STAGE-BASED MULTIVARIATE STATISTICAL ANALYSIS FOR INJECTION MOLDING

Ningyun Lu, Yi Yang, Furong Gao*,

Department of Chemical Engineering
The Hong Kong University of Science & Technology
Clearwater Bay, Kowloon, Hong Kong

Fuli Wang

School of Information Science and Engineering
Northeastern University
Shenyang, Liaoning, P. R. China

Abstract: A multistage based PCA modelling and monitoring approach is demonstrated in this paper to injection molding process, a typical multistage batch process. Analysing the changes of process correlation can lead to effective division of a batch process into several "operation" stages, in good agreement with process knowledge. This shows that multistage based sub-PCA model can be employed not only for effectively process monitoring and fault diagnosis, but also to enhance process understanding.

Keywords: Multivariate statistical analysis, Principal component analysis, Process monitoring, Injection molding, Multi-stage batch process.

1. INTRODUCTION

Batch processes become increasingly preferred choices in chemical industry, to produce higher-value-added products to meet today's rapidly changing market. It is, however, difficult to develop a first-principle or knowledge-based model for process monitoring due to the process high dimensionality, complexity, and batch-to-batch variation, and also due to limited product-to-market time. Multivariate statistical modelling methods, which require only historical process data for analysis and monitoring, and have had many successful applications for continuous processes, are attracting much interest in analysing and monitoring batch processes.

Several statistical modelling methods have been reported recently for batch processes (Wold, et al., 1987; Nomikos and MacGregor, 1994; Dong and McAvoy, 1996; Martin and Morris, 1996; Chen and Liu, 2002), all of which are based on multiway PCA (MPCA), a very popular method for modelling a batch process. These MPCA-based methods, however, are not well-suited for multistage processes because MPCA takes the entire batch data as an object and has difficulty to reveal the changes of process correlation from stage to stage. The on-line application of these MPCA-based methods requires to fill the future unavailable process data in the batch, which can affect the promptness and accuracy of on-line monitoring. Louwerse and Smilde (2000) argued for a strategy to partition reference data into several time periods for improvement of on-line monitoring. But, their method, also based on MPCA, requires also the future measurements unavailable for each remaining time period to be estimated for on-line monitoring. Their method has the same weakness as the MPCA method. Adaptive batch monitoring strategy based on recursive multiblock PCA proposed by Rännar, et al. (1996) can avoid the need of filling the future data. Its computational demand, however, can be overwhelming.

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

Considering that multiplicity of operation stage is an inherent nature of most batch processes, and to alleviate the difficulties of on-line monitoring based on multiway PCA, a stage-based sub-PCA method has been developed by the authors to extend multivariate statistical modelling methods to those multistage batch processes (Lu, et al., 2002). The key to the stage-based sub-PCA monitoring strategy is to divide a batch process into several "operation" stages, according to the changes in process correlation. Within each of these "operation" stages, the process correlation is similar; a representative stage model can be built, using the conventional two-way PCA model. This method allows two-way PCA to be "directly" applied for a batch process.

This paper is to show an industrial application of the proposed stage-based sub-PCA method to a typical multistage batch process, an injection molding process. We will demonstrate that the use of the proposed method can not only improve the ability of process monitoring and fault diagnosis, but also improve the understanding of the process. It is worthwhile to note that the stages defined by the sub-PCA method may be not equal to the real operation stages, as the covariance structure can change during a physical stage. The remainder of the paper is organized as follows: a brief description to the injection molding process is given in Section 2, followed by the introduction of sub-PCA modelling procedures and post data analysis in Section 3. The application of the method for process monitoring and fault diagnosis for injection molding process is described in Section 4. Finally, conclusions are drawn in Section 5.

2. PROCESS DESCRIPTION

Injection molding (Yang and Gao, 1999; Chen, 2002), an important polymer processing technique, transforms polymer materials into various shapes and types of products. Figure 1 shows a simplified diagram of a typical reciprocating-screw injection molding machine with instrumentations.

As a typical multistage process, injection molding operates in stages, among which, injection (or filling), packing-holding, and cooling are the most important phases. During filling, the screw moves forward and pushes melt into the mold cavity. Once the mold is completely filled, the process then switches to the packing-holding stage, during which additional polymer is "packed" at a high pressure to compensate for the material shrinkage associated with the material cooling and solidification. The packing-holding continues until the gate freezes off, which isolates the material in the mold from that in the injection unit. The process enters the cooling stage; the part in the mold continues to solidify until it is rigid enough to be ejected from the mold without damage. Concurrently with the early cooling phase, plastication takes place in the barrel where polymer is melted and conveyed to the front of barrel by screw rotation, preparing for next cycle.

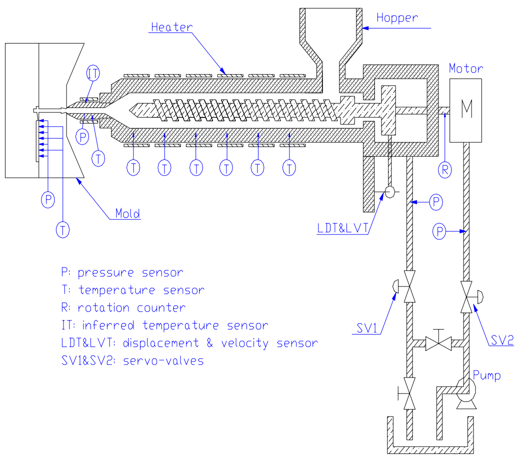


Fig. 1. Simplified illustration of injection molding machine and measuring points

As shown in Figure 1, an injection molding machine like the one in our lab is well instrumented. All key process conditions such as the temperatures, pressures, displacement and velocity can be online measured by their corresponding transducers, providing abundant process information. However, many of these process variables are correlated and time varying. In addition, different stages of operation can lead to different process behaviours, as discussed in detail in the next section. It is an ideal candidate for application of the proposed stage-based multivariate statistical modelling.

For injection molding, high degree of automation is possible. After the process conditions are properly set, the process repeats itself to produce molded part at a high rate. The process is, however, susceptible to the production of off-spec products due to various process malfunctions, drifting of process conditions, changes in materials, and unknown disturbances. Abrupt, gross faults in the key process variables can be easily and reliably detected by the conventional SPC chart. Slow drift or faults involving multiple process variables, however, can be hard to detect. These process faults, even if they are small and not common, can lead to production of large quantity of bad parts, if they are not detected earlier.

The material used in this work is high-density polyethylene (HDPE). The process variables selected for modelling are shown in Table 1. The operating conditions are set as follows: injection velocity is 24mm/sec; mold temperature equals 25ºC; seven-band barrel temperatures are set to be (200, 200, 200, 200, 200, 180, 160, 120) ºC; packing-holding time is

Table 1 Description of the process variables

No.	Variable's description	Unit
1	Nozzle Pressure	Bar
2	Stroke	mm
3	Injection Velocity	mm/sec
4	Injection Pressure	Bar.
5	Plastication Pressure	Bar
6	Injection Cylinder Pressure	Bar
7	Cavity Pressure	Bar
8	Screw Rotation Speed	RPM
9	SV1 opening	%
10	SV2 opening	%
11	Cavity Temperature	°C
12	Nozzle Temperature	°C
13	Barrel Temperature 1	°C
14	Barrel Temperature 2	°C
15	Barrel Temperature 3	°C
16	Barrel Temperature 4	°C

fixed to be 3 seconds with total cycle time around 20 seconds. Totally, 60 normal batch runs are conducted under this operating condition. Another three batch runs are conducted under abnormal conditions for the sub-PCA based process monitoring and diagnosis scheme, as detailed in Section 4.

3. MULTISTAGE SUB-PCA MODELING

3.1. Data pretreatment

Consider a batch process with J process variables measured over sampling points k ($k = 1,2,\cdots,K$); a data matrix of dimensions $J \times K$ is generated from each batch run. A set of I number of normal batch runs hence result in a three-way process data matrix, $X(I \times J \times K)$, which is the most popular data form for batch process.

For the injection molding process as illustrated in this paper, about 1000 measurements for each variable, after removing the meaningless data at the end of each batch run, result in the reference data matrix $X(I \times J \times K)$ of dimension $60 \times 16 \times 1000$. The reference data should be properly scaled before process modelling. Several kinds of scaling methods are argued for the three-way reference data sets by Westerhuis, et al. (2000). For a multistage batch process, different process variables dominate different stages; it is desirable to scale process variables within batch run to retain the inherent weights in different stages. In this work, process variables are normalized by mapping the original measurements into [0,1].

The reference data for batch process is a three-way matrix with three directions standing for batch runs, process variables and sampling points, respectively. To analyse the correlation structure in different batch runs at each sampling time, the reference three-way matrix is unfolded along the time direction, resulting in K number of time-slice matrices, $\tilde{X}^k_{I\times J}$. The conventional two-way PCA method is directly applied to these time-slice matrices to extract the correlation information.

3.2. Multistage sub-PCA modelling

The key to multistage sub-PCA is based on the recognition of the following: (1). a batch process may be divided into several stages, based on its process characteristics; (2). process correlations in two time-slice matrices is similar if the data are sampled within the same stage, despite of the fact that the process may be time varying. The changes of operation stages result in changes of the correlation structures in the time-slice matrix series; also, changes of the correlation may also indicate changes in the process stages.

For each $\tilde{X}^k$, conventional PCA can be applied directly because each batch run can be considered to be independent, and the process variables at time k for each batch run can also be viewed as independent. $\tilde{X}^k$ can then be decomposed by,

$$\tilde{X}^k = \tilde{T}^k (\tilde{P}^k)^T \; (k = 1,2,\cdots,K). \qquad (1)$$

The p-loading matrix, $\tilde{P}^k$, in fact contains the correlation information, which can be used to guide the division of the batch process and to build sub-PCA models. A special designed clustering algorithm is introduced to cluster these K numbers of p-loading matrices, $\tilde{P}^k$ ($k = 1,2,\cdots,K$), into C groups, representing C numbers of "operation" stages for a batch process. Define P_c^* ($c = 1,2,\cdots,C$) as the representative p-loading matrix for the c^{th} stage as,

$$P_c^* = \underset{k}{Min}\left(\left\|\tilde{P}^k - P_c^*\right\|^2\right) = \frac{1}{n_{stage\_c}}\sum_k \tilde{P}^k \qquad (2)$$

$$(c = 1,2,\cdots,C;\, k = 1,2,\cdots,n_{stage\_c})$$

where n_{stage_c} stands for the amount of the process data belonging to the stage *c*.

Similar to that in PCA, P_c^* is divided into two parts, $\overline{P}_c^*$ and $\tilde{P}_c^*$, for principal component subspace and residual space, respectively. In each stage c ($c = 1,2,\cdots,C$), the representative p-loading matrix, P_c^*, is then used to construct a sub-PCA model for stage c as,

$$\begin{aligned} \tilde{T} &= \tilde{X}(\overline{P}_c^*)^T \\ \hat{\tilde{X}} &= \tilde{T}\overline{P}_c^* \\ \tilde{E} &= \tilde{X} - \hat{\tilde{X}} = \tilde{X}(I - \overline{P}_c^*(\overline{P}_c^*)^T). \end{aligned} \qquad (3)$$

The stages may be associated with process time spans if the process is controlled by a time sequence. However, this may lead to occasional mis-grouping of new process data into a wrong stage, due to batch variation. Some characteristic process variables may also be used to better reflect the stage changes, for example, conversion rate for a batch reactor. Alternatively, the control limits at the edges of each stage can be relaxed to reflect the process transient nature from one stage to another.

3.3 Post data analysis

As shown in Figure 2, the p-loading clustering algorithm can divide the process into four main stages and two transient stages according to the change of process correlation. The cooling stage, a long operation stage, actually consists of plastication phase and cooling phase, which can be clearly

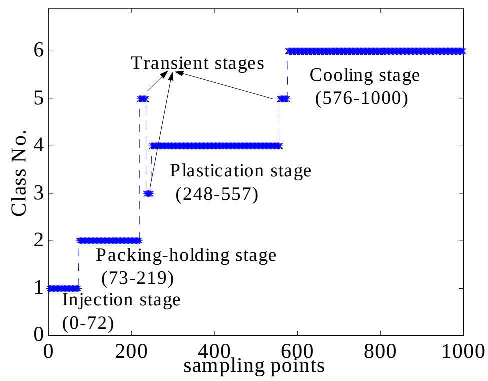


Fig. 2. Stage division of injection molding process by sub-PCA method

Table 2 Sub-PCA models in four operation stages

	Injection stage		Packing stage		Plastication stage		Cooling stage	
	.26	-.11	.36	-.15	.05	-.03	.02	.03
	.20	-.08	.38	-.16	.23	-.12	0	0
	.38	-.17	.01	-.01	.10	-.06	0	0
	.34	-.15	.35	-.15	.06	-.03	.04	.04
	0	0	0	0	.44	-.23	0	0
	.37	-.13	.06	0	0	0	.14	.15
	.02	-.01	.37	-.16	.02	-.01	0	0
*	0	0	0	0	.41	-.22	0	0
	.38	-.18	.27	-.11	.22	-.13	.55	.68
	0	0	0	0	.45	-.25	0	0
	.29	-.14	.34	-.16	.23	-.15	.20	.28
	.30	-.11	.34	-.12	.08	-.02	.10	.09
	.18	.48	.18	.48	.22	.46	.35	-.38
	.20	.49	.19	.50	.22	.47	.38	-.38
	.18	.47	.18	.47	.22	.45	.36	-.33
	.23	.39	.23	.40	.29	.37	.47	-.14
**	90.02		90.51		88.53		84.82	

***** denotes p-loading vectors.

****** denotes the percentage of explained variance by the retained principal components.

divided by sub-PCA method. A few samples in the transient response from packing-holding phase to plastication phase and from plastication phase to cooling phase form two new stages, called transient stage. Four sub-PCA models are then derived for the four main stages. This PCA analysis results in similar stage division to the actual stages used in polymer processing industry, which suggests that the stage division based on the proposed p-loading clustering method can indeed promote the process understanding.

The p-loadings of the stage PCA models are listed in Table 2. The p-loading plots, which are obtained by plotting the second loading vector against the first, indicate the correlation structure of process variables. Variables, located in the same clustering, have high correlation; variables in different clustering have weak relation (Kaspar and Ray, 1992; Yang et al., 2002). As illustrated in Figure 3, process variables (except barrel temperatures) form different clustering in different stage, indicating that these variables have different correlation structures at different stages. The variables located in the circle have small values in the p-loading vectors, indicating that they are

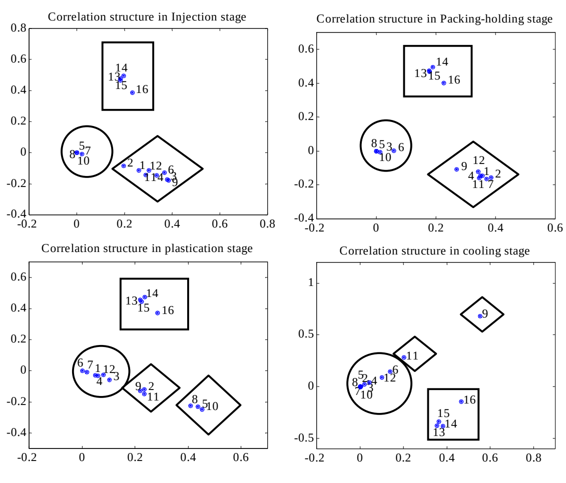


Fig. 3. Correlation structures shown in the p-loading plots. Variables in circle are “unimportant variables”; variables in rectangle are barrel temperatures; variables in diamond are characteristic variables for that stage.

“unimportant” variables for that stage. Variables enclosed by the diamonds and rectangles are dominant variables, have significant contributions to the stage PCA model. All barrel temperatures lie in the rectangle (Variable No. 13, 14, 15 and 16), forming an independent clustering indicating that they have weak relation with other process variables, which will be discussed in detail in Section 4. It is important to point out that variables in the diamonds change from stage to stage, indicating the varying process characteristics and the necessity for a stage based analysis.

4. PROCESS MONITORING AND FAULT DIAGNOSIS BASED ON SUB-PCA MODEL

Statistical process monitoring is conducted based on hypothesis tests on two indices, the *Hotelling*-T^2 and the Q statistics indices (or SPE value), in the principal component subspace and residual subspace, respectively. The confidence region of *Hotelling*-T^2 statistic can be estimated by F-distribution; while Q statistics can be well approximated by a weighted χ^2 distribution (Jackson, 1979, 1991; Westerhuis, et al., 2000). The control limits can be computed following the procedures proposed by Lu et al. (2002). The control limits estimated from I number of normal batch runs describe the normal and systematic variations of the process, provided that the reference process data can cover all normal cases.

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. The *Hotelling*-T^2 statistic reveals the abnormality, which can be described by the sub-PCA model; while the Q statistic shows the unexplained information after the process variables being projected onto the principal hyperplane. The process is monitored using the *Hotelling*-T^2 and SPE charts. The batch operation is monitored at every sampling point k with both *Hotelling*-T^2 and SPE monitoring charts. The monitoring procedure first judges which stage the new coming data belongs to, and then call the corresponding sub-PCA model to calculate the values of two indices, *Hotelling*-T^2 and SPE. The values of the two statistics for normal batch runs will be well below the control limits, while abnormal batches may have large values of the *Hotelling*-T^2 and/or SPE statistics. Once an abnormal condition is detected by the monitoring charts, the contribution plot, a commonly-used and effective diagnosis tool, is used to diagnose the fault cause for that stage.

In this work, three typical faults are intentionally introduced. Fault #1 is material disturbance by adding a few grams of polypropylene (PP) into the HDPE. Fault #2 is a barrel temperature sensor failure; while fault #3 is caused by check-ring failure, which is a common problem in injection molding. All faults can change the correlation structure, generating unexplained information by the stage PCA model. They can be promptly detected by the monitoring charts in the corresponding stage, as illustrated in Figures 4-8.

• *Fault #1*

Material disturbance is the first fault introduced to test the proposed method. A small amount of PP is added to the processing of HDPE. The T^2 and SPE monitoring charts, as shown in Figure 4, indicate that this fault can be identified soon after the starting of filling phase. In terms of the four contribution plots as shown in Figure 5, contamination of a small amount of PP into the HDPE, results in a lower cavity temperature (No. 11) throughout the cycle, as PP cools and solidifies faster than HDPE. At the same time, the viscosity of PP is higher than that of HDPE, which generates larger shear heating for PP, resulting in a higher nozzle melt temperature (No.12). The contribution plot of the packing phase is different from the others. The cavity pressure (No.7) has lower values due to the faster solidification of PP. This characteristic difference among different stages can only be revealed by such a stage-based approach.

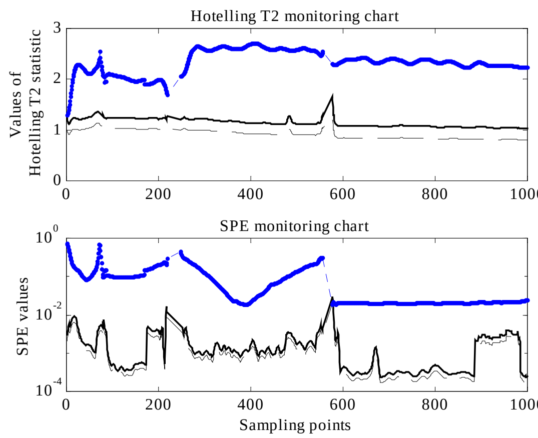


Fig. 4. T^2 and SPE monitoring charts for fault #1.
(Solid line, 99% control limit; dash line, 95% control limit)

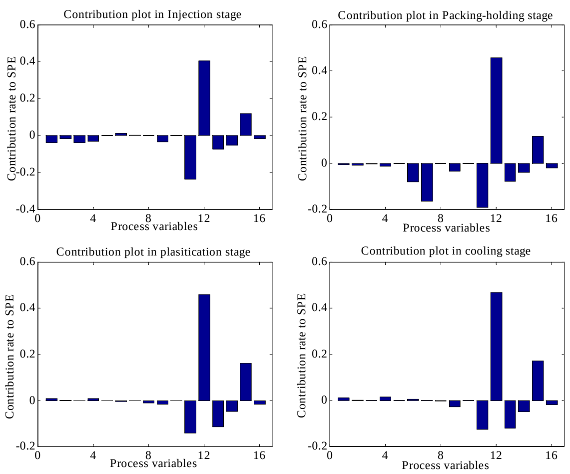


Fig. 5. Contribution plots of the four stages for fault #1

• *Fault #2*

When one thermocouple that measures the barrel temperature fails, the reading of this temperature drops, resulting in full heating of this zone. This creates excessive heats to be conducted to the neighbouring zones, even the heating of those zones are fully shutdown. This change can be quickly picked up by the *Hotelling-*T^2 and SPE monitoring

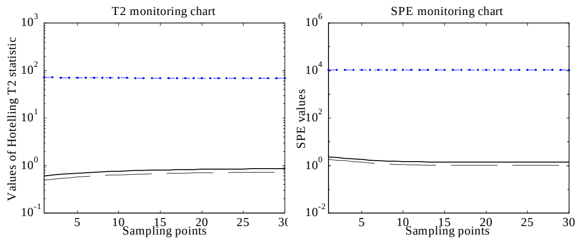


Fig. 6. T^2 and SPE monitoring charts for fault #2.
(Solid line, 99% control limit; dash line, 95% control limit)

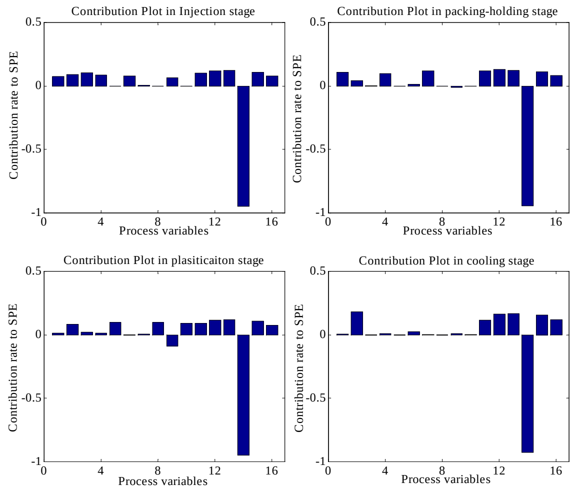


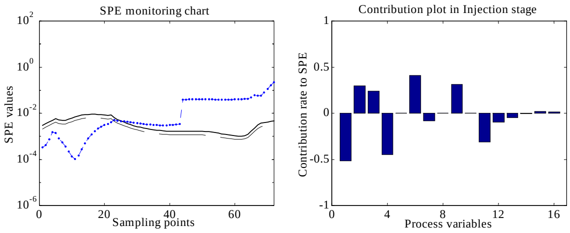
Fig. 7. Contribution plots of the four stages for fault #2

charts as shown in Figure 6. The contribution plots of the four operation stages, shown in Figure 7, clearly indicate the drop of the failed zone temperature (No. 14) and the increased temperatures of the neighbouring zones. The contribution plots in all four stages are similar, because this fault has similar impact on the four stages. As shown in Figure 3, the barrel temperatures (No.13, 14, 15 and 16) form an independent and stable clustering throughout the batch.

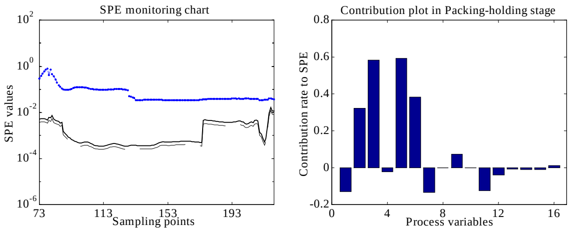
• *Fault #3*

The check-ring valve, a device that allows the polymer melt flow from the screw channel to the nozzle during plastication, closes during injection and packing stages to prevent polymer backflow from the nozzle to screw channel. Check-ring failure upsets the process correlations of different stages in different ways. As shown in Figures 8, fault #3 can be readily detected by the SPE monitoring charts. The contribution plots in the first three stages, however, are different, indicating that the fault #3 has different fault characteristics in different stages. The application of stage-based sub-PCA method is advantageous for diagnosing such a fault.

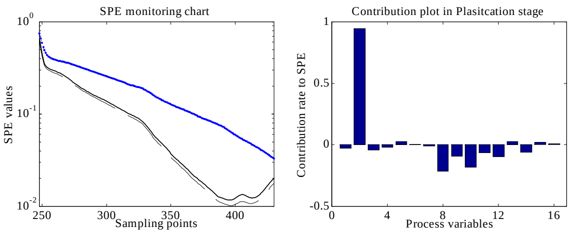
During the filling stage, smaller amount of material will be injected into the cavity, at the same injection velocity, due to the back flow associated with the failure of the checking ring valve. The nozzle pressure (No.1), injection pressure (No.4) and cavity pressure (No.7) are lower, as clearly indicated by the contribution plot of the stage. During the packing-holding phase, more material will have to be packed into the cavity to make up the shortfall in the filling, resulting in a higher stroke (No.2), higher screw speed (No.3), higher pressures (No.4, 5), as expected from the analysis of the process. This can also be clearly seen in the contribution plot. During plastication, as longer stroke has travelled in filling and packing, a longer plastication stroke (No.2) has to recovered, which is clearly seen in the contribution plot of this stage.



Monitoring result in Injection stage



Monitoring result in Packing-holding stage



Monitoring result in Plastication stage

Fig. 8. Monitoring chart and contribution plot for fault #1. (Solid line, 99% control limit; dash line, 95% control limit)

The above analysis is accorded well with the process knowledge of injection molding. For the faults that show different fault characteristics in different stages, it is desirable to analyse the contribution plots of different stages to give a reasonable cause to the fault. This suggests that the application of the sub-PCA modelling method can indeed enhance the process understanding, and improve the ability of fault detection and diagnosis.

5. CONCLUSIONS

A multistage multivariate model has been developed based on the historical data of normal batch runs for injection molding process. This modelling method divides the process into several stages, similar to what is practiced by an injection molding expert. With this multi-stage model structure, the correlation in each operation stage can be analysed in detail to enhance the understanding of the process. The experimental applications indicate that the stage-based sub-PCA modelling is effective for monitoring and detecting process faults. The most possible cause of the abnormality can also be obtained by combining the fault characteristics of different stages. The procedures presented in this paper can provide process operators with a tool for stage-division purely by data analysis. The stage-based monitoring and diagnosis can not only allow on-line monitoring without the need of predicting future data, but also can isolate and identify a fault to a specific stage of the process operation.

REFERENCES

Chen J. and Liu, K. C. (2002). On-line batch process monitoring using dynamic PCA and dynamics PLS models. *Chem. Eng. Sci.*, **57**, 63.

Chen X. (2002). A study on profiling setting of injection molding. *Ph.D. Thesis*, The Hong Kong Univ. of Sci. & Tech., Hong Kong.

Dong D. and McAvoy T. J. (1996). Batch tracking via nonlinear principal component analysis. *J. AIChE*, **42**, 2199.

Jackson J. E. (1991). A User's Guide to Principal Components. Wiley, New York.

Jackson J. E. and G. S. Mudholkar (1979). Control procedures for residuals associated with principal component analysis. *TECHNOMETRICS*, **21**, 341.

Kaspar M. H. and W. H. Ray (1992). Chemometric methods for process monitoring and high-performance controller design, *J. AIChE*, **38**, 1593.

Louwerse D. J. and Smilde A. J. (2000). Multivariate statistical process control of batch processes based on three-way models. *Chem. Eng. Sci.*, **55**, 1225.

Lu N., F. Gao and F. Wang (2002) A sub-PCA modeling and on-line monitoring strategy for batch processes. *Submitted to J. AIChE.*

Martin E. B. and A. J. Morris (1996). An overview of multivariate statistical process control in continuous and batch process performance monitoring. *Trans. of Int. Meas. & Cont.*, **18**, 51.

Nomikos P. and MacGregor J. F. (1995). Multivariate SPC charts for monitoring batch process. *TECHNOMETRICS*, **37**, 41.

Nomikos P. and MacGregor J. F. (1994). Monitoring batch processes using multiway principal component analysis. *J. AIChE*, **40**, 1361.

Rännar S., MacGregor, J. F. and Wold, S.(1998). Adaptive batch monitoring using hierarchical PCA. *Chemometrics and Intelligent Laboratory Systems*, **41**, 73.

Westerhuis J. A., Gurden S. P. and Smilde A. K. (2000). Standardized Q-statistic for improved sensitivity in the monitoring of residuals in MSPC. *J. Chemometrics*, **14**, 335.

Wold, S., P. Geladi, K. Esbensen, and J. Ohman. (1987). Multi-way principal components and PLS analysis. *J. Chemometrics*, **1**, 41.

Yang Y. and Gao F. (1999). Cycle-to-cycle and within-cycle adaptive control of nozzle pressures during packing-holding for thermoplastic injection molding. *Poly. Eng. Sci*. **39**, 2042

Yang Y., Lu N., Wang F. and Ma L. (2002). A new fault detection and diagnosis method based on principal component analysis in multivariate continuous processes. *The* 4^{th} *Proceeding Of the World Congress on Intelligent Control and Automation*, Shanghai, P. R. China, 3153.