A STAGE-BASED MONITORING METHOD FOR BATCH PROCESSES WITH LIMITED REFERENCE DATA

Ningyun Lu [1,2], Yi Yang[1], Fuli Wang[2], Furong Gao[1*]

[1]*Department of Chemical Engineering*
The Hong Kong University of Science & Technology
Clearwater Bay, Kowloon, Hong Kong

[2]*School of Information Science and Engineering*
Northeastern University
Shenyang, Liaoning, P. R. China

Abstract: A method is proposed for batch process monitoring and fault diagnosis, starting from a single batch reference data and updating with accumulation of successive batches. A moving data window method is adopted for exploring local covariance structure, stage division, and the development of monitoring models. The application to an injection molding process shows the effectiveness and feasibility of the proposed method for batch industry.

Keywords: Batch process monitoring, Principal component analysis, Multistage modeling, Injection molding.

1. INTRODUCTION

Batch processes are widely used in chemical, semiconductor, food and biology industry for producing high-value-added products to meet today's rapidly changing market. Batch processes are characterized by prescribed sequential operations in an infinite duration; they are subject to various disturbances that may affect the final product quality and the degree of reproducibility. Proper monitoring and diagnosis of the process is important for safety and quality improvement (Kourti and MacGregor, 1995; Kosanovic et al., 1996; Wold et al., 1998; Louwerse and Smilde, 2000; Sprange et al., 2002; Ündey and Cinar, 2002; Kourti, 2003).

Most batch process monitoring methods are based on such multivariate statistical projection techniques as multi-way principle component analysis (MPCA) and partial least squares (MPLS) (Nomikos and MacGregor, 1994, 1995a, 1995b). In those methods, all correlation information in process variables over the whole batch duration are extracted to develop a statistical model for the monitoring of the processes. This type of models is effective in determining whether or not a batch operation is normal as a post process analysis tool. The requirement of many cycle reference data and the drawbacks associated with on-line process monitoring may hinder its wider application to the industry.

With the existing methods, the reference data collected for modeling are expected covering statistically all normal batch-to-batch variation. This is relatively easy for batch processes with short operation duration and processes that are inexpensive to conduct many trial runs. Some slow batch processes, such as bio-related processes, however, may take exceptionally long time to complete a batch run. In this case, a method will be needed for developing a monitoring model with a minimal batch cycle, for example, one successful batch run. The model can be improved with the

* Corresponding author: E-mail: kefgao@ust.hk; Tel: +852-2358-7139; Fax: +852-2358-0054

newly available batches, without having to wait for sufficient successful batches.

This paper proposes to develop such a monitoring method starting with minimum successful batches. The initial database may contain only one successful batch run. The basic unit for modeling is a moving data window. In each window, data are arranged as a two-way matrix, where each row contains process measurements at each sampling interval, and rows are arranged according to time. Data windows are properly normalized before being used to derive a PCA model for each window to extract local covariance information. This method is termed the moving time-window PCA-based batch modeling in this paper.

The proposed moving time-window PCA is similar to the moving principal component analysis by Kano et al. (2001), which was developed for continuous processes for detecting changes of process operation condition. Lennox et al. (2001) had also presented a method called moving window PCA for batch processes. Their method, however, also requires sufficient successful batches for modeling.

As mentioned before, the PCA model of each time window contains local covariance information. Although batch process variables are time-varying, the local covariance structure in process measurements will be similar when the data of two windows have the similar underlying characteristics. This idea is similar to the method of the authors (Lu et al., 2004a), in which a batch process is divided into "stages" according to the changes of process correlation, and then a sub PCA model is built for each stage for monitoring. The differences between this proposed method and previous method lie in: (1) this paper focuses on the change of the covariance structure in time direction, not in batch direction; and (2) it requires only one reference batch for initial modeling, and the model is updating with the accumulation of new successful batch data. The details of the proposed method are given in section 2. An illustrative example is shown in section 3. Conclusions are given in the last section.

2. METHODOLOGY

2.1. Moving time-window PCA-based batch modeling

As mentioned before, it is attractive to develop a data-based model for process monitoring using limited batches. In this proposed modeling method, the reference data can be an arbitrary successful batch of history, represented as $X(N\times m)$, where N is the total sampling points in the batch run, and m is the number of process variables. As illustrated in Figure 1, a moving time window of the batch is proposed to extract the local covariance information.

The data in a window are arranged as a two-way matrix, noted as $\tilde{X}(n\times m)$, where n is the data length in a window. Obviously, a large window will result in stable local PCA models, reliable but slow fault detection; a small window can rapidly detect process abnormalities but may have excessive false alarms. In this paper, n is approximately of two or three times of the number of process variables, as recommended in the field of multivariable regression to ensure a reliable statistical model (Johnson and Wichern, 2002). Moving step can be set as small as 1 for prompt fault detection.

With this arrangement, $(N-n)$ number of windows can be resulted for each batch, designated as, $\tilde{X}^k$, $(k=1,\cdots,N-n)$. Each window should be mean-centered to provide the reference trajectories of process variables for normalizing the new batch for online process monitoring. At the same time, the measurements should be also properly scaled to eliminate the influence of different measuring units. After normalization, PCA can be applied to each moving time-window, $\tilde{X}^k=\tilde{T}^k\cdot(\tilde{P}^k)^T$. The resulted PCA loading matrices, $\tilde{P}^k(m\times m)$, contain process covariance information in the k^{th} data window.

Although the batch process variables are time varying, the covariance structure of two neighboring windows will not change much, provided that the process characteristic does not change rapidly. During the time when the process is driven by the

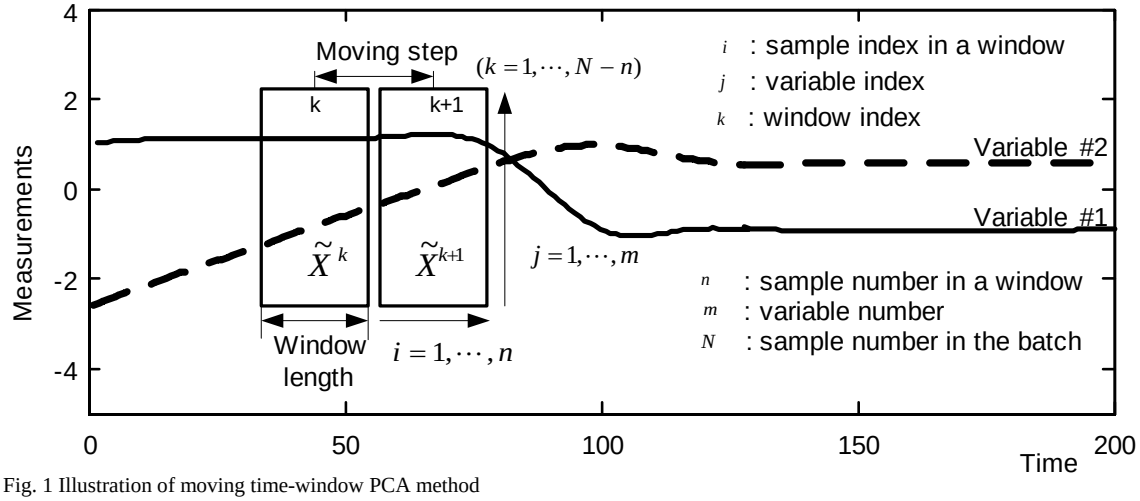


Fig. 1 Illustration of moving time-window PCA method

similar underlying characteristic, those windows will have similar covariance structures, consequently, the similar PCA loading matrices. In this way, a batch process can be divided into several stages or phases, of different process characteristics. Covariance structure changes, in corresponding to the changes of process characteristics, can be used to divide the process into stages.

There are several methods for defining the similarity of two PCA loading matrices. For instance, Krzanowski (1979) presented a PCA similarity factor as a measure of the similarity between two data spaces; and Johannesmeyer et al. (2002) discussed a statistical method for comparing two PCA models by calculating the T^2 and/or Q similarity factor. The existing methods are, however, ill-suited for partitioning simultaneously a large number of PCA models into groups according to their similarities. The PCA loading clustering algorithm (Lu et al., 2004a) is adopted here to divide the moving time-window PCA models into groups to reflect the change of process covariance structure. By the clustering algorithm, $(N-n)$ number of moving time-window PCA loading matrix $\tilde{P}^k$ are partitioned into C number of sub groups, where the loading matrices remain similar within the same group, but showing significant difference between groups. The clustering results, associated with process operation time, can be used to define process sub stages. The scheme of stage division is illustrated in Figure 2.

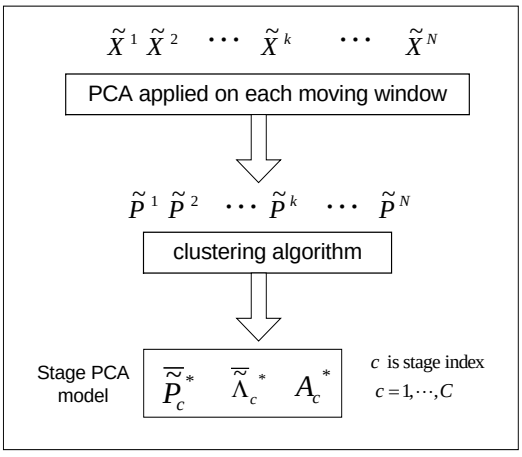


Fig. 2. Scheme of stage-division based on window's PCA loading matrices.

A stage PCA model can be developed by finding an optimal PCA loading matrix as the representative one for that stage, mathematically,

$$\begin{aligned}\tilde{P}_c^* &= \underset{k}{Min}\left\|\tilde{P}^k - \tilde{P}_c^*\right\| \\ &= \frac{1}{n_c}\sum_k \tilde{P}^k (c=1,\cdots,C; k=1,\cdots,n_c)\end{aligned}, \quad (1)$$

where n_c is the number of loading matrices belonging to stage c $(c=1,\cdots,C)$. The stage representative loading matrix, $\tilde{P}_c^*$, is divided into two parts, $\bar{P}_c^*(m\times A_c^*)$ and $\tilde{\bar{P}}_c^*(m\times(m-A_c^*))$, for principal component and residual subspaces, where the number of retained principal components, A_c^*, can be selected also by the method (Lu et al., 2004a). Similarly, the stage representative singular value matrices, $\bar{\Lambda}_c^*$, are also defined for monitoring.
For data $\mathbf{x}(1\times m)$, the principal component score and SPE can be calculated by the following stage PCA model,

$$\begin{aligned}\mathbf{t} &= \mathbf{x}\bar{P}_c^* \\ \mathbf{e} &= \mathbf{x} - \mathbf{x}\bar{P}_c^*(\bar{P}_c^*)^T \\ SPE &= \mathbf{e}^T\mathbf{e}\end{aligned}. \quad (2)$$

The initial control limit trajectories for the two statistics, Hotelling-T^2 and Q (or SPE), are estimated from the first successful reference batch. With new batches available, the control limits can be gradually updated to focus more on the batch-to-batch variation. The determination of the initial control limits and the updating procedures are given in the next.

2.2. On-line monitoring and model updating

In on-line monitoring, one should first determine which stage new data of the evolving batch belong to before calling the corresponding stage PCA model to calculate the two statistics. Since process operation time can be associated with the stage division results, one can determine the stage that new data belong to by simply checking which time span the current sampling falls to. Process monitoring is conducted by comparing the two statistics with the predetermined control limits. When the statistics go beyond the control limit, responding to an abnormality, the contribution plot (Miller et al., 1998), a commonly used diagnosis tool, can be used to show the variables impacted by the occurred abnormality.

The proposed stage monitoring method has been derived from a single reference batch, considering only within-batch information. Batch-to-batch variation information can also be explored with accumulation of batches, *e.g.*, by adjusting the stage representative PCA loading matrix and the control limit of SPE.

Initial Control limits of the two statistics

The control limits of Hotelling-T^2 are estimated for each stage, while the SPE limits are estimated within each moving window.

$$T^2 = \mathbf{t}(\bar{\Lambda}_c^*)^{-1}\mathbf{t}^T \sim \frac{A_c^*(n_c-1)}{(n_c-A_c^*-1)}F_{A_c^*,(n_c-A_c^*-1),\alpha}. \quad (3)$$

Adopting the works of Box (1954) and Jackson and Mudholkar (1979), the SPE statistic can be approximated by a weighted Chi-squared distribution, $g\chi_h^2$, where the weight g and the freedom degree h can be obtained following the same approach of

Nomikos and MacGregor (1995a). The parameters of the $g\chi^2_h$ distribution at time k are estimated from the SPE values in the moving window $\tilde{X}^k(n\times m)$, that is, $g^k = v^k/2m^k$ and $h^k = 2(m^k)^2/v^k$, where m^k is the average of the window's SPE values and v^k is the corresponding variance. Thus, SPE control limit at time k can be approximated by,

$$SPE^k_\alpha = (v^k/2m^k)\chi^2_{x(m^k)^2/v^k,\alpha}. \quad (4)$$

Stage model and the SPE control limits updating

When a new batch run follows the similar operation sequence and variable trajectories of the reference, it can be considered as a normal batch. The stage PCA models, reference trajectories and control limits, should be adjusted to include the normal batch-to-batch variation.

The stage representative PCA loading matrix as defined in Equation (1), *i.e.*, the center of the window's PCA loading matrices that belongs to stage *c*, may move with the accumulation of new successful batch data. The new center can be readily obtained by recalculating Equation (1) with the window's PCA loading matrices for the new normal batch.

The control limits detailed in the last section are derived from one reference batch, they may be too tight (or loose) in certain periods for monitoring a new batch. It is desirable to adjust the control limits by taking the batch-to-batch variation into account. For the initial SPE control limits, SPE^k_α are estimated from the SPE values of the data in the window, $\tilde{X}^k(n\times m)$. In the updating procedure, the data used for estimating the parameters in Equation (4) can be augmented to include the data of the new batch,

$$\tilde{X}^k_{new} = \begin{pmatrix} \tilde{X}^k \\ \mathbf{x}^k_{new} \end{pmatrix}, \quad (5)$$

where $\tilde{X}^k_{new}$ is gradually filled by the new data at time k of different batches. By doing so, the moving window will contain more and more batch-to-batch variation, and the SPE control limits estimated from this new data window will be correspondingly adjusted.

3. ILLUSTRATIVE EXAMPLE

The proposed modeling and monitoring method is tested on a batch process, injection molding process. Although the proposed method is developed for those long batches, the method works equally well with a relatively short batch such as the injection molding process.

3.1. Injection molding process

Injection molding (Rubin, 1972; Yang and Gao, 1999), a key process in polymer processing, transforms polymer materials into various shapes and types of products. A typical injection molding process consists of three physical stages, injection of molten plastic into the mold, packing-holding of the material into the mold under pressure, and cooling of the plastic in the mold until the part becomes sufficiently rigid for ejection. Plastication takes place in the barrel in the early cooling phase, where polymer is melted and conveyed to the front of barrel by screw rotation, preparing for next cycle.

Figure 3 shows a simplified diagram of a typical reciprocating-screw injection molding machine with instrumentations. Several normal batches are collected under the same operation condition to the previous work (Lu et al., 2004b), among which an arbitrary batch is used for modeling, and the other cycles are used for model updating. An abnormal batch with check-ring problem is also conducted to test the proposed process monitoring and diagnosis scheme. Ten process variables are selected for modeling, that is, Nozzle Pressure (No.1), Stroke (No.2), Injection Velocity (No.3), Hydraulic Pressure (No.4), Plastication Pressure (No.5), Cavity Pressure (No.6), Screw Rotation Speed (No.7), SV1 valve opening (No.8), SV2 valve opening (No.9), and Mold Temperature (No.10), respectively. Window length is set to be 30 and moving step is 1.

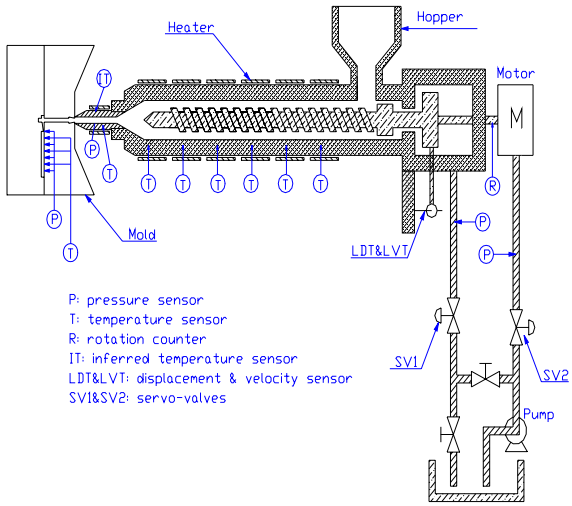


Fig. 3. Simplified illustration of injection molding machine and measuring points

3.2. Experimental results

Without using any prior process knowledge, the proposed algorithm automatically divides the trajectories of the injection molding batch into eight stages according to the change of local covariance structure, among which four long stages correspond to the four physical operation stages, *i.e.*, injection, packing-holding, plastication and cooling stages. Short new stages emerge between the four main stages, corresponding to the transitions from one major stage to the next. Dividing a batch process

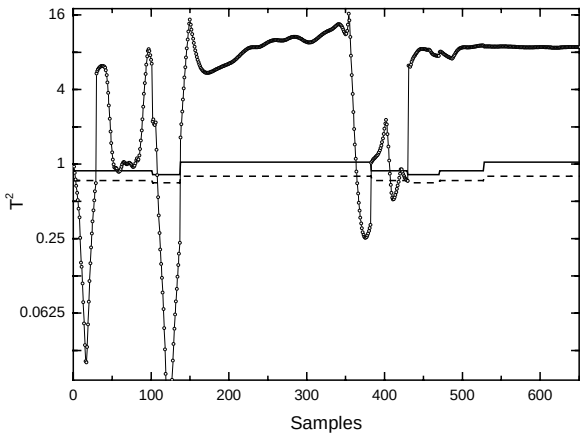
into “steady” and transient stages can not only benefit process monitoring and diagnosis, but enhance process understanding.

On-line process monitoring and fault diagnosis are conducted by judging whether the scores and SPE value of the coming measurements in a running batch are below the control limits. In the on-line monitoring of the batch with check-ring problem, both the T^2 and SPE charts can detect the fault, as shown in Figure 4. Hotelling-T^2 statistic is more sensitive than SPE because the failure of check-ring valve will not significantly deteriorate the covariance structure of time direction, however, the deviations from the reference variable trajectories result in large principal component scores, hence, have significant T^2 values.

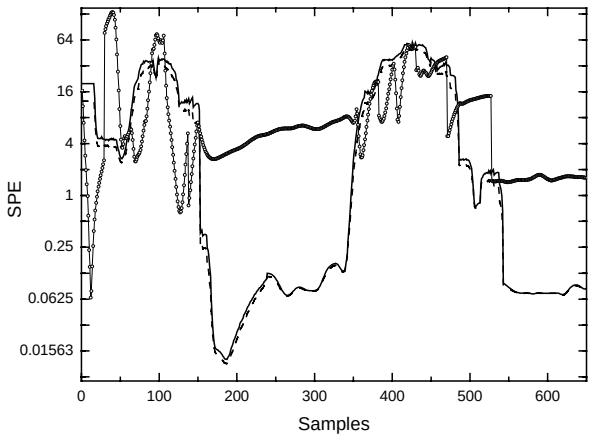
By process knowledge, the check-ring problem occurs in the injection stage, also impacts the packing-holding and plastication stages, but have little influence to the cooling stage. The monitoring results shown in the T^2 chart of Figure 4 agree well with the aforementioned. As the check-ring problem has no influence on the cooling stage, the plot for this long stage is not given to allow more detailed presentation of the results in the affected stages. The SPE chart of Figure 5 shows, the monitoring of the same fault with control limits updated with ten successful cycles. A comparison of Figures 4 and 5 show the adjustment of the control limits, by considering the batch-to-batch variation. The results are similar, indicating that it is viable to monitor such a process starting with just one cycle data. The diagnosis result is shown in the contribution plot in Figure 5, where Nozzle Pressure (No.2), Stroke (No.3), Injection Velocity (No.4), Hydraulic Pressure (No.4), Cavity Pressure (No.6) and Mold Temperature (No.10) are seriously impacted by the detected fault. This fault pattern is well agreed with the check-ring problem. Detailed description on the check-ring problem can be found in reference (Lu et al., 2003).

4. CONCLUSION

A new batch monitoring method has been proposed for those cases where there exist difficulties in collecting sufficient cycles in limited time. The proposed method uses a single batch reference data to extract local covariance information by applying



(a)



(b)

Fig. 4. Monitoring charts of a faulty batch with check-ring problem.
(a). Hotelling T^2 monitoring chart;
(b). SPE monitoring chart.
(Solid line, 99% control limit; Dash line, 95% control limit)

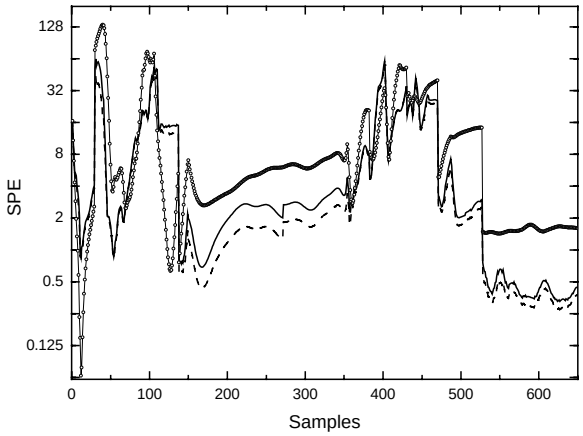


Fig. 5. SPE monitoring chart with updated control limits for the batch with check-ring problem.
(Solid line, 99% control limit; Dash line, 95% control limit)

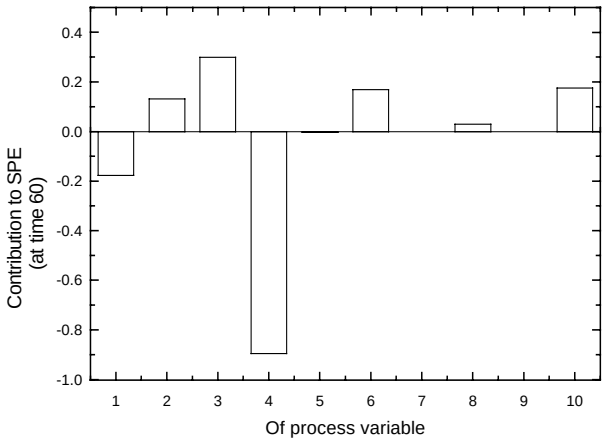


Fig. 6. Contribution plots for the batch with check-ring problem.

PCA on a moving time-window that scans process trajectory over the batch duration. Process stages are determined by analyzing the change of process covariance structure, by partitioning the window's PCA loading matrices using a clustering algorithm. A sub PCA model has been developed for each stage according to the clustering results. Model updating has also been discussed with newly available batches. The proposed modeling method can not only give a valid monitoring scheme with a minimal reference batch, but also it can divide the batch into stages. The division of a batch process without the requirement of prior process knowledge can improve process monitoring efficiency in terms of reduction of computation resources, also enhance process understanding, and consequently benefit fault diagnosis.

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