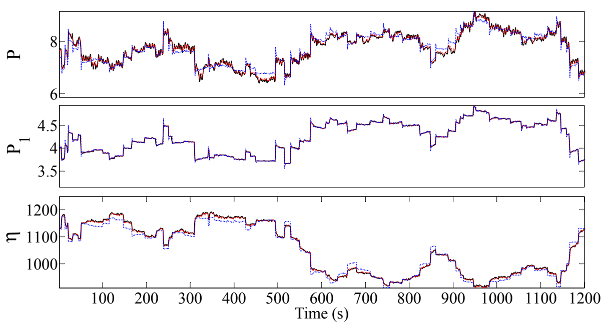


Fig. 4: Modeling result of the NFIR and the NARX on unseen LDPE(A) data under normal conditions. Solid black line: actual output; red dashed line: NARX model output; blue dashed line: NFIR model output.

A. Process Monitoring

An attempt to monitor an extrusion process using PCA directly will lead to unavoidable difficulties because of the nonlinear and dynamic nature of the process [7], [24], [25]. In this subsection, the monitoring results of applying the proposed model-based PCA on the residual matrix is investigated. A PCA model was produced using the residual matrix **E**, which is composed of the errors between the model predicted outputs and the measured outputs. The proposed NFIR-PCA approach for process monitoring is further compared to both conventional linear DPCA and the NARX-PCA in this section.

The number of principal components, r, was determined according to its variance contribution. Thus, two principal components which could capture 79.1% of the variance of the of the total variance of the 3 error variables were chosen for the NFIR-PCA model. Compared to NARX-PCA, two linear principal components captured 86.2% of the total variance. By contrast, one principal component was required for the linear DPCA model and 96.4% of the total variance was explained. After establishing the PCA model, on-line monitoring of the extrusion process requires the T^2 statistic to monitor system variations in the PCA model space, and a second Q statistic to monitor system variations in the PCA residual space. The 99% confidence limits for the T^2 and Q statistics are determined respectively as discussed in [21].

For the recorded 2000 reference samples, Table II summarizes the Type I error, or false alarm rate, for the T^2 and the Q statistics of the linear DPCA, the NARX-PCA and the NFIR-PCA methods for a confidence of 99%. These results imply that the Type I errors for the T^2 statistic of linear DPCA is far lower than expected, which is later shown to result in its insensitivity of detecting process fault. This can be attributed to that the principal component in linear DPCA

TABLE II: Number of Type I errors For Reference Data From Linear DPCA, NFIR-PCA And NARX-PCA With 99% Control Limits

Method	#PC(s)	Variance Contribution	T^2	Q
Linear DPCA	1	96.4%	0 %	2.2%
NARX-PCA	2	86.2%	1.9%	0.9%
NFIR-PCA	2	79.1%	2.0%	0.7%

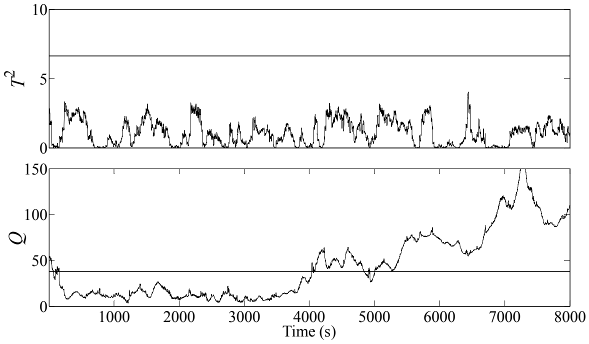
is unable to describe the nonlinear behavior in the extrusion process and that the assumption of the monitored variables follow a Gaussian distribution no longer holds.

Monitoring results of the proposed method for the testing data set 1) the unseen LDPE(A) fault free data; 2) the unseen LDPE(B) faulty data are shown in Fig. 5. The straight lines represent the 99% control limits. Fig. 5c shows all the unseen LDPE(A) data (the first 4000 samples) is under the control limit, which implies the NFIR model is capable to capture the nonlinear and dynamic behavior. Moreover, for the second fault data set, both T^2 and Q statistics of NFIR-PCA in Fig. 5c show the data samples are beyond the control limit (50 samples after the new material introduced) implying the NFIR model is no longer validated for different material. In contrast, the T^2 of linear DPCA and the Q of the NARX-PCA are not sensitive to this disturbance. The application study therefore indicated that using linear principal components and incorrect distribution function to describe nonlinear dynamic behavior may render the monitoring statistics insensitive or increase the false alarms. It also demonstrated that the monitoring ability of the NARX-model structure, which relies on the past values of the process outputs, is compromised when the process outputs are affected by process faults.

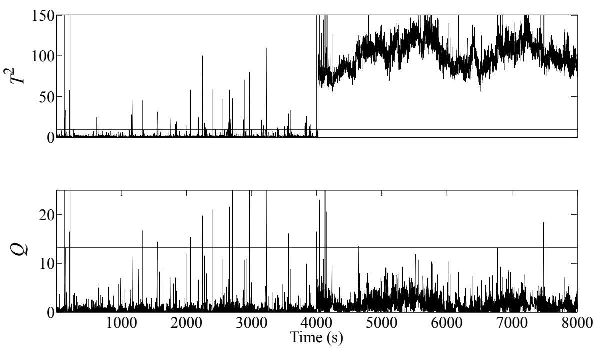
VI. CONCLUSIONS

This paper has studied the incorporation of NFIR model into the multivariate statistical process control framework, motivated by the fact that monitoring processes with linear dynamic model may lead to insensitive statistics or false alarms. The application of the NFIR model to remove the nonlinear and dynamic information from the monitored variables, together with the use of PCA to monitor the resulting residuals can thus help to circumvent the above problems. The benefit of applying the NFIR model instead of the NARX is that the NFIR model requires no feedback of the process output, and hence its model residual is able to reflect the process faults more closely.

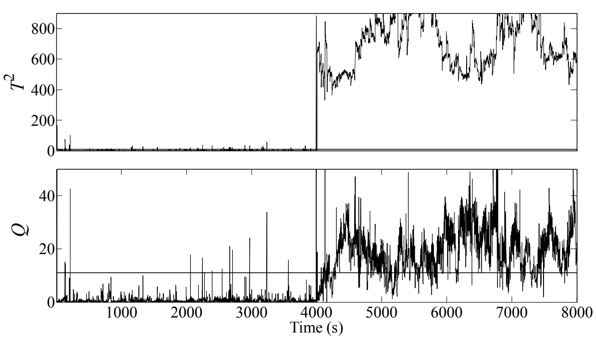
A further contribution of this paper has been to apply the Fast Recursive Algorithm for model identification. In comparison with the traditional subset selection method, such as the orthogonal least square algorithm (OLS), the FRA is able to select the most important and relevant model terms more efficiently without compromising model accuracy [17], [19], [26]. Unlike DPCA, which makes use of all the potential time-lagged data variables, the FRA selects only the most important ones for the NFIR model. The effectiveness of the proposed model-based PCA approach



(a) Linear DPCA



(b) NARX-PCA



(c) NFIR-PCA

Fig. 5: Process monitoring results on the unseen normal data (the first 4000 samples) and the faulty data (after 4000 samples) using (a) DPCA; (b) NARX-PCA; (c) NFIR-PCA

has been demonstrated by the monitoring results for data recorded from a polymer extrusion process.

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