Monitoring Batch Processes Using Multiway Principal Component Analysis

Paul Nomikos and John F. MacGregor
Dept. of Chemical Engineering, McMaster University, Hamilton, Ontario L8S 4L7, Canada

Multivariate statistical procedures for monitoring the progress of batch processes are developed. The only information needed to exploit the procedures is a historical database of past successful batches. Multiway principal component analysis is used to extract the information in the multivariate trajectory data by projecting them onto low-dimensional spaces defined by the latent variables or principal components. This leads to simple monitoring charts, consistent with the philosophy of statistical process control, which are capable of tracking the progress of new batch runs and detecting the occurrence of observable upsets. The approach is contrasted with other approaches which use theoretical or knowledge-based models, and its potential is illustrated using a detailed simulation study of a semibatch reactor for the production of styrene-butadiene latex.

Introduction

Recent trends in North American and in most industrialized countries have been toward the manufacture of higher-value-added specialty chemicals that are produced mainly in batch reactors. Examples include specialty polymers, pharmaceuticals, and biochemicals. There are also many other batch-type operations, such as crystallization and injection molding, which are very important to the chemical and manufacturing industries. Monitoring these batch processes is very important to ensure their safe operation and to assure that they produce consistent high-quality products. In this article, we present a new multivariate procedure for monitoring the progress of all such industrial batch processes.

General batch issues like scheduling, operation planning, optimization, qualitative control decisions, and developing operating policies have been discussed by Birewar and Grossmann (1989), Cuthrell and Biegler (1989), Crook et al. (1990), Stephanopoulos et al. (1990), Rippin (1992), and MacGregor et al. (1984). Nonlinear feedback control of product quality has been discussed by Kravaris et al. (1989), Kozub and MacGregor (1992a), and Peterson et al. (1992).

Currently some of the difficulties limiting our ability to provide adequate monitoring include: the lack of on-line sensors for measuring product quality variables, the finite duration of batch processes, the presence of significant nonlinearities, the absence of steady-state operation, and the difficulties in developing accurate mechanistic models that characterize all the chemistry, mixing and heat-transfer phenomena occurring in these processes. Most of the existing industrial approaches for achieving consistent and reproducible results from batch processes are based on the precise sequencing and automation of all the stages in the batch operation. Monitoring is usually confined to checking that these sequences are followed and that certain reactor variables, such as temperatures and reactant feedrates, are following acceptable trajectories. In some cases, on-line energy balances are used to keep track of the instantaneous reaction rate, and the conversion or the residual reactant concentrations in the reactor (Wu, 1985).

Current research approaches to monitoring batch processes have focused on the use of either fundamental mathematical models or detailed knowledge-based models (Frank, 1990). The first takes advantage of a mechanistic model to describe the process, and the monitoring procedure is based on state estimation methods. The second relies on the knowledge of the operators and engineers about the process to formulate artificial intelligent algorithms.

State estimation approaches

The approaches using fundamental models are usually based on state estimation methods (Jazwinski, 1970), which combine a fundamental model of the process with on-line measurements

to provide on-line, recursive estimates of the underlying theoretical states of the batch process (Iserman, 1984; Schuler and De Haas, 1986). The fundamental model usually consists of a set of nonlinear differential equations which describe the deterministic part of the process.

The simplest approach to monitoring is to formulate a state estimator based on the deterministic model that should be satisfied during normal operation. Generally, observers or Kalman filters are used to reconstruct the states and the outputs of the system, and then tests on the output errors or innovations are used to detect faults (Willsky, 1976). If only a finite number of faults or events can occur, then several state estimators based on models incorporating different sets of plausible events can be seen in parallel. The most likely status of the process at any instant can then be evaluated using generalized likelihood ratio tests on the innovations (Basseville, 1988) or by computing the posterior probability of each model being valid. A high probability of a particular state estimator being valid would lead to an alarm and an indication of the probable cause. King (1986) presented an interesting use of this approach to detect hazardous batch reactor conditions that could lead to a runaway by monitoring undesirable side reactions using temperature measurements and parallel Kalman filters.

In some industries, such as the aerospace industry, there often exist very good state models which not only describe the system, but also provide detailed representations of how model uncertainties, disturbances, and possible faults affect the system. In these situations, robust fault detection and isolation (FDI) methods have been developed (Patton et al., 1989), which transform the observer equations and decouple the system to construct residuals which are affected only by the faults of interest. A bank of observers can then be used, where each observer is made sensitive to a different fault or group of faults, while being insensitive to common disturbances, modeling errors, and other faults. Tests to detect specific faults are then performed on these residuals.

An alternative approach that is well suited to chemical and biochemical batch reactors, which are subject to stochastic disturbances such as impurities and parameter variations, is to incorporate one's knowledge about these stochastic states into the state model and estimator. This step is also a key point in making the state estimator provide unbiased and robust estimates of the deterministic states (MacGregor et al., 1986). Monitoring the progress of batch processes then consists of tracking the development of important deterministic state variables (such as conversion, composition, particle size, and molecular weight) with time to check that they are following satisfactory trajectories. If unacceptable deviations in any of these states are detected, then not only can an alarm be given, but an assignable cause can usually be found in the behavior of the stochastic states (such as impurity concentrations have increased or the heat-transfer coefficient has dropped). Such an approach has been used by Kozub and MacGregor (1992b) to monitor polymer and latex property development in semibatch emulsion polymerization. On-line energy balances have also been effectively implemented in this manner by using Kalman filters (MacGregor, 1986; De Valliere and Bonvin, 1989, 1990; Bonvin et al., 1989; Schuler and Schmidt, 1992).

All these state estimation approaches to monitoring are "directional" in nature, in that they build into their models the possible faults or reasons for deviations from normal behavior. Although they are potentially very powerful approaches for monitoring batch processes, they present a number of problems in practice. Detailed theoretical models and on-line sensors related to product quality are necessary, if one wishes to track key quality states. Such detailed models and robust sensors are time-consuming and difficult to develop, and the state estimation approaches are computation-intensive. The detection and diagnostic abilities of these estimators will also depend highly on one's prior knowledge of the possible faults and disturbances that may occur, since these must be explicitly built into the estimator as part of the stochastic state vector or included as plausible events in one of the parallel filters. Events or disturbances that are omitted from the model may lead to biased estimates and faulty diagnosis, if they occur.

Knowledge-based approaches

Knowledge-based approaches use expert system and artificial intelligence methods to process the data. In rule-based expert systems, the process model is represented by a set of qualitative and quantitative governing descriptions based on the knowledge about the process available from operators and engineers. Associated with each behavioral description there is also a set of causality assumptions. These behavioral and causal descriptions are arranged in a hierarchical structure, and diagnostic rules for each node in the hierarchy are generated from these descriptions (Ramesh et al., 1989; Birky and McAvoy, 1990).

Additional structure and quantitative analysis can be brought to these rule-based expert systems through the use of probability theory or fuzzy logic to represent the uncertainties associated with the models and the diagnostic hypotheses (Petti et al., 1990; Rojas and Kramer, 1992; Terpstra et al., 1992). An advantage of these approaches is that they do not require detailed theoretical models of the process. However, formulating the behavioral and causal descriptions, and the diagnostic hierarchy with its probabilistic or fuzzy rules may be just as difficult and time-consuming as using the fundamental model approach. Recently, Fathi et al. (1993) incorporated state and parameter estimation modules within the diagnostic reasoning of a knowledge-based system to overcome the deficiencies of both approaches and to increase the diagnostic ability of the system.

Another approach to the problem is through the use of artificial neural networks with various nonlinear functions (such as sigmoid, gaussian, and wavelets) which have been demonstrated to be good pattern classifiers and thus potentially capable of diagnosing faulty conditions (Venkatasubramanian and Chan, 1989; Himmelblau, 1992; Leonard and Kramer, 1992; Bakshi and Stephanopoulos, 1993). Their main drawback is that to develop such neural network classifiers, a training set must be available which contains an abundance of faults, something which is rarely available in real processes.

Most rule-based expert systems and neural network classifiers have been developed for continuous processes that are intended to operate at various steady states. To handle unsteady-state processes, such as batch operations, a variety of methods have been developed recently for extracting information on temporal shapes or time profiles, and classifying process behavior based on this information using rule-based expert systems (Janusz and Venkatasubramanian, 1991; Konstantinov and Yoshida, 1992; Holloway and Krogh, 1992;

Cheung and Stephanopoulos, 1992). Their main drawbacks are the lack of a statistical basis for interpreting the data and classifying the results, and the complexity of the approaches when dealing with more than a few variables.

A multivariate statistical approach

In this article, we present an alternative approach to monitoring batch processes based on the use of empirical models developed from a multiway principal component analysis (MPCA) of existing batch data. The approach is based on the philosophy of statistical process control (SPC), under which the behavior of the process is characterized using data obtained when the process is operating well and is in a state of control. Subsequently, future unusual events are detected by referencing the measured process behavior against this 'in-control" model and its statistical properties. In this sense, the present approach is "nondirectional" in that it will detect any deviation from normal behavior and may not be as powerful as the state estimation and knowledge-based approaches in detecting those specific faults that are built into their models. On the other hand, it is not sensitive to the assumptions of these "directional" approaches, and the only information needed to develop the monitoring procedure is a historical database of past successful batches.

Although, theoretical models of batch processes and on-line sensors for the quality properties are not usually available, nearly every batch process does have frequent observations available on many easily measured process variables, such as temperatures, pressures, flow rates, and agitator power. Measurements on up to 30 or more variables may be available every few seconds throughout the entire history of a batch. Furthermore, a history of many past successful and some unsuccessful batches is usually available. From these data, it should be possible to build an empirical model to characterize the operation of successful batch runs (to build a "fingerprint" for successful batches) and to develop statistical tests for deviations from such normal operation.

The major difficulty is how to handle the large number of multivariate observations taken throughout the batch history. Although it is not unusual to measure more than 20 variables around a batch process, this does not mean that 20 independent things are taking place. The measured variables are autocorrelated in time and extremely highly correlated with one another at any given time. Furthermore, not only is the relationship among all the variables at any one time important, but so is the entire past history of the trajectories of all these variables. To accommodate this kind of data, a multivariate statistical projection method (MPCA) is used to compress the data and to extract the information by projecting the data into a low-dimensional space that summarizes both the variables and their time histories during successful batches. The progress of a new batch is then monitored by comparing the progress of the projections of its variable trajectories in the reduced space with the statistical distribution of the trajectories from the past successful batches.

This approach leads to the development of some new multivariate SPC control charts whose presentation and interpretation are no more difficult than conventional Shewhart charts (Shewhart, 1931), and yet they are much more powerful in their ability to detect even subtle changes in batch process operations. These ideas represent extensions of the multivariate monitoring procedures developed by Kresta et al. (1991) and Skagerberg et al. (1992) for monitoring continuous processes to nonlinear and finite duration batch processes.

Only the monitoring and detection aspects of the problem are tested in this article. As with most "nondirectional" SPC procedures no assignment as to the cause of the event is provided. Once a significant deviation from normal operating performance has been detected, it is usually left to the engineers and operators to use their process knowledge to provide a quick diagnosis of possible causes and to respond in an appropriate manner. However, with the multivariate statistical procedures proposed here, it is also possible to provide the operators with much more diagnostic information by interrogating the underlying MPCA model. Some of these diagnostic approaches have been proposed by MacGregor et al. (1994).

Multiway Principal Component Analysis

Principal component analysis (PCA) is a well known multivariate statistical method (Mardia et al., 1989; Jackson, 1991), which has as its objective the explanation of the variance-covariance structure of a multivariate dataset through a few linear combinations of the original variables with special properties in terms of variances. It decomposes a matrix $X(I \times J)$, where there are J measurement variables for I objects into a series of R principal components ($X = \sum_{r=1}^{r=R} t_r p_r'$), with each characterized by a loading vector (p_r) and a score vector (t_r). The principal components represent the selection of a new coordination system obtained by rotating the original variables and projecting them into the reduced space defined by the first few principal components, where the data are described adequately and in a simpler and more meaningful way. The principal components are ordered such that the first one describes the largest amount of variation in the data, the second one the second largest amount of variation, and so on. With highly correlated variables, one usually finds that only a few principal components are needed to explain most of the significant variation in the data. The number of principal components to retain can be determined by using cross validation (Wold, 1978; Eastment and Krzanowski, 1982).

The loading vectors (p_r) are orthonormal and provide the directions with maximum variability. The t scores from the different principal components are the coordinates for the objects in the reduced space. They are uncorrelated and therefore are measuring different underlying "latent structures" in the data. By plotting the scores of one principal component vs. another, one can easily see which of the objects have similarities in their measurements and form clusters, and which are isolated from the others and therefore are unusual objects or outliers.

The power of PCA arises from the fact that it provides a simpler and more parsimonious description of the data covariance structure than the original data. Its success in several different areas is partially related to the nonlinear iterative partial least squares (NIPALS) algorithm (Geladi and Kowalski, 1986; Wold et al., 1987a) for the calculation of the principal components. It is a simple, fast and effective algorithm to extract the principal components in a sequential manner and is a variant of the power method for calculating eigenvectors of a matrix (Goldberg, 1991). PCA has been ap-

plied to a broad spectrum of sciences, like biology, psychology, chemistry, quality and process control, and economics, revealing its robustness and potential strength to analyze large datasets.

In many cases, especially in sciences like chemistry, psychometrics, and image analysis, the data from an experimental study takes the form of three-way arrays. This is also the case in the batch monitoring problem. To understand the nature of the data available with which to monitor batch processes, consider a typical batch run in which $j = 1,2, \ldots, J$ variables are measured at $k = 1,2, \ldots, K$ time intervals throughout the batch. Similar data will exist on a number of such batch runs $i = 1,2, \ldots, I$. All the data can be summarized in the $\underline{X}(I \times J \times K)$ array illustrated in Figure 1, where different batch runs are organized along the vertical side, the measurement variables along the horizontal side, and their time evolution occupies the third dimension. Each horizontal slice through this array is a $(J \times K)$ data matrix representing the time histories or trajectories for all the variables of a single batch (i). Each vertical slice is an $(I \times J)$ matrix representing the values of all the variables for all the batches at a common time interval (k).

A method which can handle such data is MPCA (Wold et al., 1987b), which is statistically and algorithmically consistent with PCA and has the same goals and benefits. The relation between MPCA and PCA is that MPCA is equivalent to performing ordinary PCA on a large two-dimensional matrix formed by unfolding the three-way array $\underline{X}$ in one of three possible ways. In this work, we will unfold $\underline{X}$ in such a way as to put each of its vertical slices $(I \times J)$ side by side to the right, starting with the one corresponding to the first time interval. The resulting two-dimensional matrix has dimensions $(I \times JK)$. This unfolding allows us to analyze the variability among the batches in $\underline{X}$ by summarizing the information in the data with respect both to variables and their time variation.

The objective of this version of MPCA is to decompose the three-way array $\underline{X}$ into a series of principal components consisting of score vectors (t_r) and loading matrices (P_r), plus a residual matrix $\underline{E}$ (Figure 1). It accomplishes this decomposition in accordance with the principles of PCA and separates the data in an optimal way into two parts. The noise or residual part $(\underline{E})$ which is as small as possible in a least squares sense, and the systematic part $(\Sigma_{r=1}^{R} t_r \otimes P_r)$ which expresses it as one fraction (t) related only to batches and a second fraction (P) related to variables and their time variation.

The MPCA algorithm derives directly from the NIPALS algorithm and has the following formulation:

i. Scale $\underline{X}$ by subtracting from each column its mean and dividing by its standard deviation.
ii. Choose arbitrary a column of $\underline{X}$ as t.
iii. $\underline{E} = \underline{X}$

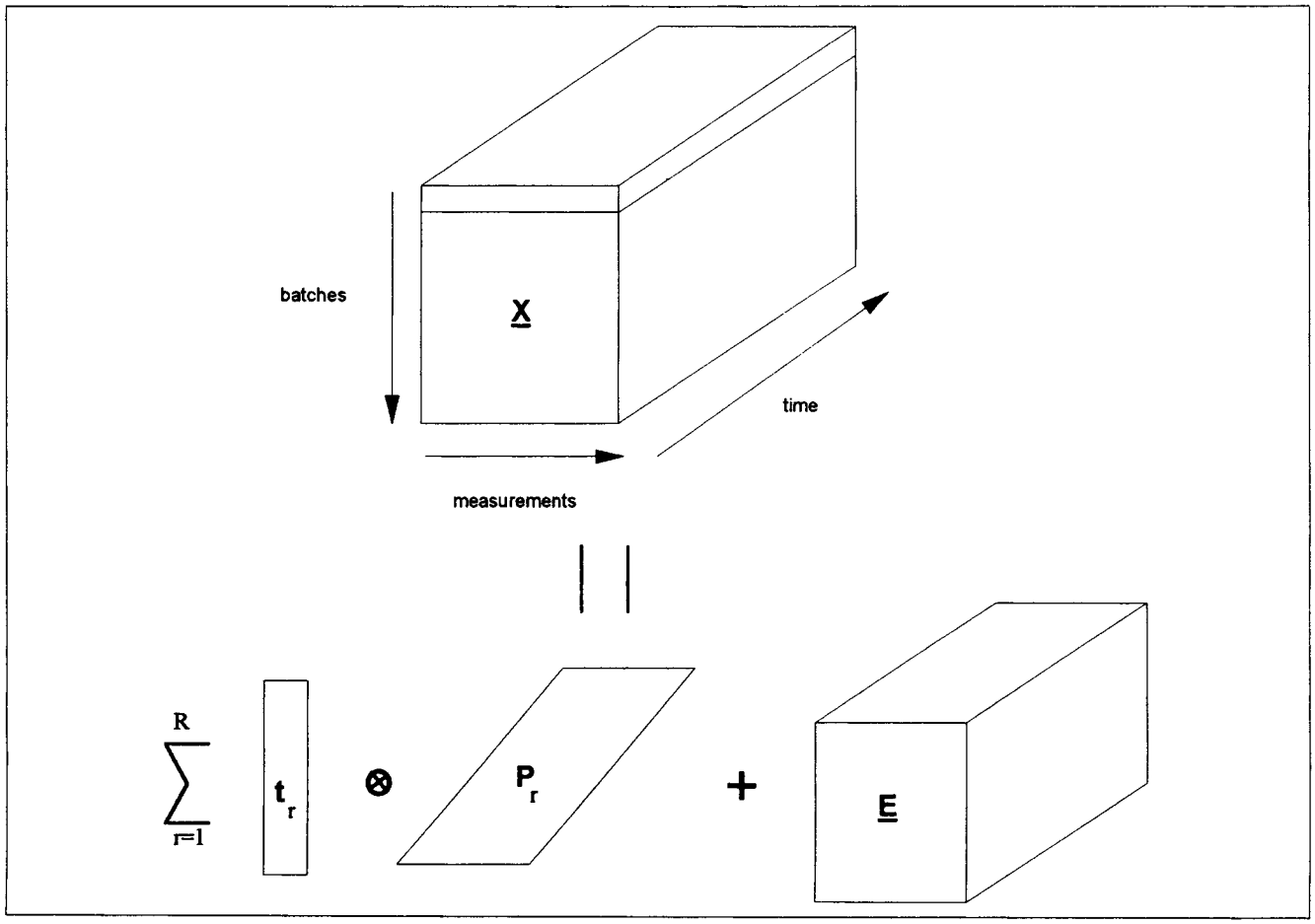

Figure 1. Arrangement and decomposition of a three-way array by MPCA.

1. $P = \underline{E}' \cdot t$
2. $P = P/\|P\|$
3. $t = \underline{E} \circ P$
4. If t has converged then go to step 5, otherwise go to step 1.
5. $\underline{E} = \underline{E} - t \otimes P$.

iv. Go to step 1 to calculate the next principal component.

The matrix operations in the above algorithm are:

$$\underline{E}'(j,i,k) = \underline{E}(i,j,k)$$

$$P = \underline{E}' \cdot t \quad P(k,j) = \sum_{i=1}^{I} \underline{E}'(j,i,k) t(i)$$

$$\|P\| = \sqrt{\sum_{k=1}^{K} \sum_{j=1}^{J} P(k,j)^2}$$

$$t = \underline{E} \circ P \quad t(i) = \sum_{j=1}^{J} \sum_{k=1}^{K} \underline{E}(i,j,k) P(k,j)$$

$$\underline{X} = t \otimes P \quad \underline{X}(i,j,k) = t(i) P(j,k)$$

Figure 2 shows clearly that this version of MPCA explains the variation of the measured variables about their average trajectories as calculated from the reference database. Subtracting the average trajectory from each variable removes the major nonlinear behavior of the process. The ith elements of the t-score vectors corresponds to the ith batch and summarize the overall variation in this batch with respect to the other batches in the database over its entire duration. The P loading matrices summarize the time variation of the measurement variables about their average trajectories, and their elements are the weights, which when applied to each variable at each time interval within a batch, give the t scores for that batch.

MPCA, unlike PCA which has been applied to a variety of problems, has been mainly used in image analysis (Geladi et al.,1989) and in few cases in chemometrics (Smilde and Doornbos, 1991), where the data from an experiment take the form of a three-way array. MPCA, because of its equivalence with PCA, shares the same benefits of information extraction and data projection. In the following sections, these features of MPCA are utilized to analyze and compare past batch runs and to develop on-line monitoring schemes for new batches.

Analysis of Historical Batch Data Using MPCA

In this section we illustrate how MPCA can be used to perform a post analysis on completed batch runs to discriminate between similar and dissimilar batches. Such an analysis can be used to improve operating policies and to understand some of the major sources of batch-to-batch variation. We consider a simulation study of a semibatch emulsion polymerization reactor. This simulation has been used as a framework, where we have perfect knowledge and command of the process operation, to develop the ideas of the present statistical procedure and to test out its abilities to detect simulated operational problems.

The simulated data are based on the semibatch emulsion

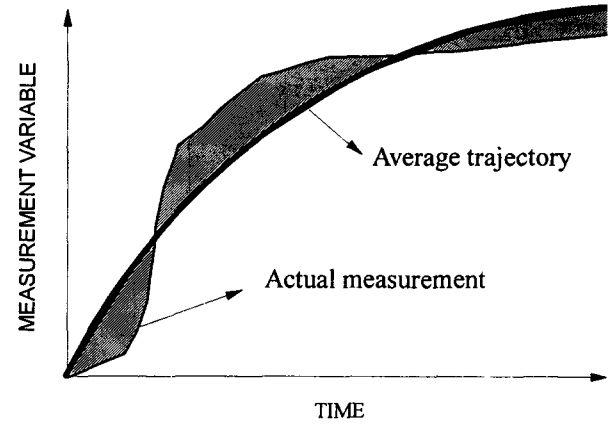

Figure 2. Shaded area indicating the variation that MPCA explains.

polymerization of styrene-butadiene to make a latex rubber (SBR). The simulations were performed using a detailed mechanistic model developed by Broadhead et al. (1985). The batch is initially charged with seed SBR particles and with all its 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. Impurities in the initial charge of the organic phase and in the butadiene feed to the reactor were added to introduce meaningful disturbances for this study. Autocorrelated variations and noise were added to the monomer feed rates throughout each batch, and measurement noise was added to the temperature measurement of the feeds. The batch duration is 1,000 min, and measurements are taken every 5 min (200 time intervals) on the flow rates of styrene (1) and butadiene (2), on the temperatures of the feeds (3), the reactor (4), the cooling water (5), and the reactor jacket (6), and on the density of the latex in the reactor (7). Also, estimates of the total conversion (8) and the instantaneous rate of energy release (9) were obtained from an on-line dynamic energy balance around the reactor and jacket.

A base recipe was chosen, and 50 batches were simulated to create a reference database of normal batches by introducing typical variations in the base case conditions (such as initial charge of seed latex, amount of chain transfer agent, and level of impurities). 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 quality measurements define the acceptable quality region of the product, and a "good" or normal batch is taken to be one which falls under three standard deviations around the mean for each quality measurement.

Two additional batches with product just barely out of this specification region were simulated: one with an initial organic impurity contamination in the butadiene feed, 30% above that of the base case; the other with the same problem, but this time the contamination, 50% above the normal level, started halfway through the batch operation. These "bad" batches, having the same cause for their abnormal operation, will help investigate the ability of MPCA to detect a fault occurring at

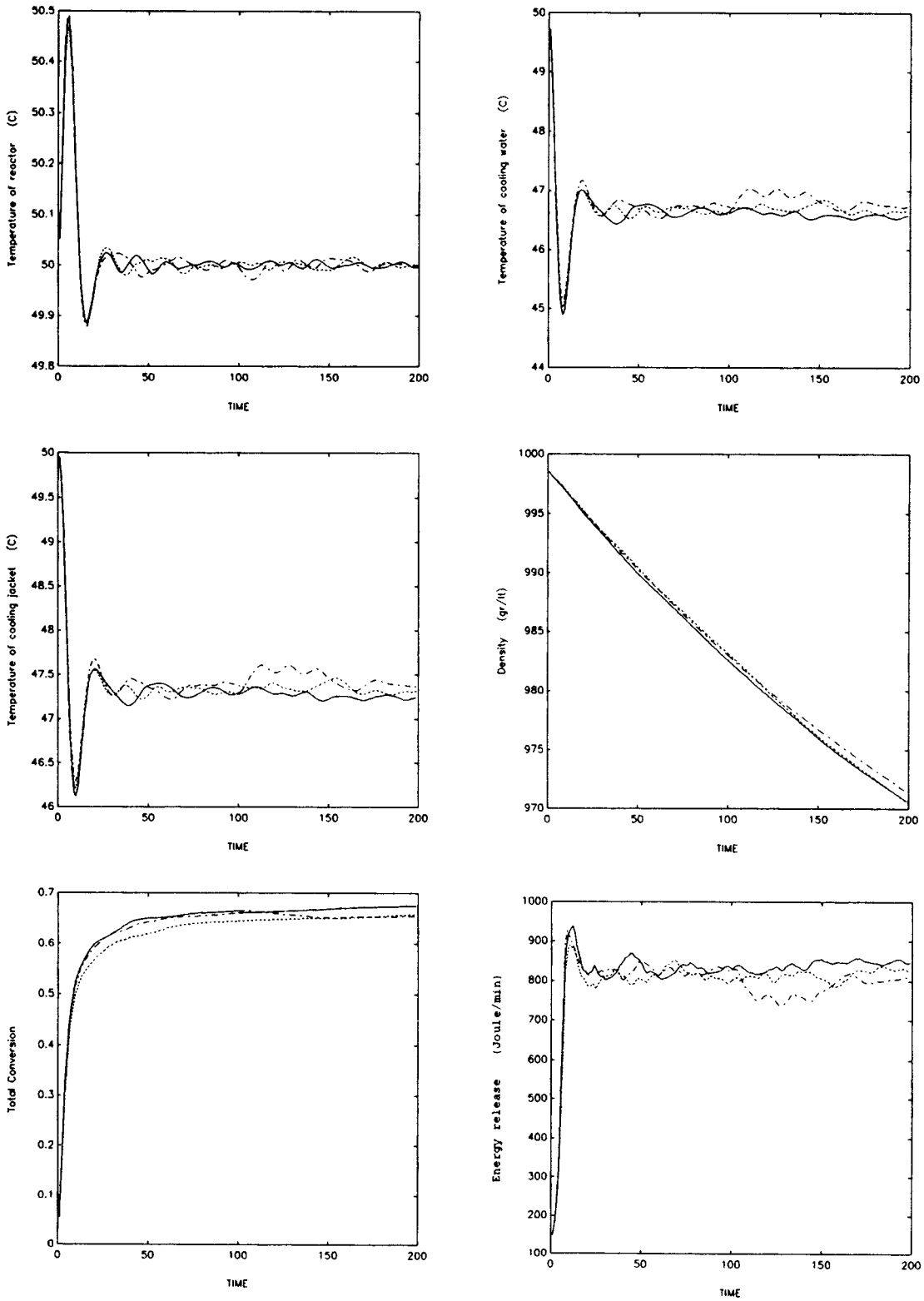

Figure 3. Trajectories of measurement variables for a normal batch (——), a batch with initial problem (· · · ·), and a batch with problem halfway through its operation (----).

different times without confounding the results because of any differences in the cause of the abnormal operation.

In both cases, there was not an abrupt fault which is often easily detectable by examining the plots of the individual variables. They were more incipient faults, typical in industry, where the abnormal operation is slowly developing and none of the individual measurements reveal clearly the fault. The trajectories for the individual variable measurements for the

two bad batch runs and a normal one are shown in Figure 3, where there is not much observable difference among these runs. If all the trajectories from the database of the 50 good batches were plotted on this figure, any differences between these and the bad batches would be difficult to detect through a visual inspection of these individual plots.

By adding these two bad batches as the last (51 and 52) objects in the normal database, a MPCA was applied to the three-way array $\underline{X}$ with dimensions $52 \times 9 \times 200$. The projections of these 52 batches into the score plane of the first two principal components (t_1,t_2) are shown in Figure 4, where the two faulty batches fall well outside the cluster of good batches, clearly indicating that their temporal development was different. All batches with a similar history should cluster in the same region of the reduced space described by the principal components.

This example demonstrates the ability of MPCA to discriminate between normal and abnormal batch operation through simple to interpret plots and to detect any systematic variability in the measurements of a batch operation. Consequently, this classification to normal and abnormal batches that MPCA provides for this example answers the question if the measurements contain the appropriate amount of information for classification of a batch as similar or dissimilar to the typical normal batch operation. This is the most important question, which shall be investigated first in any monitoring scheme, and MPCA provides a simple and easy way to answer it.

Having established the "observability" of faults in the post analysis of past data, the next step is to build a model that summarizes the information contained in the database of good batches about the normal operation of the process and to use this model as the statistical reference framework to classify a new batch as normal or abnormal. This classification will then be based on the similarity and statistical consistency of the trajectory measurements of a new batch with the historical reference distribution of trajectories from normal operation as summarized by this model.

Performing an MPCA on the data from the 50 good batches $[\underline{X}(50 \times 9 \times 200)]$, three principal components, as determined by cross validation (Krzanowski, 1982; Nomikos and MacGregor, 1994), were necessary to describe the predictable variation of all the variables about their average trajectories and hence to provide a model that describes adequately the normal operation of a batch run. Figure 5 shows the score plot in the space of the first two latent vectors (t_1,t_2) for the 50 good batches, and similar to this are the score plots for any other two of the three latent vectors. The scatter character of these plots indicates that all these batches belong to the same "normal" population, and none of them lies far away from the cluster. The area that this population occupies defines the normal operational region in the reduced space; the closer a batch is to the origin of this reduced space, the more similar is its operation to the average batch run. The sum of squares of the residuals from this model for each of the 50 batches $[Q_i = \Sigma_{k=1}^{K} \Sigma_{j=1}^{J} \underline{E}(i,k,j)^2]$ are given in Figure 6. These Q_i values represent the squared perpendicular distance of the $(J \times K)$ dimensional point for the ith batch from the reduced space defined by the three principal components of the MPCA model. Figure 6 shows that all batches have been explained adequately, since none of them has an unusually large residual exceeding the 99% confidence interval (Jackson and Mudholkar, 1979).

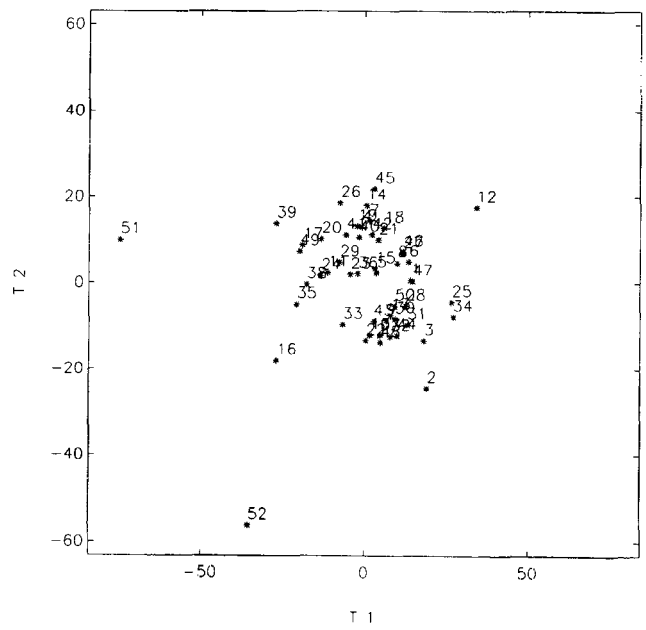

Figure 4. MPCA is able to discriminate between abnormal (51,52) and normal batches.

These t and Q plots show that the MPCA model describes adequately the normal database and exhibits certain "normal" statistical properties essential for the development of the on-line monitoring procedure.

The MPCA model attempts to explain all the predictable variation in the normal operating batch data. It is informative to examine the percentage of the total variation in each variable and at each time, which is explained by the three principal

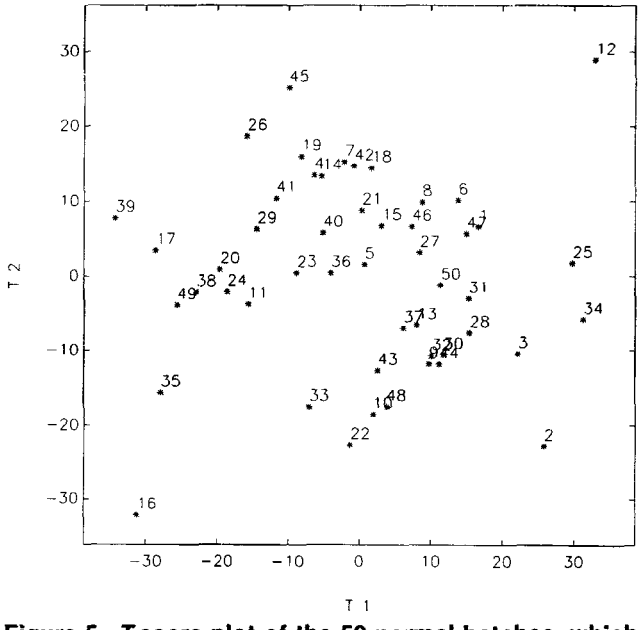

Figure 5. T-score plot of the 50 normal batches, which defines the normal operational region in the reduced space.

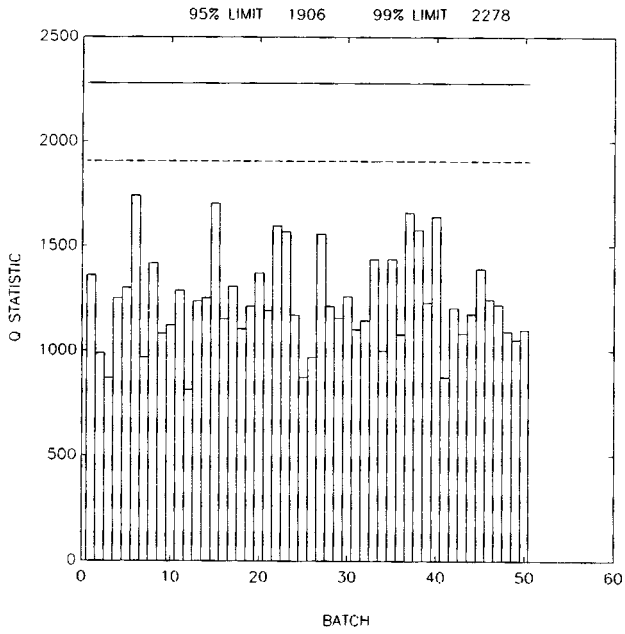

Figure 6. Sum of squares of the residuals (Q), with their 95% and 99% confidence limits.

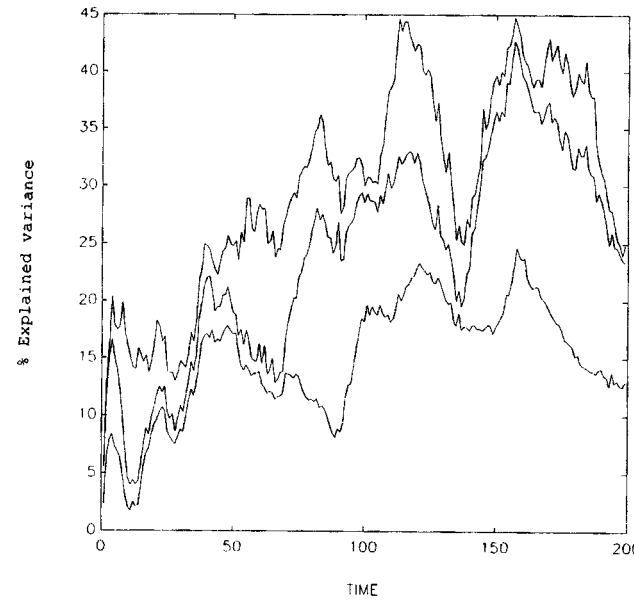

Figure 8. % Explained variance with respect to time for each of the three principal components, plotted on a cumulative basis.

components. Figure 7 shows that the dominant variables in the first principal component are the density (7) and the total conversion (8). The temperatures around the reactor (5,6) and the rate of energy release (9) are explained mostly by the second and third principal components. Variables with mainly a stochastic character, such as the flow rate of the styrene (1) and the temperature of the feeds (3), are largely ignored by MPCA. Only the flow rate of the butadiene (2) contributes to the model, due to the fact that it is carrying the incoming organic impurities. The amount of variance accounted for by each principal component as function of time is shown in Figure 8. Note that on a relative basis, the second principal component concentrates more than the other two principal components on the variability at the last half part of the batch operation. These plots give insight into the process operation and provide information for understanding the MPCA model so that it can be used more effectively to monitor new batches and detect faults.

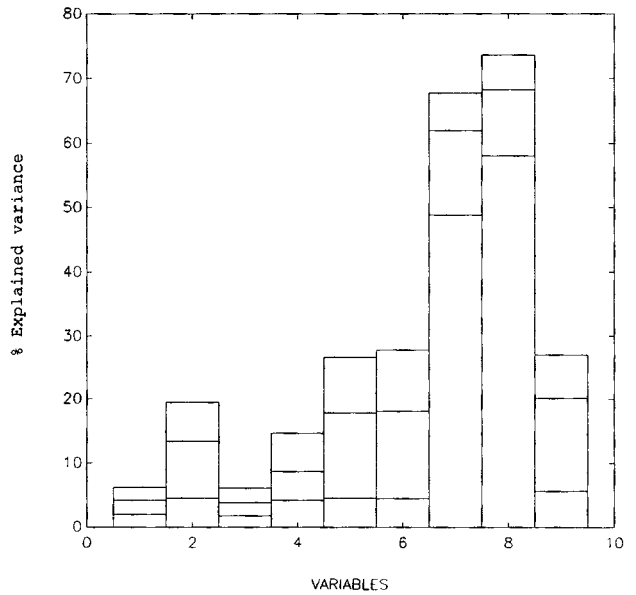

Figure 7. % Explained variance with respect to the measurement variables for each of the three principal components, plotted on a cumulative basis.

On-Line Monitoring of Batch Processes

In this section, we develop a method based on MPCA for monitoring the progress of batch processes in real time. The philosophy behind this method is very much that of traditional SPC methods, whereby the future behavior of the process is compared against a reference distribution based on past history. In this case, the reference distribution is the history of past successful batch runs, which produced good-quality product and exhibited no unusual faults or operating problems during their progress. In fact, one way of selecting the reference distribution is to take the history of previous batch runs and omit all those batches that one would like the monitoring scheme to have pinpointed as being different. The MPCA model is then built on the data from these reference batches. The central idea is to use the results of this analysis as the reference distribution to characterize the normal operation of the process and extract directly from this the statistical information needed to evaluate the behavior of new batches.

The on-line evolution of a new batch is monitored in the reduced space defined by the principal components of the MPCA model. The P loading matrices contain all the structural information about how the variable measurements should deviate from their mean values at each interval. The predicted t scores for each of the R principal components and the residuals E for a new batch X_{new} $(K \times J)$ are given by:

$$t_r = X_{new} \circ P_r$$

$$E = X_{new} - \sum_{r=1}^{R} t_r \otimes P_r$$

where X_{new} is the measurement matrix after mean centering and scaling as in the reference database, and t_r (scalar) is the score corresponding to the rth principal component.

A problem arises in the on-line application of the two prediction equations of MPCA: the matrix X_{new} is not complete. If the process is at the kth time interval, X_{new} has only its first k rows complete, and it is missing all the future observations. Several approaches have been studied to overcome this deficiency (Nomikos and MacGregor, 1994). The objective of all these approaches is to fill in the future values in the X_{new} matrix in such a way that the predicted t scores at each time will be as close as possible to those that would be predicted, if one had the full X_{new} matrix.

The approach presented here, which has shown good attributes for detecting a fault in a clear and quick manner, is based on assuming that the future deviations in X_{new} from the mean trajectory will remain constant at their current values for the duration of the batch. This is similar to the assumption made in model-predictive control algorithms, such as the dynamic matrix control (DMC) algorithms, where the future values of the disturbances are assumed to remain constant at their current values over the prediction horizon considered. Therefore, in monitoring a new batch on-line, the following procedure is used:

i. Take the new vector of measurements at time interval k.

ii. Subtract the mean and divide by the standard deviation, which corresponds at the kth time interval from the normal database to get the vector with the current deviations.

iii. Set the rows of X_{new} from k onward equal to the current deviation vector.

iv. $t_{r,k} = X_{new} \circ P_r$; $E = X_{new} - \Sigma_{r=1}^{R} t_{r,k} \otimes P_r$; $SPE_k = \Sigma_{j=1}^{J} E(k,j)^2$

v. Return to step i.

The score values ($t_{r,k}$) represent the projection of X_{new} at time k onto the R-dimensional plane defined by the reference MPCA model. If a new batch is progressing in a manner that is consistent with the past reference distribution of good batches, then it should appear to be coming from the same MPCA model. Thus, its residuals [$E(k,j)$] should be small, and its score values ($t_{r,k}$) should continue to fall within the region of variation defined by the reference distribution.

There are two ways in which a new batch can exhibit deviations from the MPCA model. Its score values ($t_{r,k}$) can move outside the acceptable range of variation defined by a control region, or its residuals [$E(k,j)$] could become large and the batch will be placed well outside, perpendicular to the reduced space. In the first case the model is still valid, but the magnitude of the variation during the new batch is too great. In the second case, however, the model is no longer valid, because a new event, not in the reference set, has occurred and the new batch does not project onto the reduced space adequately. In the later case, the squared prediction error (SPE_k) will become larger than a control limit defined by applying the model to the good batches in the historical database.

Thus, the residuals account for any variability which is not described sufficiently in the database of good batches. The best way to monitor the residuals is to use the SPE, which is the sum of squares of errors directly related to the latest on-line measurements from the process, since the sum of squares of the residuals [$Q = \Sigma_{k=1}^{K} \Sigma_{j=1}^{J} E(k,j)^2$] is heavily confounded with the error associated with the assumption about how to treat the future observations. We are interested in pinpointing the particular interval where something is going wrong and its duration, and the SPE is a very good indicator to accomplish this. Figure 9 gives a graphical description of each quantity ($t_{r,k}$, SPE_k) that one has to track for monitoring on-line the operation of a new batch.

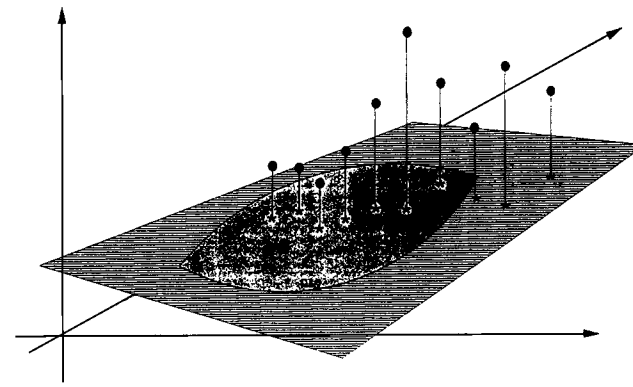

Figure 9. Batch operation in the reduced space of MPCA.

The stars on the reduced space are the t scores, and the area inside the ellipse depicts the normal operational region. The sum of squares of the residuals are the normal distances from the reduced space.

The results of applying such a monitoring scheme to a new "normal" batch and the two "bad" batches from the SBR emulsion polymerization simulation are shown in Figures 10, 11 and 12, respectively. The four charts in these figures are the most useful ones for monitoring the behavior of new batches. The top left plot in each figure shows the progress of the squared prediction errors (SPE), and the top right plot shows the progress of one of the latent vectors (t_r). The bottom left plot shows the progress of the batch in the joint space of the first two latent variables (t_1,t_2). The final plot in the bottom right corner is a plot of a Hotelling statistic (D), which provides a measure of the directed distance of the position of a new batch in the reduced space from the origin of normal operation.

The control limits shown in each plot correspond to approximately 95% and 99% confidence regions based on the historical reference distribution of good batches. These were calculated using the idea of the external reference distribution (Box et al., 1978). Each of the 50 good batches in the reference database was passed through the on-line monitoring algorithm given above, as if they were new batches, and their scores ($t_{r,k}$) and squared predictions errors (SPE_k) were collected at each time interval k. This provided 50 observations, on each of the t scores and squared prediction errors, at each time interval k. These observations were used to construct the control regions for future observations, under the assumption that whatever mechanism gave rise to the observations in our sample is still operating in the same manner for the future observations.

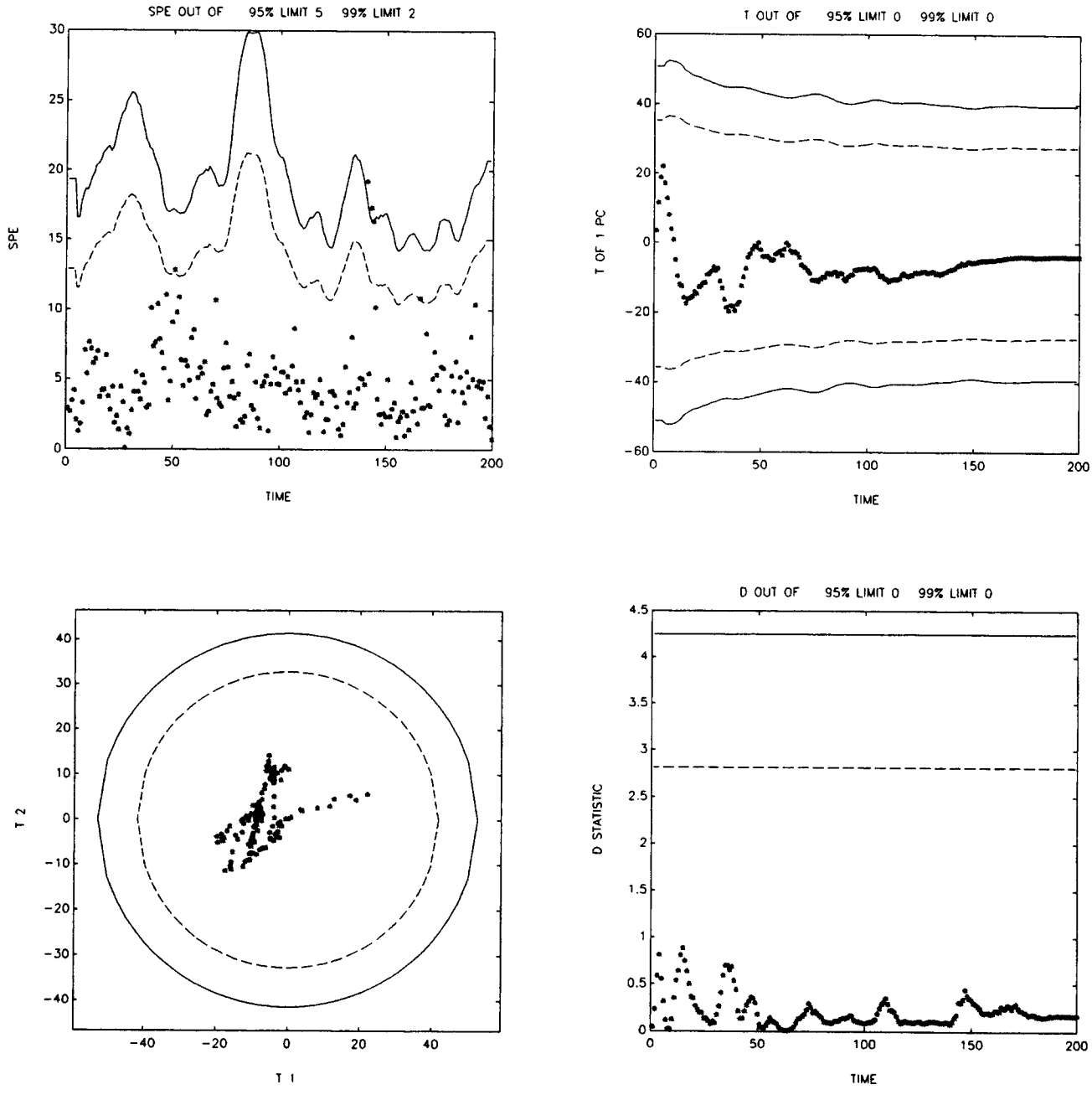

Figure 10. Monitoring charts with their 95% and 99% control limits for a normal batch run.

The distribution of the $t_{r,k}$'s was found to be adequately approximated by a normal distribution. This was to be expected since any linear combination of random variables, according to the Central Limit Theorem, should tend toward a normal distribution. Under this assumption, all the control limits associated with the t scores were derived using normal distribution theory statistics (Hahn and Meeker, 1991). The elliptical contours in the joint (t_1,t_2) plots and the Hotelling statistics (D) are based on the multivariate normal distribution theory (Anderson, 1984; Johnson and Wichern, 1988):

$$D = t_k' S^{-1} t_k \frac{I(I-R)}{R(I^2-1)} \sim F_{R,I-R}$$

where R is the number of principal component used for the MPCA model, I the number of batches in the normal database, t_k is the vector containing the scores from all the principal components at time interval k, and S is the estimated covariance matrix of the t scores from the post analysis of the good database. This is a diagonal matrix because the t scores from different principal components are uncorrelated.

As can be seen from the individual t plots, the limits change throughout the duration of the batch, reflecting a greater degree of variation at certain times (Figures 10–12). Rather than trying to show how the joint elliptical contours change with time on the joint latent variable space plots (t_1,t_2), we constantly display the control contours appropriate for the end

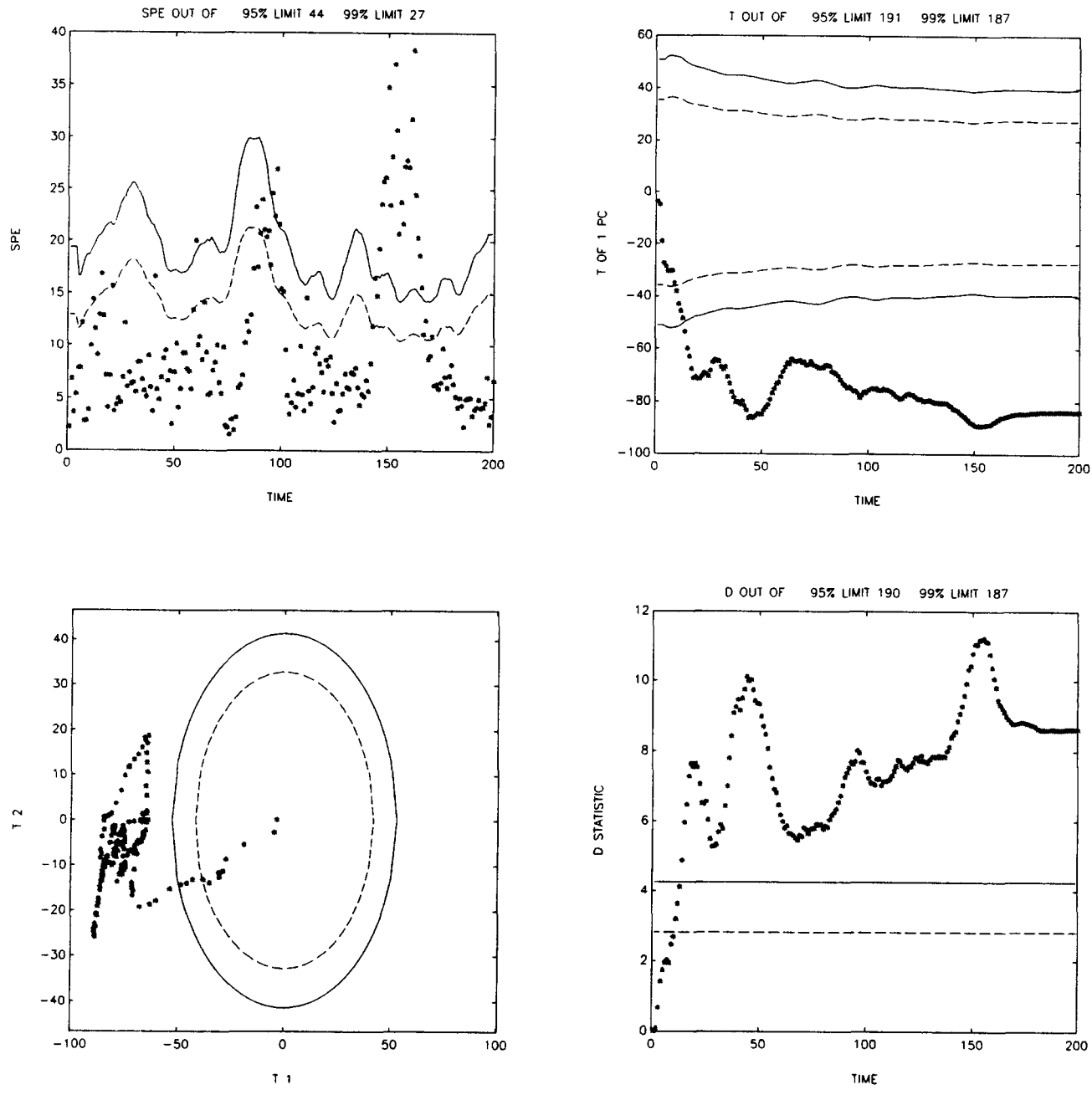

Figure 11. Monitoring charts with their 95% and 99% control limits for a batch run with initial problem.

of the batch. The hypothesis tested by these control ellipsoids at each time interval is the classification of a batch as normal or abnormal, based on the measurements available until that time interval and the assumed future behavior of the batch. Similarly, the control limits for the Hotelling statistic D are also based on that appropriate for the final time and have the same interpretation.

Assuming that the prediction errors $E(k,j)$ are also normally (but not independently) distributed, the SPE_k is a quadratic form which can be well approximated by a $g \cdot \chi^2_h$ distribution where g is a constant and h is the effective degrees of freedom of the chi-squared distribution (Box, 1954). The values of g and h can easily be estimated by matching the moments of the $g \cdot \chi^2_h$ distribution with the moments of the 50 observations of the SPE from the reference distribution at each time interval k, and the control limits are obtained from the chi-squared tables. More details on the calculation of control limits for all these plots are provided by Nomikos and MacGregor (1994).

The interpretation of the monitoring charts in Figures 10, 11 and 12 is straightforward. The new "normal" batch has all its latent vector plots and its SPE well within the control limits, implying that at no point during the batch operation there is any evidence that everything is not proceeding well. The batch with the impurity contamination in the butadiene feed starting right from time zero is clearly flagged as a batch with problems within the first 15 time intervals. Several of its SPE values exceed the 99% limit, but the clearest detection is provided by the charts associated with its t scores. The reason

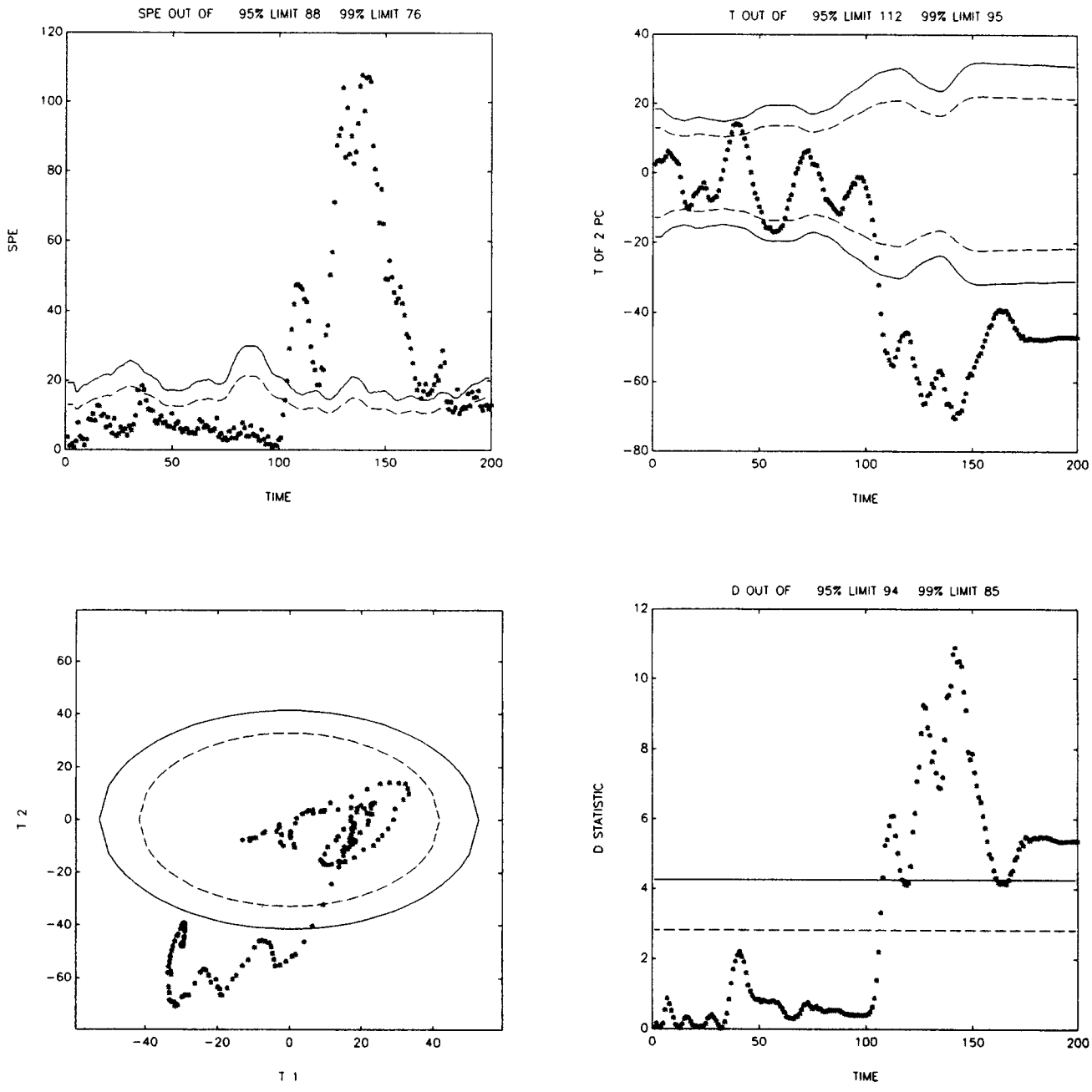

Figure 12. Monitoring charts with their 95% and 99% control limits for a batch run with problem halfway through its operation.

that the problem shows up most clearly in the individual t_1 plot comes from the fact that the major variables contributing to the first principal component (Figure 7) are the total conversion and the measured latex density, both of which show abnormally low values at the start of a batch when impurities are present.

In the other "bad" batch with an impurity contamination in the butadiene feed at the midpoint of the batch (time interval 100), the problem is most clearly alarmed in the SPE plot. This indicates that a type of variation or fault has been encountered that was not present in the reference database, which is indeed the case here. None of the batches in the normal database had a sudden change in the level of the organic impurities in the feeds halfway through its operation. Most of them had small perturbations in the level of the organic impurities right from the beginning of the batch. It is also interesting to see that it is now the second principal component (t_2) that most clearly detects the problem. This is reasonable because as one can see from Figure 8, the second principal component is dominated by information over the last part of the batch operation, where the fault occurred.

These examples demonstrate that the proposed charts preserve the ideas of SPC charts and can detect easily and quickly an abnormality. One has to closely watch the SPE and D control charts, which provide complementary information about the process operation and, if something is going wrong,

to use the other t-score charts to get a better understanding of the fault. Very effective methods for diagnosing possible causes for the detected deviations have been presented by MacGregor et al. (1994) and Miller et al. (1993). These diagnostic methods rely on interrogating the underlying PCA model and plotting the contributions of each variable to any increase in the SPE or to any movement in the principal components $(t_1,t_2, \ldots)$ over the time period of interest.

Given the case with which these multivariate monitoring charts were able to detect the simulated faults, one might expect that the faults would also be apparent in the trajectories of the individual variables. But as discussed earlier and illustrated in Figure 3, the faults, resulting in products that barely violate the specification regions, are not readily apparent in the individual trajectories. The problem with the one-at-a-time inspection of each variable trajectory is that one is only looking at the magnitude and possibly the trends of the deviations in that one variable. However, the true process is multivariable, and all the variables are highly correlated with one another. The power of the proposed monitoring scheme results from the fact that MPCA uses the joint covariance matrix of the variable trajectory deviations. By doing this, it utilizes not just the magnitude and trends of the deviation of each variable from its mean trajectory, but also the correlation among all of the deviations over the history of the batch. It is this correlation structure among the variables that appears to be most important in detecting faults. When a fault occurs, the relationship among the trajectory deviations often changes substantially, even though their individual magnitudes may not be large.

We would like to point out that the post analysis of a database of batches and the estimation of confidence limits for the monitoring charts have substantial computational requirements, although the calculations are very simple. By relying on large databases, one simply has to process a large amount of data. On the other hand, once this off-line analysis has been completed, the computational requirements for the on-line monitoring algorithm are extremely light and simple.

Conclusions

A new approach to monitoring the progress of batch processes has been presented. Rather than utilizing detailed engineering knowledge about the process, as in model-based and knowledge-based approaches, this approach utilizes only the information contained in the historical database of past batches. Such information is readily available for any computer monitored industrial batch process. A simulation of a styrene-butadiene batch reactor has been used to develop the ideas and to test the abilities of the proposed method, while an industrial example can be found in Nomikos and MacGregor (1994).

Multiway principal components analysis (MPCA) is used to extract the information from the trajectories of all the measured process variables, and to project it onto a low dimensional space defined by the latent vectors or principal components. The data reduction is tremendous, since all the information from a database of batches is captured in a few matrices which define the reduced space. A post analysis of past batches enables one to classify similar and dissimilar batches by examining the clustering of their projections onto this hyperplane. New batches can be monitored in real-time, using a sound statistical framework, by tracking their progress in this reduced space.

The approach is based on the basic concepts of Statistical Process Control (SPC), whereby the future behavior of a process is monitored by comparing it against that observed in the past when the process was performing well, that is in a state of statistical control. Control limits for the monitoring charts are derived from the statistical properties of this historical reference distribution of past "good" batches. Therefore, the approach relies upon the idea that future "good" batches should have similar behavior to past ones. The proposed monitoring charts are in accordance with the SPC requirements for charts that can be easily displayed, interpreted, and can quickly detect a fault.

As in all inferential approaches, the fundamental assumptions of "comparable" runs and "observable" events of interest must hold for the method to work. The first assumption states that the method is valid as long as the reference database is representative of the process operation. If something changes in the process (for example, new catalyst), then one has to build a new database which embodies the change and reapply the method. The second assumption expresses the requirement that the events which one wishes to detect must be "observable" from the measurements that are being collected. No monitoring procedure can detect events that do not affect the measurements.

The power of the statistical approach presented here lies in the fact that it utilizes the unsteady-state trajectory data on all measured variables in a truly multivariate manner, as to account not only for the magnitude and trend of the deviations in each measured variable from its average trajectory, but also for the high degree of correlation in both time and among the deviations in all the variables. The objective of the monitoring procedure is to detect and eliminate faults from future appearance, and thereby shrink the control limits and work towards a more consistent production of quality product.

Extensions of these methods, which not only utilize the historical data on the measured process variable trajectories, but also the measured feed-stock properties and other variable initial conditions, as well as the final product quality measurements at the end of each batch, are being developed. Those approaches utilize Multi-way Projection to Latent Structures (MPLS) methods (Wold et al., 1987b) that allow one to combine matrices and arrays that are interrelated.

Notation

D = Hotelling statistic
E = residual matrix for a new batch
$\underline{E}$ = residual matrix for historical database
$F_{R,I-R}$ = F distribution with R and $I-R$ degrees of freedom
g = constant associated with the distribution of the squared prediction error
h = degrees of freedom for chi-squared distribution
i = index for batches
I = total number of batches
j = index for measurement variables
J = total number of measurements variables
k = index for time intervals
K = total number of time intervals
p = loading vector
P = loading matrix
Q = sum of squares of the residuals
r = index for principal components
R = total number of principal components
S = covariance matrix of t scores

SPE = squared prediction error
t = score for a new batch
$\mathbf{t}$ = score vector
X_{new} = new batch
$\underline{X}$ = historical database

Greek letter

χ^2_h = chi-squared distribution with h degrees of freedom

Matrix

bold small letters = column vectors
bold capital letters = matrices
underline bold capital letters = three-way arrays
$'$ = transpose

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