Preprints of the 12th IFAC Symposium on Computer Applications in Biotechnology
The International Federation of Automatic Control
16-18, 2013, December. Mumbai, India

Online Monitoring for Uneven Length Batch Processes using Function Space Principal Component Analysis

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Abstract: Online batch process monitoring has been a challenging task, as batch processes do not operate around a nominal steady state operating point. Various monitoring approaches where future batch trajectory is filled with average (nominal) batch trajectory have been proposed. Predicting future trajectory for a batch process is a difficult task. Recently a multiway principal component analysis (MPCA) based approach that does not involve future trajectory prediction was proposed. In this paper a new technique based on function space principal component analysis (FSPCA) is proposed for online batch process monitoring. The main advantage of the proposed FSPCA based methodology is its ability to detect incipient and small to medium magnitude faults and its relevance for uneven length batch processes. Efficiency and effectiveness of the proposed algorithm is demonstrated via a fed-batch penicillin cultivation process simulation. The diagnostic performance of the proposed approach is significantly better compared to MPCA based approaches.

Keywords: Principal components analysis (PCA), Multiway principal component analysis (MPCA), Function space principal component analysis (FSPCA), Fault diagnosis and monitoring

1. INTRODUCTION

Batch processes are dominant in industries such as, biochemical, pharmaceutical, chemical, polymer, food industry, etc. Batch processes have a definite start and ending with a series of steps or tasks to be performed with fixed operating conditions and fixed processing time. Thus, batch processes are characterized by time varying variable correlation structure and parameters. Therefore, apart from high dimensionality and highly correlated measurement, batch process monitoring bring in additional complications due to the following reasons: i) the batch processes do not generally operate around a nominal steady state operating point, ii) historical data for batch processes are three dimensional, and iii) batches may have varying duration, i.e. uneven length batch. The lack of a reliable online monitoring mechanism in a batch process would have very significant impact on plant economy in terms of time, raw material and energy lost in faulty batches. Thus, it is important to monitor and maintain product quality for batch processes in an online fashion and online batch process monitoring has been an active area of research and a wide variety of techniques have been proposed for fault diagnosis of batch process.

Statistical process control (SPC) based monitoring methods have been at the forefront when it comes to batch process monitoring. Initial attempts towards monitoring batch process using multivariate statistical methods were involving unfolding of the three dimensional data into two dimensions. The unfolding can be carried out in different ways, i.e. batch-wise unfolding or variable-wise unfolding. Monitoring approaches based on both the types of unfolding have been proposed in the literature (Lu *et al.*, 2004; Nomikos & MacGregor, 1994; Rännar *et al.*, 1998). Once historical data of various batches is organized in a two-dimensional matrix, conventional principal component analysis (PCA) based monitoring charts can be used for batch process monitoring. However, simple unfolding can be implemented only for batches of fixed duration. For uneven length batch processes, methods based on synchronization that require dynamic time warping (DTW) or correlation optimized warping (COW) (Patel & Gudi, 2009; Tomasi *et al.*, 2004) have been proposed. A modified approach based on Multiway PCA (MPCA) proposed in (Lee *et al.*, 2004) does not require time synchronization and yet works for uneven length batch processes.

Another methodology, to enable data unfolding, is to capture dynamics of a batch process by a fixed number of orthogonal basis functions. Such a methodology is known as function space principal component analysis (FSPCA) and it can be used for monitoring of uneven length batch processes (Chen & Liu, 2001). However, this FSPCA methodology is applicable for offline batch process monitoring. In this paper, an online monitoring approach based on FSPCA is proposed for monitoring of uneven length batch processes. It has been shown that because of function approximation, the proposed methodology has better diagnostic performance compared to MPCA based approach. Simulations involving fed-batch penicillin cultivation process were carried out to demonstrate effectiveness of the proposed FSPCA based online batch process monitoring approach.

The remainder of the paper is organized as follows. First the MPCA based approach for online batch process monitoring is

discussed in section 2. The FSPCA method along with relevant data pre-processing methods such as, batch-wise unfolding, basis function and FSA, are explained in section 3. The proposed FSPCA methodology for online monitoring is explained in detail in section 4. Finally, the simulation case study involving a fed-batch penicillin cultivation process simulation is presented in section 5, followed by concluding remarks in section 6.

2. MULTIWAY PCA

Multiway PCA approach, which uses batch-wise unfolding for batch process monitoring, was proposed by Nomikos and MacGregor (1994, 1995). The MPCA approach involves detection of deviations from the mean trajectory by subtracting mean of each variable at each time from the unfolded data matrix. However, this MPCA approach had several difficulties: i) prediction future batch data, ii) assumption of constant variance-covariance structure, iii) assumption of equal batch duration. To overcome these limitations a modified approach based on MPCA was proposed by (Lee, et al., 2004). This modified monitoring approach is explained briefly in the next subsection.

2.1 Online batch process monitoring by MPCA

Historical batch process data is three dimensional in nature. These dimensions can be represented by batches (I), variables (J) and time (K). First, the three dimensional historical data $\mathbf{X}_{I\times J\times K}$ is unfolded batch-wise to obtain $\mathbf{X}_{I\times JK}$ and variables at each time are scaled to zero mean and unit variance. Next, the data matrix is rearranged variable-wise giving $\mathbf{X}_{IK\times J}$. PCA is then applied to this matrix and scores matrix $\mathbf{T}_{KI\times R}$ and loadings matrix $\mathbf{P}_{J\times R}$ are obtained, where R is the number of principal components retained. Next, the scores at each time, $(\mathbf{T}_k)_{I\times R}$ is obtained and from Tk matrix, the covariance matrix at each time, $(\mathbf{S}_k)_{R\times R}$, is calculated. Thus, in this approach, the covariance matrix is obtained at each time instance and it need not be constant. More details on the online batch process monitoring by MPCA are given in (Lee, et al., 2004).

3. FUNCTION SPACE PCA

As stated earlier, function space analysis based principal component analysis had been proposed for offline monitoring of uneven length batch processes. In this section FSPCA methodology is explained along with involved pre-processing methods such as data unfolding, function space analysis, etc.

3.1 Function space analysis

For a batch process, each variable in each batch can be represented as a time trajectory. The batch-wise unfolding would then give a data matrix shown in (1). Each time trajectory of variable x_j for batch i is represented by $f_{i,j}(t)$ and these time trajectories can be of different length. The sampling time of the batch process is considered to be k. The original process variable can be mapped to new feature variables in function space.

$$\mathbf{X}(t)_{(I\times J)} = \begin{bmatrix} f_{1,1}(t) & f_{1,2}(t) & \cdots & f_{1,J}(t) \\ f_{2,1}(t) & f_{2,2}(t) & \cdots & f_{2,J}(t) \\ \vdots & \vdots & \ddots & \vdots \\ f_{I,1}(t) & f_{I,2}(t) & \cdots & f_{I,J}(t) \end{bmatrix} \quad (1)$$

where, I is the number of batches and J is the number of variables. Here, t varies from start of a batch to end of the batch, i.e. $t = [t_{\text{start}}, t_{\text{end}}]$, i.e. $t = t_{\text{start}} : k : t_{\text{end}}$. The main concept behind approximation using function space analysis is explained here briefly.

A set of linearly independent, orthonormal functions can be obtained such that they span the function space, i.e. a basis for the function space can be obtained (Ramsay & Silverman, 2005). Many such basis functions are available, e.g. Legendre polynomials, Fourier basis function, Bernstein polynomials, generalized orthogonal basis functions, etc. By approximation theory any function $f(t)$, which is assumed to be continuous and square integrable over a range space, can be expanded in the basis function as shown in (2).

$$f(t) \cong \hat{f}(t) = \sum_{i=0}^{N-1} c_i \phi_i(t) \quad (2)$$

where, $\{\phi_i(t)\}$ is a basis for the function space, $\{c_i\}$'s are coefficients and N is the number of basis functions used for approximation of $f(t)$. This $\hat{f}(t)$ is called the best approximation of $f(t)$ with respect to the basis $\{\phi_i(t)\}$. Any basis can be selected depending on the application and nature of the function (Ramsay & Silverman, 2005; Reiss & Ogden, 2007).

Approximation of trajectory of any variable of a batch process ($f(t)$) can be obtained in terms of N basis functions and corresponding coefficients as follows:

The basis function matrix $\mathbf{\Phi}$ can be generated as in (3). Then least squares estimate of the coefficients can be obtained from (4).

$$\mathbf{\Phi} = \begin{bmatrix} \phi_0(t_1) & \phi_1(t_1) & \cdots & \phi_{N-1}(t_1) \\ \phi_0(t_2) & \phi_1(t_2) & \cdots & \phi_{N-1}(t_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(t_K) & \phi_1(t_K) & \cdots & \phi_{N-1}(t_K) \end{bmatrix} \quad (3)$$

$$\hat{\mathbf{c}} = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T f(t) \quad (4)$$

where, $\hat{\mathbf{c}}$ is a vector containing estimated coefficients $\{c_i\}$'s given in (2). Selection of the number of basis functions to be used for approximation can be obtained based on the approximation effectiveness measure defined in (Chen & Liu, 2001).

3.2 Function space PCA

In this subsection, function space PCA methodology is explained in brief. The first step in applying function space PCA is to obtain a function approximation for each process variable across all batches with same number of basis functions (N). Note that the number of basis functions used for approximation of each variable may be different and will depend on the amount of variability in the variable. After function approximations are obtained, a two dimensional data matrix for trajectory coefficients can be written as (5). Thus, uneven length batch data is approximated using even length of coefficient matrix, making it possible to unfold three-dimensional historical data into a two-dimensional matrix.

$$\mathbf{C}_{I\times N} = \begin{bmatrix} [c]_{I\times N_1} & [c]_{I\times N_2} & \cdots & [c]_{I\times N_J} \end{bmatrix} \quad (5)$$

where, $N = \sum_{j=1}^{J} N_j$ and $[c]_{I\times N_j}$ is a trajectory coefficient matrix for variable j for all batches.

FSPCA based monitoring procedure takes the matrix **C** as representative historical data and a statistical model is obtained by applying PCA on **C**. Multivariate statistical control limits Q and T^2 are then obtained for monitoring of batches processes. When data for a new batch is available, its function approximation is obtained using the same number of basis function as used for function approximation of historical database. The new array of coefficients is then projected on to the principal components retained in the statistical model and compared against control limits for Q and T^2 (See Section 3.3 and 3.4, respectively). If none of the control limits are violated, then the product is of desired quality. However, if any one of the control limits is violated, then the product quality is not satisfactory and further analysis is required to ascertain the cause of bad product quality.

3.3 Q limit for FSPCA

Once a statistical model is build using the normal operation coefficient matrix, the next task is to define control limits that can be used for the monitoring of batch processes. The limits should be drawn for the variability along the principal axes retained (k) in the FSPCA model as well as for the variability along the principal axes not included ($n - k$) in the FSPCA model. These control limits are called Hotelling's T^2 and Q limits respectively.

Any significant deviation in the direction of ($n - k$) PCs (corresponding to smallest singular values), can be indicative of a fault. This deviation, i.e., the residual vector, can be calculated for the new measurement **x**, as in (6).

$$\text{Res} = \left(\mathbf{I} - \mathbf{P}\mathbf{P}^T\right)\mathbf{x} \quad (6)$$

where, **I** is an identity matrix and **P** is the loadings matrix. The value of Q statistic is defined as in (7).

$$Q = \text{Res}^T\text{Res} \quad (7)$$

The control limit for the Q statistic is chosen as 95% confidence limit from the normal operating residual values (Jackson & Mudholkar, 1979).

3.3 T^2 limit for FSPCA

Hotelling's T^2 statistic effectively captures normal operating region for the multivariate data in PCA. For the statistical models that are built using FSPCA, a similar statistic can be used to characterize the normal behavior of a batch process. The T^2 value for a PCA model is defined as in

$$T^2 = \mathbf{x}^T\mathbf{P}\mathbf{D}_\lambda^{-1}\mathbf{P}^T\mathbf{x} \quad (8)$$

where, $\mathbf{D}_\lambda$ is a diagonal matrix containing first k eigenvalues corresponding to the principal components retained in the statistical model. The control limit for the T^2 statistic is chosen as 95% confidence limit from the normal operating scores values (Ku *et al.*, 1995).

Although, the FSPCA based monitoring procedure is well equipped to handle unequal length batch processes, it is applicable only for offline monitoring. To overcome this limitation, a new online monitoring approach based on FSPCA is proposed in this paper. The proposed algorithm is discussed in the next section.

4. PROPOSED ONLINE MONITORING ALGORITHM

The FSPCA approach for batch process monitoring applies batch-wise unfolding to the historical three-dimensional data. One major disadvantage of this approach is that sense of time is lost due to unfolding and online monitoring is not possible. Thus, it is important to incorporate the notion of time while monitoring, if online monitoring is to be performed. Here a notion of time sliced model is proposed for FSPCA to overcome this limitation. Using time sliced model, statistical control limit for each time slice can be calculated and these control limits can be used for online monitoring and diagnosis. This approach of obtaining time sliced model is explained in detail in the next subsection.

4.1 Time Sliced FSPCA model

The first step towards online monitoring using FSPCA is to define time slice duration (t_s) based on duration of the batch process. The time slice duration should be chosen such that it is small enough to perform online monitoring and large enough to avoid unnecessary computational load. This aspect is discussed again in detail later along with a simulation case study. An FSPCA model is then obtained for each of the time slice duration.

The historical data for a batch process can be unfolded as given in (1). Each $f_{ij}(t)$ for different batches may have different length, while for a given batch (i), the duration will be same. A time slice matrix ($\mathbf{X}_S$) can be formed by substituting $t = t_{start} : k : t_s$. It is recommended that t_s should be

an integer multiple of k. A function approximation for batch trajectories of time slice matrix is then obtained, as per the discussions given in Section 3. Once coefficient $\mathbf{C}_S$ for the time slice matrix $\mathbf{X}_S$ is obtained, a statistical model is built by applying PCA on the coefficient matrix. The statistical control limits (Q and T^2) obtained here are the control limits at time t_s. Similarly the control limits for every nt_s times (where n is an integer) need to be calculated for each of the corresponding time slice matrix. A step-by-step modeling procedure is given below:

1. Obtain three-dimensional data matrix $\mathbf{X}_{I\times J\times K}$.
2. Select a time slice duration t_s and set $n = 1$.
3. Perform unfolding on the matrix X, to obtain a time slice matrix $\mathbf{X}_S = \mathbf{X}(nt_s)$ of dimension $I\times(Jnt_s/k)$.
4. Obtain a function approximation of trajectories in the time slice matrix $\mathbf{X}_S$ to generate coefficient matrix $\mathbf{C}_S$.
5. Build a statistical model by applying PCA on the coefficient matrix $\mathbf{C}_S$.
6. Calculate control limits for Q and T^2 and denote them as $Q(n)$ and $T^2(n)$.
7. Increase n by 1.
8. Repeat from step 2, until nt_s is greater than the maximum batch duration.

It is important to note here that if nt_s is greater than duration of any batch, then complete batch data should be taken while generating the time slice matrix.

Thus, in this proposed approach an incremental model is built for every nt_s duration and control limit for every time slice $Q(n)$ and $T^2(n)$ are obtained.

4.2 Online Monitoring using proposed FSPCA model

The proposed online monitoring algorithm evaluates plant condition at every time slice interval. The online measurements are collected for a time slice period and its function approximation is obtained using the same number of basis functions (N) as used during modeling. The coefficients thus obtained are projected onto the time slice FSPCA model obtained and residual (Q) and T^2 values are calculated. If any one of the control limits is violated, it can be indicative of a fault and a fault is detected at time nt_s. A step-by-step monitoring procedure is given below:

1. Set $n = 1$.
2. Collect online batch data for nt_s duration.
3. Obtain function approximation of each measurement trajectory using the same number of basis functions used while modeling.
4. Project the obtained coefficient vector on to the PCs retained in statistical model.
5. Calculate Q and T^2 values.
6. If any one of the control limits is violated, a fault is detected at time nt_s.
7. Increase n by 1.
8. Repeat from step 2, until the end of the batch.

The proposed online monitoring algorithm is expected to perform better for incipient faults as well as faults which are non-stationary. To demonstrate effectiveness of the proposed FSPCA based online monitoring approach, simulations were carried out. These simulation results are summarized in the next section.

5. SIMULATION CASE STUDIES

Applicability and usefulness of the proposed FSPCA based approach for online batch process monitoring is demonstrated using a simulation case study involving fed-batch penicillin cultivation process.

The proposed approach is validated on fed-batch penicillin fermentation process. The simulations were carried out using the PenSim v2.0 simulator (Birol *et al.*, 2002), which is available at http://www.chee.iit.edu/~cinar/software.html, developed by a research group of Illinois Institute of Technology, USA. The fed-batch process schematic is shown in Fig. 1. In the PenSim v2.0, there are provisions to change the duration of a batch and to introduce various faults. Faults can be introduced in aeration rate, agitator speed and substrate feed rate.

Here the total duration of a batch was randomly selected between 390 to 420 hours. Historical data was generated for 100 normal batches with sampling time of 0.2 hours. A total of 11 measurements were considered available online and the list of measured variables is given in Table 1. Small variations were added to simulation initial conditions to mimic real plant operating condition during normal operation. Measurement noise was added to all the variables such that signal to noise ratio is 5%. This was done exactly in the same manner as reported in (Lee, et al., 2004) so that a fair comparison can be made. Statistical models were developed using MPCA and the proposed FSPCA approach based on these 100 normal batches. The Bernstein polynomials (first 15 polynomials) were used as a basis for the function space.

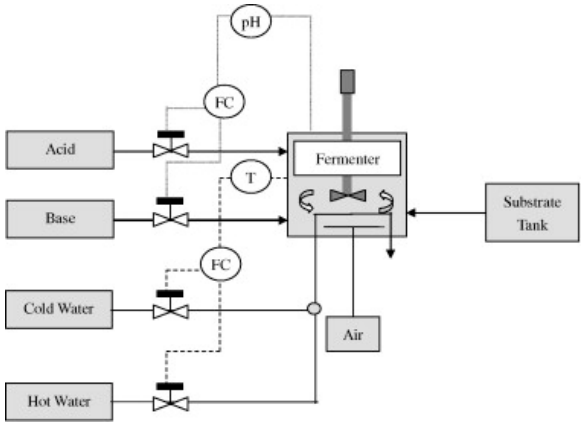

Figure 1: The fed-batch penicillin fermentation process

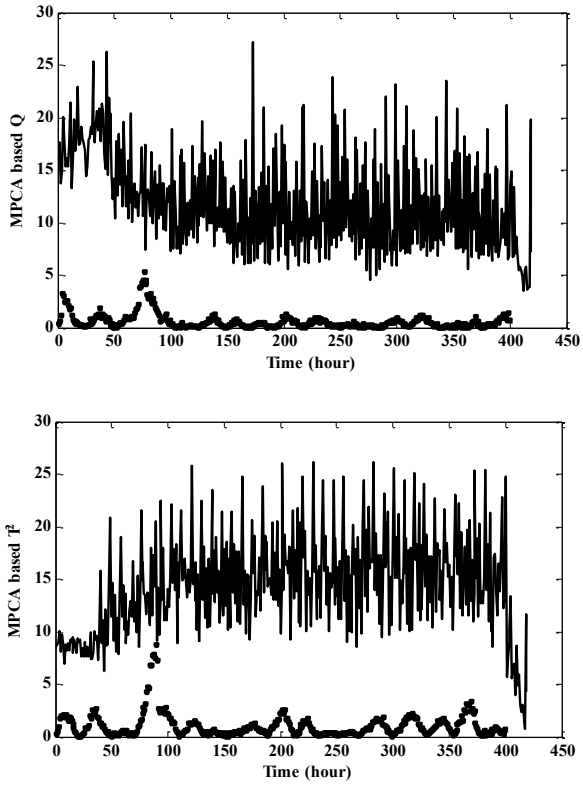

Figure 2: Modified MPCA based control charts for a ramp fault in agitator speed

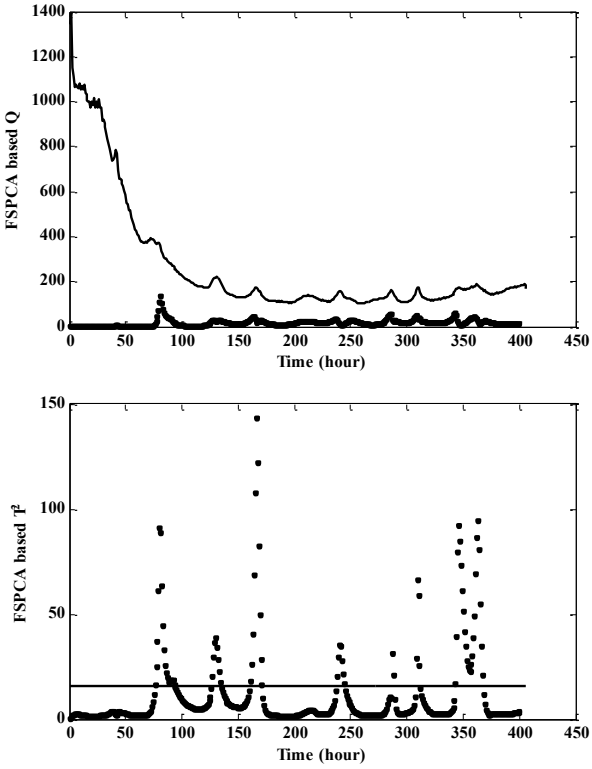

Figure 3: The proposed FSPCA based control charts for a ramp fault in agitator speed

Solid lines indicate 95% confidence limit and dots are online Q and T^2 values in Fig. 2 to Fig. 5.

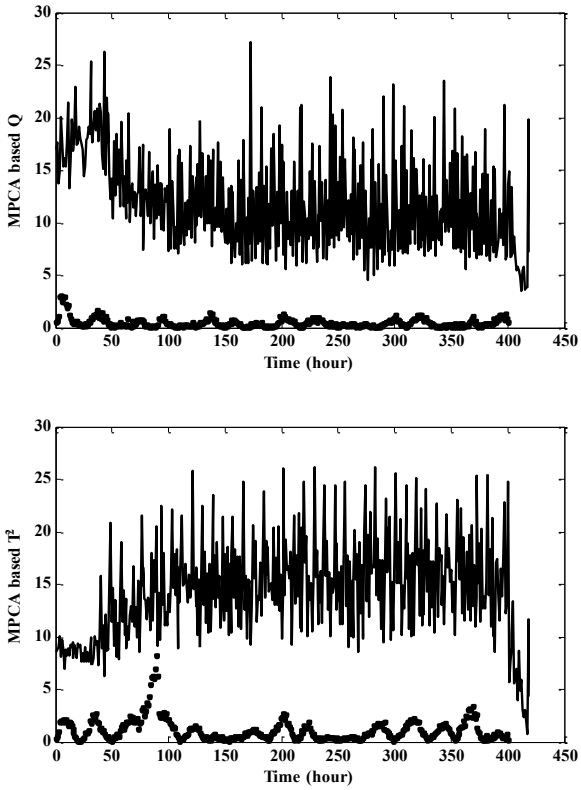

Figure 4: Modified MPCA based control charts for a ramp fault in aeration rate

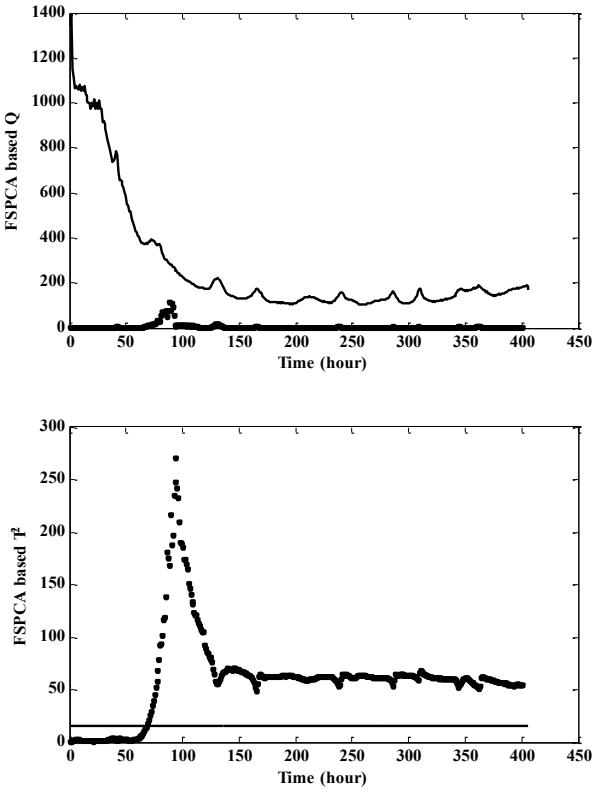

Figure 5: The proposed FSPCA based control charts for a ramp fault in aeration rate

Table 1: List of measured variables for the fermentation process

Number	Variables
1.	Aeration rate (l h^{-1})
2.	Agitator speed (W)
3.	Substrate Feed rate (l h^{-1})
4.	Substrate Feed Temp (K)
5.	Dissolved Oxygen Concentration (% saturation)
6.	Culture Volume (l)
7.	Carbon dioxide Concentration (mmol l^{-1})
8.	pH
9.	Bioreactor Temperature (K)
10.	Generated Heat (Kcal)
11.	Cooling Water Flow rate (l h^{-1})

Table 2: Faults introduced in fed-batch fermentation process

Fault	Fault Type	Mag. of Fault	Fault Time (h)	MPCA	Proposed FSPCA
Aeration Rate	Step	5.0	30-180	☑	☑
		-5.0	70-180	☑	☑
	Ramp	0.025	50-90	☒	☑
		0.03	70-100	☒	☑
Agitator Speed	Step	5.0	30-100	☑	☑
		-5.0	50-90	☑	☑
	Ramp	0.13	50-90	☒	☑
		0.3	50-90	☒	☑
Substrate Feed Rate	Step	-15	50-170	☑	☑

The time slice duration was considered to be 1 hour, i.e. monitoring of batch process was carried out every hour. It is sufficient to monitor this 400-hour batch process condition every hour without compromising on diagnostic performance along with acceptable computational load and hence the time slice duration should be selected based on the nature of the batch process. As the proposed FSPCA methodology accounts for variability in the data for every time slice period, it is expected that it will result in better diagnostic performance for incipient faults.

To evaluate performance of monitoring methodologies based on MPCA and the proposed FSPCA, several fault cases were also simulated. These fault conditions are listed in Table 2. Either a sudden step or a slowly varying ramp type faults were introduced in aeration rate, agitator speed and substrate feed rate. As can be seen from Table 2, MPCA is not able to identify ramp type of faults (marked as ☒), i.e. incipient faults. Compared to that FSPCA is correctly able to detect all faulty operations. The same has been demonstrated using monitoring plots shown in Fig. 2 through Fig. 5. Based on Q and T^2 plots for MPCA and the proposed FSPCA method, it can be seen that MPCA is not able to detect a ramp fault in agitator speed and aeration rate. On the other hand, the proposed FSPCA algorithm is easily able to detect these faults. Thus the proposed FSPCA algorithm is better suited for detecting slowly varying incipient faults.

6. CONCLUSION

In this paper an online monitoring algorithm based on FSPCA is proposed. FSPCA employs batch-wise unfolding of three-dimensional data and online monitoring cannot be performed using conventional FSPCA algorithm. Here, a time slice modelling approach is proposed based on FSPCA, which is better suited at capturing time varying batch process dynamics. It has been shown that FSPCA is better suited for monitoring of slow incipient faults compared to modified MPCA approach proposed earlier.

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