Batch Tracking via Nonlinear Principal Component Analysis

Dong Dong and Thomas J. McAvoy
Dept. of Chemical Engineering and Institute for Systems Research,
University of Maryland, College Park, MD 20742

Batch processes are very important to the chemical and manufacturing industries. Techniques for monitoring these batch processes to ensure their safe operation and to produce consistently high-quality products are needed. Nomikos and MacGregor (1994) presented a multiway principal component analysis (MPCA) approach for monitoring batch processes, and test results show that the method is simple, powerful, and effective. MPCA, however, is a linear method, and most batch processes are nonlinear. Although data treatment techniques can remove some nonlinearity from the data, nonlinearity is still a problem when using MPCA for monitoring. In this article a nonlinear principal component analysis (NLPCA) method (Dong and McAvoy, 1993) is used for batch process monitoring. Results show that this method is excellent for this problem. Another interesting extension of this approach involves multistage batch process monitoring, which is illustrated through a detailed simulation study.

Introduction

The current trend toward the production of low-volume/high-cost materials has generated high interest in the use of batch and semibatch processes. Examples include reactors, crystallizers, distillation towers, injection molding processes, and other processes involved with the manufacture of polymers. Many important batch process issues have been extensively studied including design, simulation, optimization, and control (Lewin and Lavie, 1990; Luyben, 1990; Filippi-Bossy et al., 1989; Luus, 1993; Modak, 1993). However, techniques for monitoring batch processes, which are important to ensure their safe operation and to assure that they produce consistent high-quality products, need additional study (Nomikos and MacGregor, 1994). Some methods like first principle approaches (Iserman, 1984; Willsky, 1976; Schuler and Schmidt, 1992) and knowledge-based methods (Ramesh et al., 1989) are powerful, but they also have some problems in practice. For example, the first principle methods need a detailed theoretical model and sometimes such a model is unavailable; the knowledge-based methods can require a complicated knowledge base, the development of which can be very difficult. In a pioneering paper Nomikos and MacGregor (1994) presented a multiway principal component analysis (MPCA) approach for monitoring batch processes, and test results show that the method is simple and powerful. The only information needed in their approach is a historical database of past successful batches. Because of the wide use of process computers, such a database is easy to obtain. The key point of their approach is to use MPCA to compress the normal batch data and extract information by projecting the data onto a low-dimensional space that summarizes both the variables and their time histories. The progress of a new batch is then monitored by comparing the progress of the projections in the reduced space with those from normal-batch data. Their approach is an extension of the multivariate procedures using PCA developed by Kresta et al. (1990) for monitoring continuous processes. To deal with batch-process data, MPCA is used in place of PCA. But both PCA and MPCA are linear methods and most batch processes are nonlinear. There are two potential problems in using linear PCA and MPCA on nonlinear processes. One problem is that the linear methods may not be efficient in compressing nonlinear data. If more than three components are needed to describe the data, the PCA or MPCA approaches become cumbersome because too many plots are needed. Another problem is that the results of using PCA and MPCA may be inadequate because minor components can contain important information on nonlinearities (Xu et al., 1992). If the minor components are discarded, this impor-

Correspondence concerning this article should be addressed to T. J. McAvoy.

tant information is lost; if the minor components are kept, the linear methods may contain too many components to be useful for solving the problem.

In this article a nonlinear principal component analysis (NLPCA) method (Dong and McAvoy, 1996) is used for batch-process monitoring. Results show that the proposed method is excellent for this problem. Some batch processes are operated in different stages, and the batch variables can have different correlation structures for the different stages. Kosanovich et al. (1994) found that batch patterns could not be classified if one did not consider the different stages in the development of the batch-process model. In addition to giving results for a single-stage batch process, results for multistage batch-process monitoring are also given. The example presented involves a two-stage batch process, and it is shown that some abnormal situations cannot be detected if one ignores the different stages. These results also indicate that it is important to consider basic process knowledge in the design of data-based batch-monitoring methods.

The article is organized as follows: in the next section a brief review of PCA and NLPCA is given. In the third section the methodology of batch-process monitoring using NLPCA is introduced, and an example of a semibatch reactor for the production of styrene-butadiene latex is used to illustrate the method. In the fourth section multistage batch-process monitoring is discussed and an example of an exothermic batch chemical reactor is used for illustration. Finally, conclusions are given.

PCA and NLPCA

The concepts of linear and nonlinear principal components are illustrated in Figure 1. The data points are two-dimensional so they may be more easily visualized. Figure 1a illustrates the concept of a linear principal component. The linear principal component line minimizes the sum of squares of all the orthogonal deviations between the straight line and the data. Next consider higher dimensional data. A data set X that contains n samples of m variables can be expressed in terms of l linear principal components with $l \leq m$ as

$$X = TP' + E, \tag{1}$$

where $T = [t_1, t_2, \ldots, t_l]$ is defined as the matrix of principal component scores, P is defined as the matrix of principal component loadings, and E is the matrix of residuals. The principal loadings determine the direction of the principal component lines, and the principal scores are the coordinates of the data points on the principal component lines. Figure 1b illustrates the concept of a nonlinear principal component. The nonlinear approach is the same as the linear approach, except that it summarizes the data with a smooth curve that is determined by nonlinear relationships among all the variables. This smooth curve minimizes the squared orthogonal deviations between the data and the curve. A data set X that contains n samples of m variables can be expressed in terms of l nonlinear principal components, with $l \leq m$ as

$$X = F(T) + E, \tag{2}$$

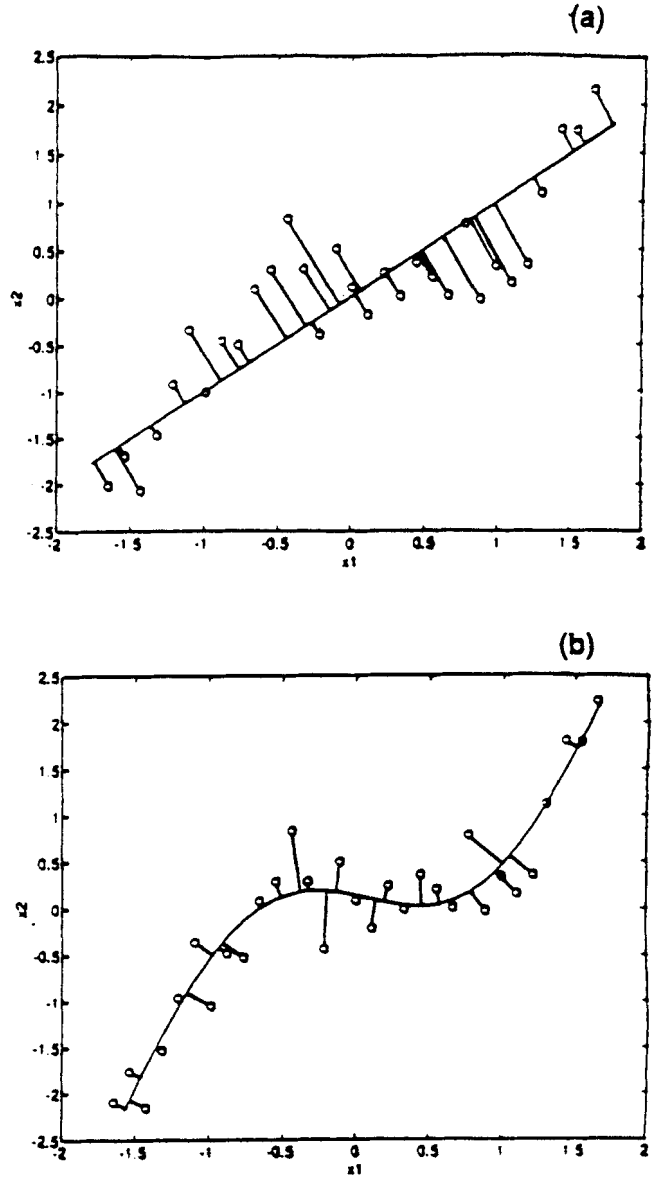

Figure 1. (a) Linear principal component minimizes the sum of squared orthogonal deviations using a straight line; (b) nonlinear principal component minimizes the sum of square orthogonal deviaitons using a smooth curve.

where $T = [t_1, t_2, \ldots, t_l]$ is defined as the matrix of nonlinear principal component scores, and F is defined as the nonlinear principal component loading function. Figure 1 illustrates that the nonlinear principal component approach is better than the linear principal component approach in modeling the data, and it can capture the nonlinear relationship among the variables. In the nonlinear principal component analysis method proposed by (Dong and McAvoy, 1996) there are two steps. In the first step, the principal curve algorithm (Hastie and Stuetzle, 1989) is used to generate a table of results that contains the original data, the nonlinear principal scores, and data reconstructed from the nonlinear principal components by assuming $E = 0$ in Eq. 2. In the second step, two three-layer neutral networks are developed from the table to ob-

tain the NLPCA model. For new process data, their scores and reconstructed data can be easily gotten by using the NLPCA model. The detailed methodology of the approach can be found in (Dong and McAvoy, 1996).

Batch-Process Monitoring Using NLPCA

The basic methodology for continuous process monitoring using PCA was proposed by (Kresta et al., 1990). Good process data, obtained when the process operates fault free, are used to develop the PCA model. It is assumed that these data contain enough information to cover the range of good process operation. For monitoring the progress of the process and detecting the occurrence of faults, the squared prediction error (SPE) and principal component score charts are plotted and monitored. If the scores or the SPE move outside the region over which the model was developed, the conclusion is that some change or fault has occurred in this process. Using the same methodology as Kresta et al. (1990), Dong and McAvoy (1996) have discussed the use of NLPCA, instead of PCA, for monitoring nonlinear continuous processes.

PCA and NLPCA are powerful methods for monitoring continuous processes. However, when applying them to monitoring batch processes, there is a problem. For a continuous process, the data that define the normal operation range can be arranged in a matrix. For batch-process monitoring, a three-way array is required for the process data, with time being the additional dimension. For every batch run, J variables are measured at K time intervals throughout the batch. A number of such batches are needed to cover the normal batch operation range. Suppose there are I such batches, then all the data form a three-way array $X(I \times J \times K)$ illustrated in Figure 2. PCA cannot be applied directly to this three-way array. MPCA (Wold et al., 1987) is an extension of PCA that can handle such an array of data. MPCA decomposes the X array into a summation of the product of score vectors (t_r) and loading matrices P_r, plus a residual matrix E that is minimized in a least-squares sense, as

$$X = \sum_{r=1}^{R} t_r \otimes P_r + E, \tag{3}$$

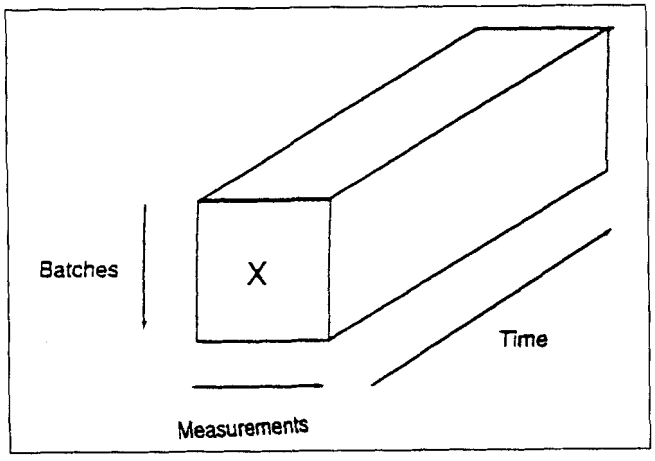

Figure 2. Normal-batch processes data: a three way array.

where R is the number of principal components used in the analysis. The score space represents the major variability over the batches for all variables and for all points in time. The loading matrix summarizes the major time variations of the variables over all the batches. The relationship between MPCA and PCA is very interesting. MPCA is equivalent to performing ordinary PCA on a large two-dimensional matrix formed by unfolding the three-way array (Wold et al., 1987; Geladi, 1989; Stahle, 1989). The following two-dimensional matrices can be formed by three possible unfolding approaches.

- Variables × time for each specific batch.
- Batches × variables at each specific time.
- Batches × times for each specific variable.

The first unfolding approach allows one to analyze the variability among the batches by summarizing the information in the data with respect both to the measured variables and their time variation. The second unfolding approach is useful for analyzing the variability among samples, and the third approach can be used to get information about the variability among the batch variables. In this article, the first unfolding approach is used because it can provide information on the variability among the batches that can be used directly for batch process monitoring (Nomikas and MacGregor, 1994). The dimension of the resulting matrix is $(I \times JK)$ by the first unfolding approach. After unfolding, NLPCA can be used directly on the batch-process data. Several issues are very important for batch-process monitoring using NLPCA. These include data scaling, on-line issues, and special problems for multistage batch processes. Two examples are considered in this article.

Example 1

The data for this example are provided by MacGregor (Nomikos and MacGregor, 1994). The process involves a semibatch emulsion polymerization of styrene-butadiene to make a latex rubber (SBR). The batch is initially charged with seed SBR particles and with an initiator, chain transfer agent, emulsifier, water, and a small amount of styrene and butadiene monomers. Styrene and butadiene monomers are then fed to the reactor, at an approximately constant rate for the rest of the batch procedure. The batch duration is 1,000 min, and measurements are taken every 5 min on 9 process variables such as the flow rate of styrene and the temperature of the feed. By introducing typical variations in the base-case conditions, such as the initial charge of seed latex, the amount of chain transfer agent, and the level of impurities, 50 batches were simulated to create a reference database of normal batches. The resulting latex and polymer properties, composition, particle size, branching, cross-linking, and polydispersity, of these 50 batches were consistent with the variations one might see during a sequence of industrial-batch runs. These batches define the normal batch operation range. Two additional batches with product out of this normal range were simulated, one with an initial organic impurity contamination in the butadiene feed, 30% above that of the normal case, the other with the same problem that started halfway through the batch operation, with the contamination being 50% above the normal level. In addition to these two bad batches, another normal batch was simulated, and these three batches

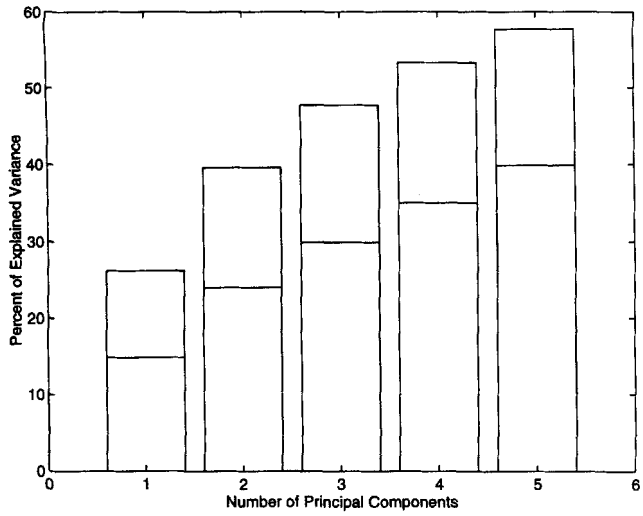

Figure 3. Explained variation by PCA and NLPCA.

Upper bar, NLPCA; lower bar, PCA.

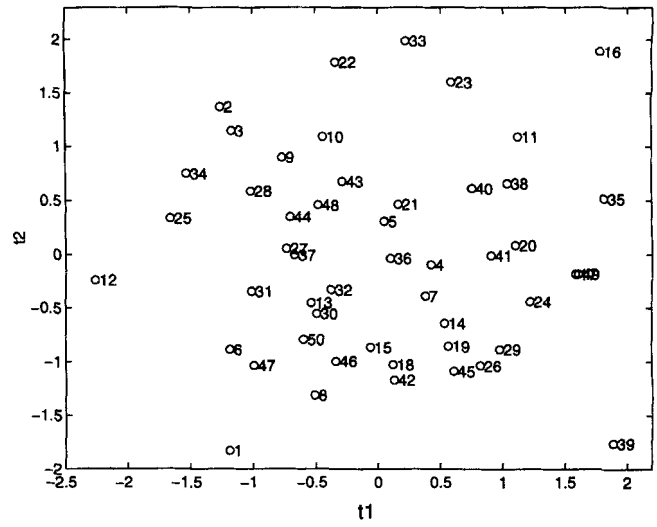

Figure 4. Scores obtained by NLPCA for the 50 normal batches.

were used as tests to investigate the ability of NLPCA to detect a fault.

The first step is to unfold and scale the normal batch-process data. The normal batch-process data matrix $X(50\times 200\times 9)$ is unfolded to a matrix with dimension (50×1800), and then the data are scaled to zero mean and unit variance. The mean of this matrix is the average trajectory of the 50 normal batches, and the scaling involves subtracting the average trajectory from each variable. This treatment of data can remove some nonlinearity among batch variables, but nonlinearity may still be a problem.

The second step is to analyze the unfolded and scaled data using NLPCA to get the NLPCA model. Figure 3 shows the variation explained by PCA and NLPCA, where it can be seen that NLPCA produces better results than PCA. For example, using two principal components, PCA can explain 25.5% of the variation, while NLPCA can explain 39.6% of the variation. Cross-validation indicates that for PCA three principal components are sufficient for modeling the data, while for NLPCA only two principal components are needed. So for process monitoring, only one score plot (t_1 vs. t_2) is needed if NLPCA is used, but for PCA three score plots are needed. Figure 4 shows the scores for the 50 normal batches, where it can be seen that the scores cluster in a normal range, and none of them lies far away from the cluster.

Now consider monitoring a new batch on-line. Here an important problem is to design an on-line strategy. When using the first unfolding method, the model covers the entire trajectory, since the model inputs involve the complete trajectories for one batch. One can calculate a score and an SPE for a new batch only after a trajectory is complete. For a new batch, data are only available from the beginning of the batch to the current time, and thus the data are not complete. Since all the future observations are missing when the batch is being made, a requirement for an on-line strategy is to replace the future observations with appropriate values such that the predicted scores at each time will be as close as possible to those that would be calculated if the complete trajectories were available. Nomikos and MacGregor (1994) presented an on-line strategy that is similar to the dynamic matrix control (DMC) algorithm for this prediction. We also use this strategy, which is based on assuming that the future deviations of the observations from the mean trajectory remain constant at their current values for the rest of the batch run. Using this on-line strategy one can calculate a score and an SPE for a new batch at every sampling time. If a new batch is good and consistent with the normal batches from which the NLPCA model was developed, its scores should fall within the normal range and its SPE should be small. For an abnormal batch, there may be two kinds of abnormalities. For the first kind of abnormality the basic relationships among the batch variables do not change, but several batch variables have a larger than normal change. For this kind of abnormality, the SPE remains small, but the scores will move outside the region over which the model was developed. The second kind of abnormality results when the relationship among the batch variables changes. For this kind of abnormality the SPE will increase, because the new measurements cannot be explained by the NLPCA model.

Figures 5 to 7 show the results for monitoring the three test batches. The control limits shown in each plot correspond approximately to the 95% and 99% confidence regions based on the reference distribution for normal batches, and they are determined by using the methodology presented by Nomikos and MacGregor (1994). The scores can be well approximated by a normal distribution and the SPE can be well approximated by a $\alpha\cdot\chi_\nu^2$ distribution. Because there are 50 normal batches, each of them is passed through the preceding on-line strategy as if they were new batches, to produce 50 SPEs at each sampling time. The values of α and ν for each sampling time can be estimated by matching the moments of the $\alpha\cdot\chi_\nu^2$ distribution with the moments of the 50 SPEs. Figure 5 shows the result for the good test batch. Figure 5a is the score plot and Figure 5b is the SPE plot. Both the scores and the SPEs are well within the control limits, indicating that the data from this new batch are consistent with those from normal batches. The monitoring results for the test batch with an initial impurity problem are shown in Figure 6. Some SPE values exceed the 99% control limit, which indicates that the data from the new batch are not

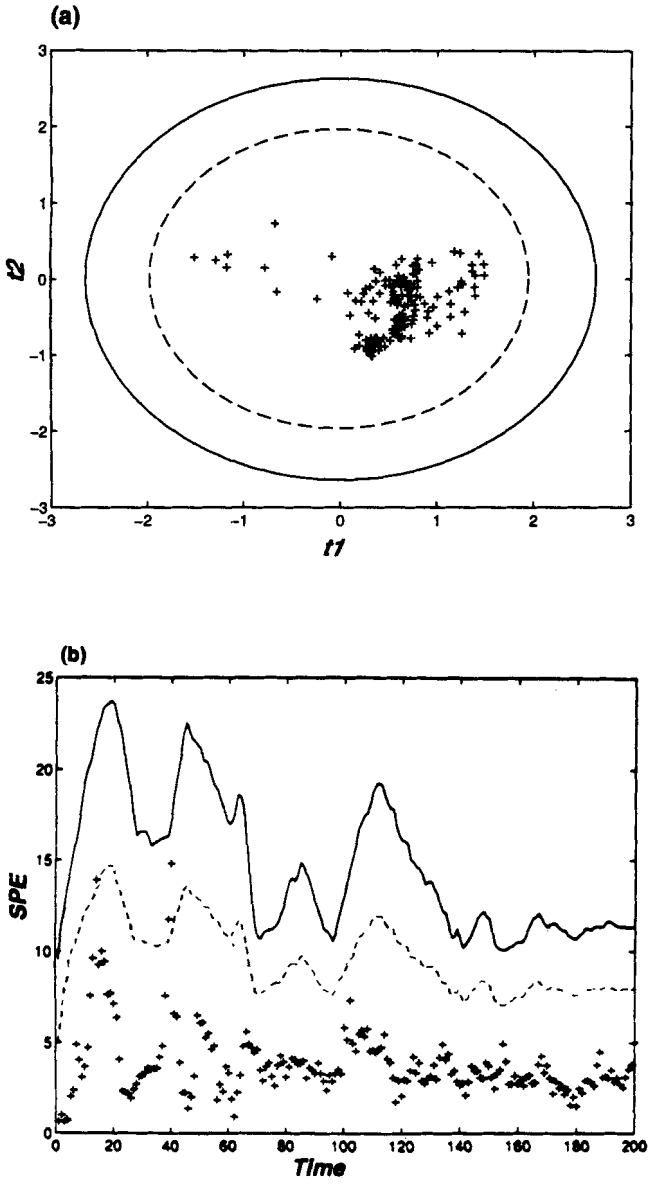

Figure 5. On-line monitoring for a good batch using the NLPCA approach.

(a) Score plot; (b) SPE plot. Dotted line, 95% control limit; solid line, 97% control limit.

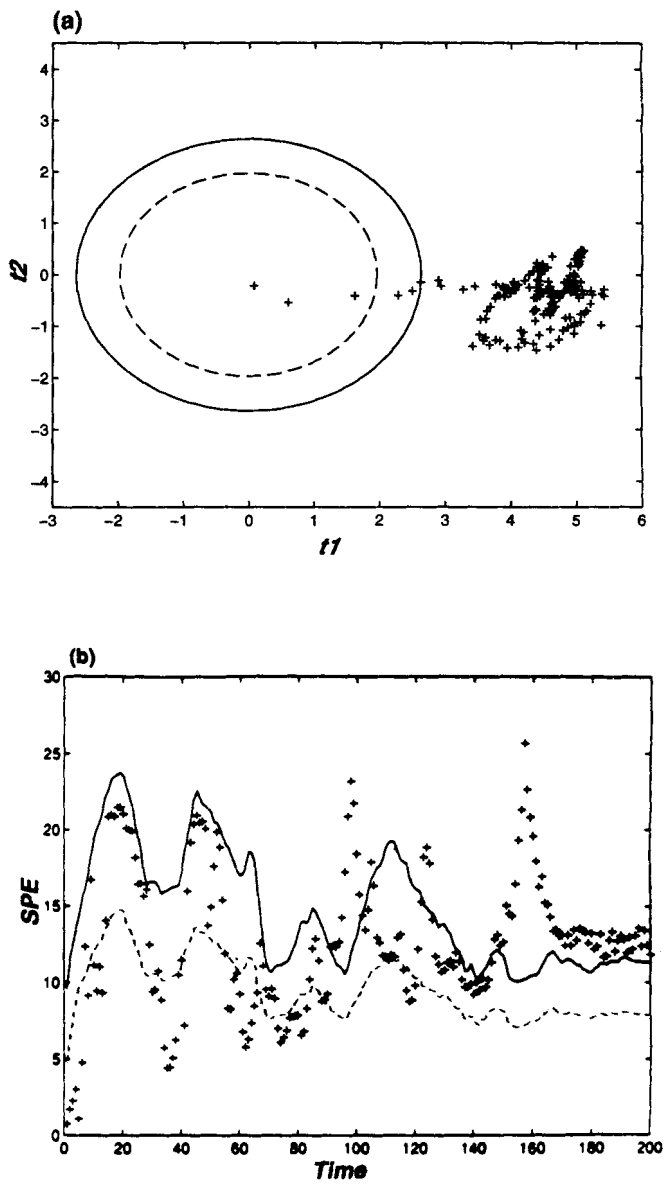

Figure 6. On-line monitoring for a bad batch with an initial impurity problem using the NLPCA approach.

(a) Score plot; (b) SPE plot. (Dotted line, 95% control limit; solid line, 99% control limit.)

consistent with the data from normal batches. As can be seen, the scores quickly move outside the control limit, clearly indicating that there is an abnormality at the start of this batch. For the test case with the impurity occurring halfway through the batch, Figure 7 shows the monitoring results. As can be seen after 100 sampling times (which is halfway through the batch), both the scores and the SPE values quickly move outside the control limits, which clearly indicates that there is an abnormality in this batch. Figures 6 and 7 illustrate the fact that different faults produce significantly different score trajectories. This fact has been noted by Nomikos and MacGregor (1994) and Lewin (1995). The different score trajectories facilitate the diagnosis of process faults.

The results show that NLPCA provides a very good approach for batch-process monitoring. Although for this problem the linear PCA approach also gives very good results (Nomikos and MacGregor, 1994), the NLPCA has an advantage. For nonlinear processes, NLPCA required fewer components for a given explained percent variance, and as a result for process monitoring the number of plots required is less. This feature can be very important when the linear approach requires four or more plots. If the NLPCA method is applied to linear data, then it yields the same results as normal PCA. This is a nice feature of the nonlinear approach presented in this article. In our experience the calculations for NLPCA require more computer time than PCA since an iterative optimization procedure is involved (Dong and McAvoy, 1996).

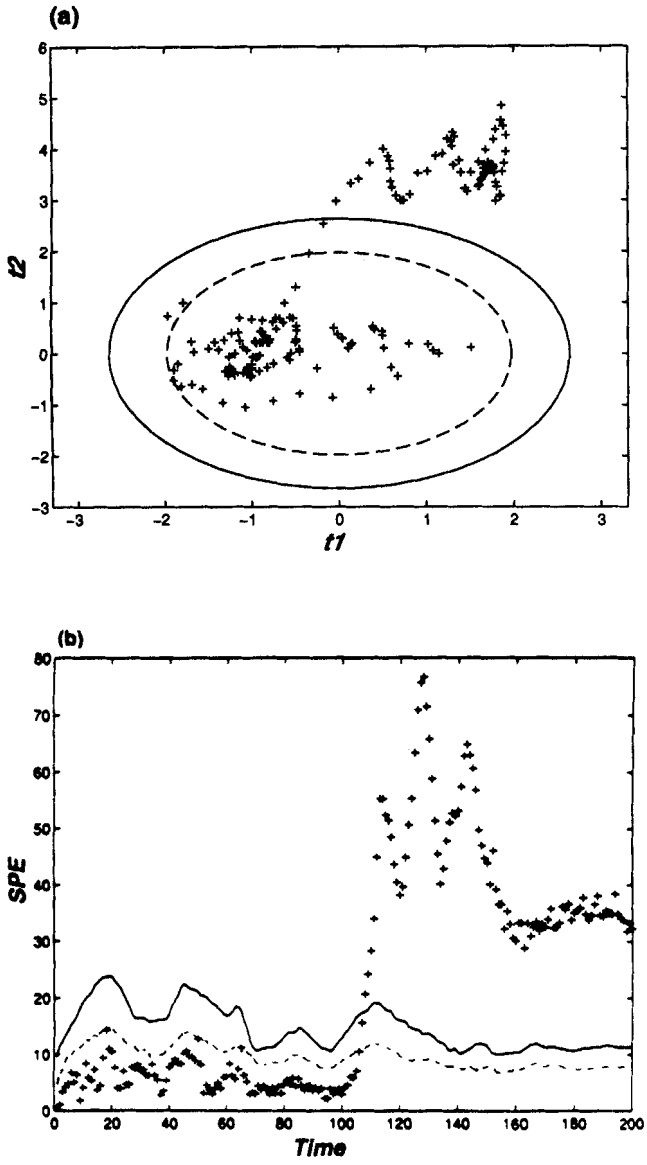

Figure 7. On-line monitoring for a bad batch with impurity occurring halfway through the batch using the NLPCA approach.

(a) Score plot; (b) SPE plot. Dotted line, 95% control limit; solid line, 99% control limit.

Multistage Batch-Process Monitoring

Many industrial batch processes are operated in different stages. For example, the first stage can be a heating stage, and the second can be a holding stage. More complicated batch processes can involve up to four stages (Joseph and Hanratty, 1993). Kosanovich et al. (1994) analyzed a two-stage batch process using MPCA and got very interesting results. Usually the input variable profiles vary greatly from one stage to the next, and the control strategies for implementing input profiles are also different. Thus, the variations in and the correlation structures of the batch variables are different for different stages.

Using NLPCA for batch-process monitoring is a data-based method. It is important to incorporate process knowledge in the design of such data-based methods. For multistage batch processes, the basic phenomenon is that there are different correlation structures for the different stages. Based on this knowledge, it is natural to consider using different models for the different stages in order to achieve better results (Kosanovich et al., 1994). The effectiveness of this consideration and the detailed method for multistage batch-process monitoring are illustrated by the following example.

Example 2

This example involves a two-stage jacketed exothermic batch chemical reactor based on a model published by Lewin and Lavie (1990). The first stage is a startup stage, where the reactor contents are brought from their initial conditions to the desired operating level. The second stage is a maintenance stage, where the desired nominal operating conditions are maintained until the end of a batch. During the first stage, steam is used to raise the reaction temperature to the desired level, after which cooling water is used to remove the heat of reaction. For this process, the first stage is completed as quickly as possible in order to make the total batch time short. However, Lewin and Lavie (1990) found that because of limited cooling capacity in the jacket, the operation time for the first stage must exceed some minimum value to prevent the reactor temperature from going out of control in the second stage. The reaction system given by Lewin and Lavie (1990) involves two consecutive first-order reactions originally used in Luyben (1990):

$$A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} C. \tag{4}$$

The mass balances and the heat of the reaction can be expressed by the following equations,

$$dC_A/dt = -k_1 C_A \tag{5}$$

$$dC_B/dt = k_1 C_A - k_2 C_B \tag{6}$$

$$\sum_{j=1}^{2} \Delta H_j(C_j, T, P) = k_1(T) C_A \lambda_1 + k_2(T) C_B \lambda_2, \tag{7}$$

where k_1 and k_2 are rate constants,

$$k_1 = \alpha_1 e^{Ea_1/RT} \qquad k_2 = \alpha_2 e^{Ea_2/RT}, \tag{8}$$

T is the temperature of the reaction, P is the pressure, C_i is the amount of species i at time t, ΔH_j is the heat of reaction j, Ea_1 and Ea_2 are the activation energies, and α_1 and α_2 are the frequency factors. The initial conditions are listed in Table 1, and are the same as those of Lewin and Lavie (1990) and Luyben (1990). In Table 1 T_j and T_m are the tempera-

Table 1. Nominal Initial Conditions

Variable	Value	Variable	Value
T	80°F (27°C)	C_B	0.0 mol B/ft^3
T_m	80°F (27°C)	T_c	80°F (27°C)
T_j	80°F (27°C)	T_h	260°F (127°C)
C_A	0.8 mol A/ft^3 (28 mol A/m^3)		

Table 2. Nominal Kinetic Parameters

Variable	Value	Variable	Value
α_1	729 min_{-1}	Ea_2	$-20{,}000$ Btu mol^{-1}
α_2	6,567.6 min_{-1}	λ_1	$-40{,}000$ Btu mol^{-1}
Ea_1	$-15{,}000$ Btu mol^{-1}	λ_2	$-50{,}000$ Btu mol^{-1}

tures of the jacket and metal wall, respectively, and T_h and T_c are the hot and cold supply temperatures, respectively. The nominal kinetic parameters, taken from Luyben (1990), are given in Table 2. The batch duration is 300 min, and the safe startup time is 100 min, as determined using the method proposed by Lewin and Lavie (1990). Measurements on nine variables such as reactor temperature and flow rate of the coolant, are taken every 2 min. By introducing typical variations in initial conditions and reactor conditions, such as the inlet cooling water temperature, the initial concentration of A, and the heat-transfer coefficients, 50 normal batches are simulated. The variations in these normal batches are consistent with those experienced during a sequence of industrial-batch runs, and they define the normal-batch operation range. Two additional batches are simulated to test the ability of NLPCA to detect a fault. One is a normal batch, and all its variations are in the normal range. Another is a bad batch with a kinetic deterioration starting at 150 min into the batch. The kinetic deterioration is simulated as a gradual process in which there is a 150 Btu/mol (158 kJ/mol) decrease for both activation energies over 30 min.

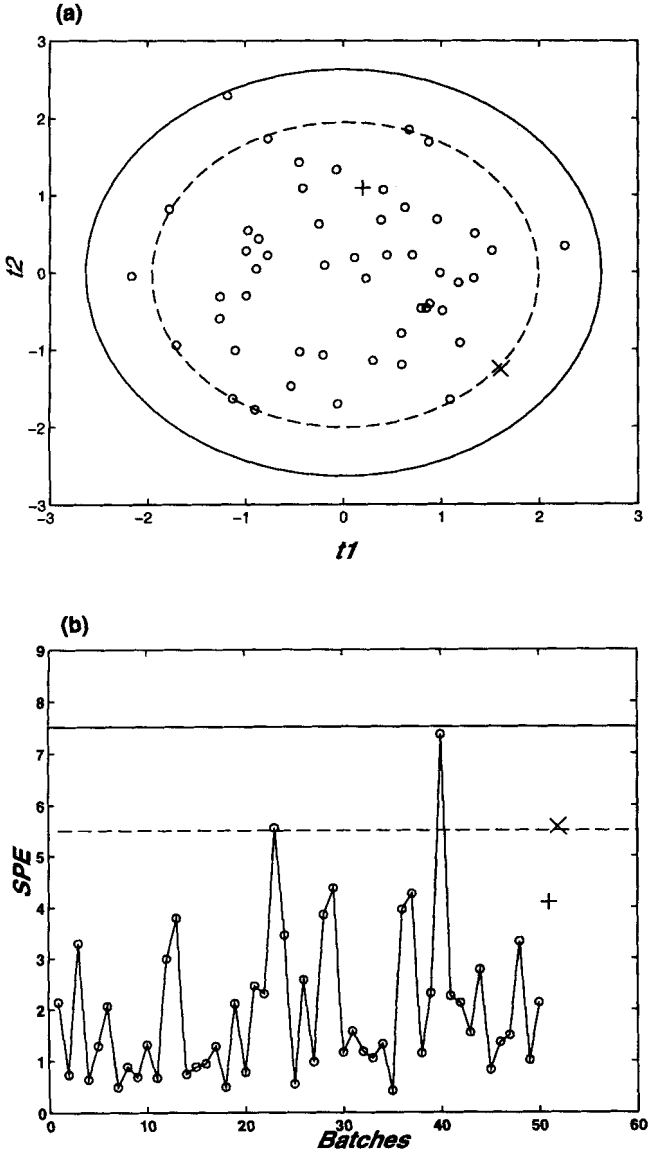

Figure 8. (a) Scores for the 50 normal batches and the two test batches; (b) SPE values for the 50 normal batches and the two test batches using the NLPCA approach.

Dotted line, 95% control limit; solid line, 99% control limit.

The same procedure employed in Example 1 is used to build the NLPCA model. First, a single model for the complete two-stage process is considered. The normal batch process data matrix $X(50\times150\times9)$ is unfolded to a matrix with dimension $(50\times1{,}350)$. Then the data are scaled to zero mean and unit variance, and PCA and NLPCA are used to analyze the unfolded, scaled data. Cross-validation indicates that for PCA five principal components are needed, while for NLPCA three principal components are needed. The NLPCA model is built using three nonlinear principal components. Figure 8a shows the scores of the first two nonlinear principal components for the 50 normal and the two test batches obtained from NLPCA. The control limits shown in the plot correspond to the 95% and 99% confidence regions, which are determined by the scores of the 50 normal batches. The final score for the normal test batch is within the normal operation range, but the final score of the bad test batch does not fall outside the cluster of normal batches. Figure 8b shows the SPE values of 50 normal batches and the two test batches. The SPE of the bad test batch is still in the 99% confidence region. Thus, the model fails to classify the bad batch from normal batches.

Next, two separate models for each stage are used. Figure 9 shows scaled batch variables for a normal batch. The two stages of operation are clearly visible, with the first 100 min being the startup stage, and the subsequent time being the maintenance stage. This suggests division of the data into two

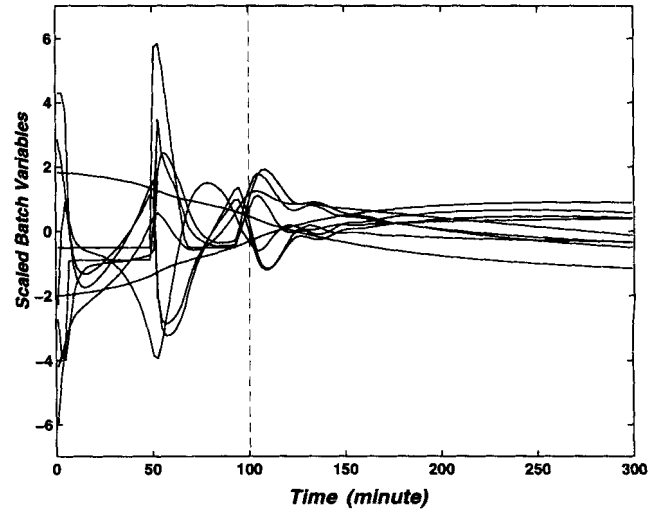

Figure 9. Scaled-batch variables for a normal batch.

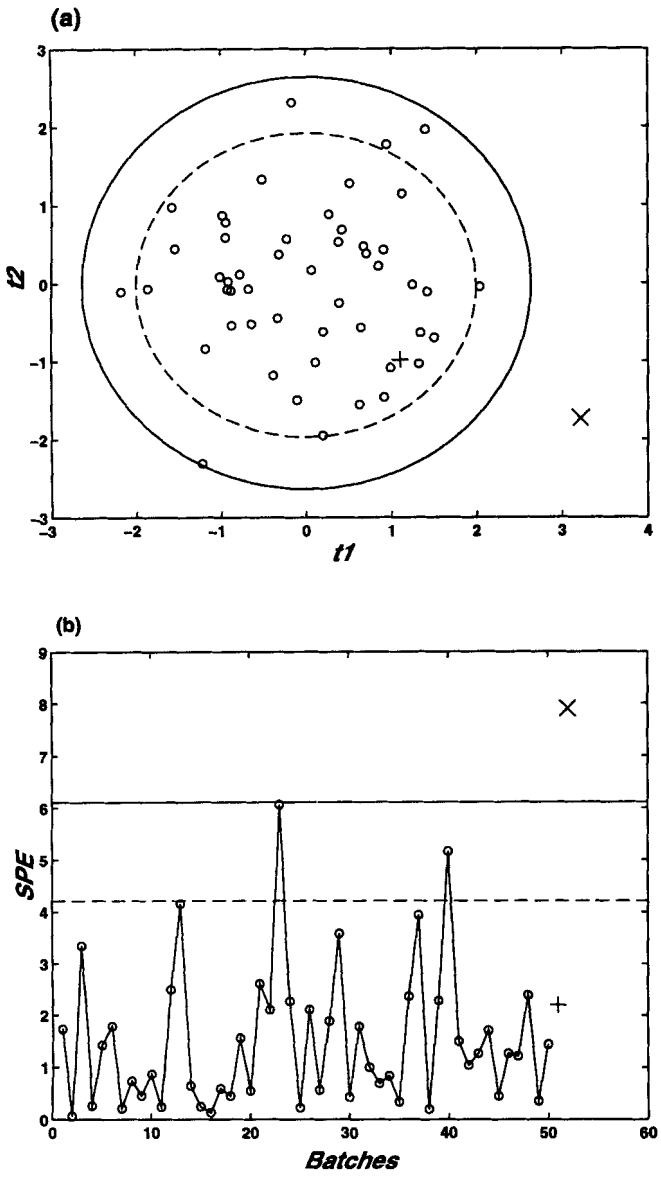

Figure 10. Results for the NLPCA approach: (a) scores for the second stage; (b) SPE values for the second stage.

Dotted line, 95% control limit; solid line, 99% control limit.

parts consistent with the stages (Kosanovich et al., 1994). Following this approach the X data, which are $(50\times150\times9)$, are divided into two parts $X1(50\times50\times9)$ and $X2(50\times100\times9)$. Two NLPCA models are built using the same procedure as before. For the second-stage model, two nonlinear principal components are used. The scores for the second stage are shown in Figure 10a. This plot shows that the bad test batch falls outside the 99% confidence region, and the normal test batch is well within the normal region. The SPE values for the 50 normal batches and two test batches for the second stage are shown in Figure 10b. It can be seen that the SPE values for all normal batches, including the test normal batch, are within the 99% confidence region. This result indicates that the model is appropriate for all normal batches, and that it correctly flags the bad test batch. Thus, the two-stage models have the ability to classify a bad batch from normal batches. In order to compare NLPCA with a linear approach, two-stage MPCA models are also built. For the second-stage model, three principal components are used, and this number is determined by the cross-validation. Figure 11a shows the scores for the first two linear principal components for the 50 normal batches and the two test batches. As can be seen, the score for the bad test batch does not fall outside the 99% control limit. Figure 11b shows the SPE values for the 50 normal batches and the two test batches. The SPE for the bad test batch is still within the 99% confidence region. Thus, the linear model is not as good as the nonlinear model in detecting the bad batch from normal batches.

Using the two-stage models for on-line monitoring is straightforward. The only difference from Example 1 is that one needs to shift from the first-stage model to the second-stage model when the second stage begins. Figures 12 and 13

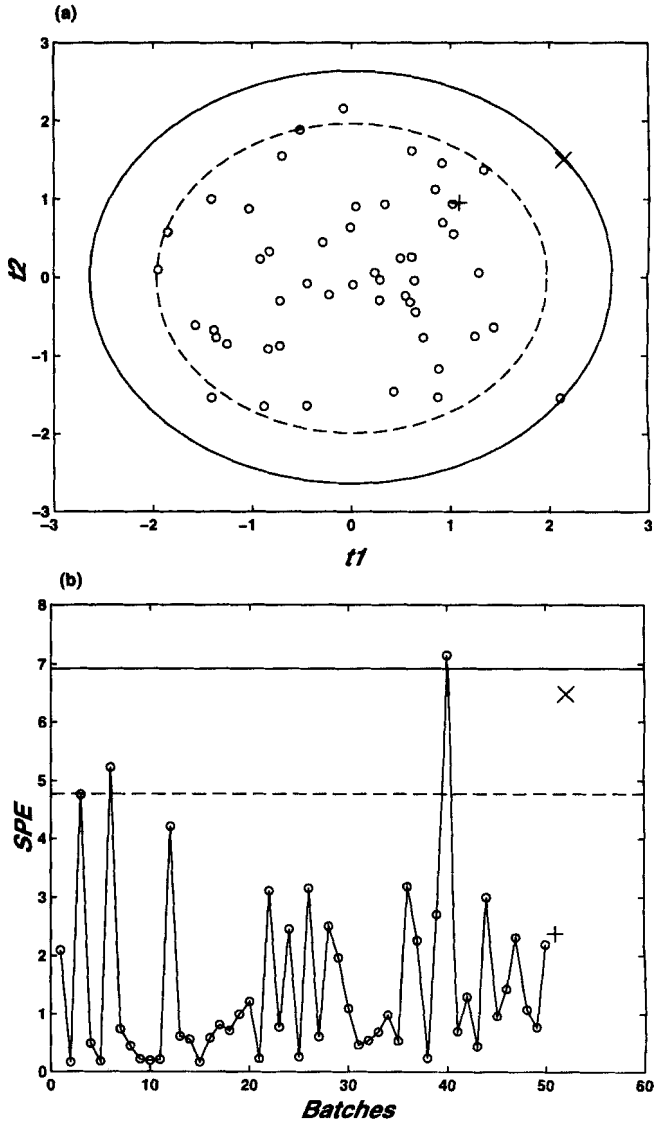

Figure 11. Results for the linear PCA model.

(a) Scores for the second stage; (b) SPE values for the second stage. Dotted line, 95% control limit; solid line, 99% control limit.

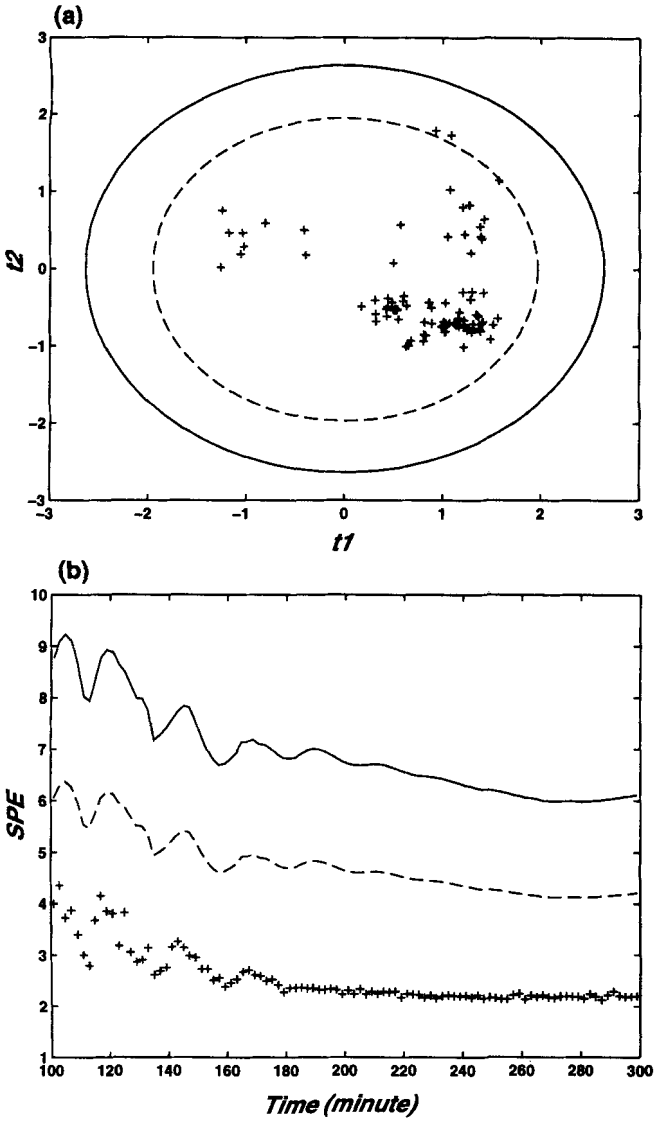

Figure 12. On-line monitoring for a normal test batch using the NLPCA approach.

(a) Score plot; (b) SPE plot. Dotted line, 95% control limit; solid line, 99% control limit.

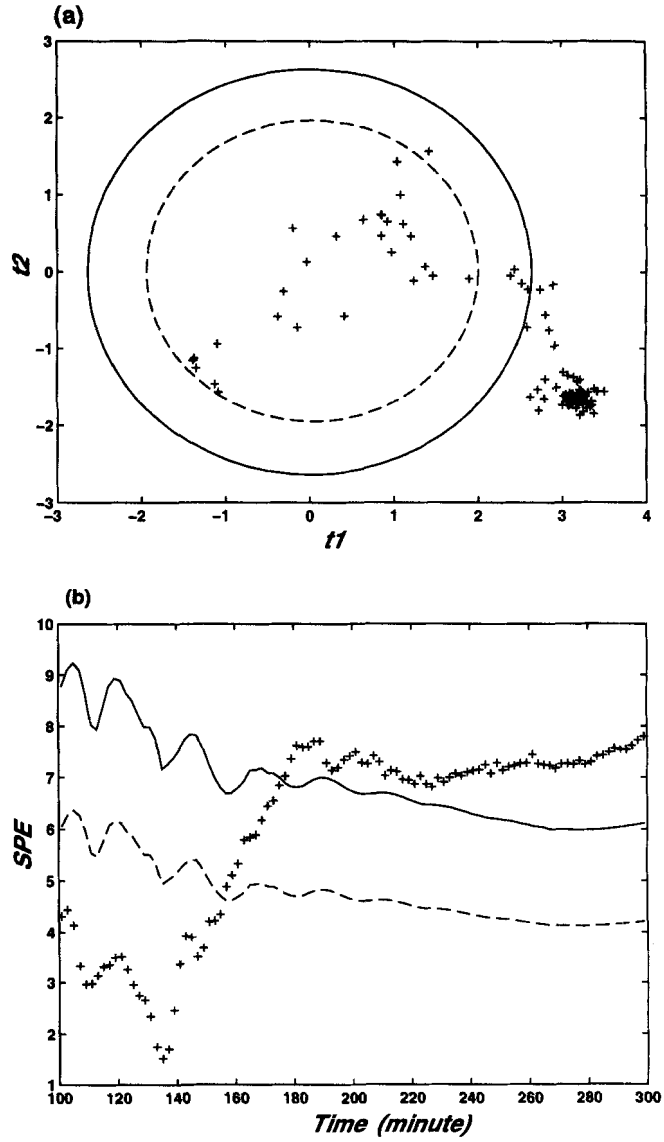

Figure 13. On-line monitoring for a bad test batch using the NLPCA approach.

(a) Score plot; (b) SPE plot. Dotted line, 95% control limit; solid line, 99% control limit.

show the results for on-line monitoring using the two-stage models, and the control limits shown in each plot correspond to the 95% and 99% confidence regions. Only the results for stage two are shown because the fault begins in this stage. Figure 12 shows the results for the normal test batch. Figure 12a is the score plot and Figure 12b is the SPE plot. Both the scores and the SPEs are well within the control limits, indicating the data from this new batch are consistent with those from normal batches. For the test batch with kinetic deterioration starting at 150 m (during the second stage of the batch), Figure 13 shows the results. As can be seen after 150 min, both the score and the SPE values begin to move outside the control limit. Because the kinetic deterioration is simulated as a gradual fault, the SPEs and the scores finally move outside the 99% confidence limit after 180 min. From the results it is clear that the two-stage models are more appropriate for monitoring this batch process, which agrees with the results of Kosanovich et al. (1994). It can also be seen that better results are achieved using the NLPCA models than linear PCA models. The two-stage model can be used easily for on-line monitoring and the gradual fault is detected effectively.

Conclusion

In this article the usefulness of NLPCA for batch-process monitoring is illustrated. Based on a method proposed by Nomikos and MacGregor (1994), a three-way array of normal batch process data is unfolded to a matrix, and then NLPCA is used to project the matrix down to a low-dimensional space defined by nonlinear principal components. Since most information in normal batch-process data is captured by the nonlinear principal components, a new batch can be monitored by tracking its progress in this low-dimensional space. Two examples are used to illustrate the effectiveness of *NLPCA* for batch process monitoring. For the first example, a one-

stage batch process, NLPCA works very well. For the second example, a two-stage batch process, the results show that dividing the data into two parts is very useful, and NLPCA achieves excellent results by using two models. The results for the two-stage example also illustrate that for this data-based method, integrating process knowledge into process monitoring approaches, namely using two models, is very helpful. The nonlinear PCA technique discussed in this article converges to ordinary PCA when the underlying data are linear.

Acknowledgment

This material is based upon work supported by the National Science Foundation under grant NSF D CDR 8803012, and NSF EEC 94-02384.

Literature Cited

Dong, D., and T. J. McAvoy, "Nonlinear Principal Component Analysis—Based on Principal Curves and Neural Networks," *Comput. Chem. Eng.*, **20,** 65 (1996).

Filippi-Bossy, C., J. Bordet, J. Villermaux, S. Marchal-Brassely, and C. Georgakis, "Batch Reactor Optimization by Use of Tendency Models," *Comput. Chem. Eng.*, **13,** 35 (1989).

Geladi, P., "Analysis of Multi-way (Multi-mode) Data," *Chemometrics Intell. Lab. Syst.*, **7,** 11 (1989).

Hastie, T., and W. Stuetzle, "Principal Curves," *J. Amer. Stat. Assoc.*, **84**(406), 502 (1989).

Iserman, R., "Process Fault Detection Based on Modeling and Estimation Method, a Survey," *Automatica*, **20,** 387 (1984).

Joseph, B., and F. W. Hanratty, "Predictive Control of Quality in a Batch Manufacturing Process Using Artificial Neural Network Models," *Ind. Eng. Chem. Res.*, **32,** 1951 (1993).

Kosanovich, K. A., M. J. Piovoso, K. S. Dahl, J. F. MacGregor, and P. Nomikos, "MultiWay PCA Applied to an Industrial Batch Process," *Proc. ACC*, p. 1294 (1994).

Kresta, J., T. E. Marlin and J. F. MacGregor, "Choosing Inferential Variables Using Projection to Latent Structures (PLS) with Application to Multicomponent Distillation," *Proc. AIChE Meet.*, Chicago (Nov. ,1990).

Lewin, D. R., "Predictive Maintenance using PCA," *Contr. Eng. Pract.*, **3**(3), 415 (1995).

Lewin, D. R., and R. Lavie, "Designing and Implementing Trajectories in an Exothermic Batch Chemical Reactor," *Ind. Eng. Chem. Res.*, **29,** 89 (1990).

Luus, R., "Optimization of Fed-Batch Fermentors by Iterative Dynamic Programming," *Biotechnol. Bioeng.*, **41,** 599 (1993).

Luyben, W. L., *Process Modeling, Simulation and Control for Chemical Engineers*, McGraw-Hill, New York (1990).

Modak, M. J., "Choice of Control Variable for Optimization of Fed-Batch Fermentation," *Chem. Eng. J.*, **52,** b59 (1993).

Nomikos, P., and J. MacGregor, "Monitoring of Batch Processes Using Multi-way PCA," *AIChE J.*, **40,** 1361 (1994).

Ramesh, T. S., J. F. Davis, and G. M. Schwenzer, "Catcracker: An Expert System for Process and Malfunction Diagnosis in Fluid Catalytic Cracking Units," AIChE Meeting, San Francisco (Nov., 1989).

Schuler, H., and C. U. Schmidt, "Calorimetric-State Estimators for Chemical Reactor Diagnosis and Control: Review of Methods and Applications," *Chem. Eng. Sci.*, **47,** 899 (1992).

Stahle, L., "Aspects of the Analysis of Three-Way Data," *Chemometrics Intell. Lab. Syst.*, **7,** 95 (1989).

Willsky, A. S., "A Survey of Design Methods for Failure Detection in Dynamic Systems," *Automatica*, **12,** 601 (1976).

Wold, S., P. Geladi, K. Esbensen, and J. Ohman, "Multi-way Principal Components and PLS Analysis," *J. Chem.*, **1,** 41 (1987).

Xu, L., E. Oja, and C. Y. Suen, "Modified Hebbian Learning for Curve and Surface Fitting," *Neural Networks*, **5,** 441 (1992).

Manuscript received Aug. 17, 1995, and revision received Dec. 27, 1995.