Novel approach for process plant monitoring,

Nadeem Muhammed Khalfe

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Using statistical data compression important process changes can be quickly detected and identified


Often it is time-consuming to monitor conditions in modern complex process plants since there is an abundance of instrumentation that measures thousands of process variables every few seconds. This has caused a “data overload” and due to the lack of appropriate analyses this wealth of information is underutilized. Operating personnel typically use only a few variables to monitor the plant’s performance. Fortunately, groups of variables often move together because more than one variable may be measuring the same driving principle governing the process behavior.

Multivariate statistical methods such as principal component analysis (PCA) are capable of compressing the information into low-dimensional spaces that retain most of the information. Using this method of statistical data compression a multivariate monitoring procedure has been developed to efficiently monitor performance of large processes and rapidly detect and identify important process changes. A graphical interface was developed that facilitates plotting the real-time plant condition by a single point. The location of this point will indicate if the plant is running in normal or abnormal zones and diagnose on line any fault in the process. Also, the graphical interface points out the process parameters that are out of their normal operating window and make the process abnormal. This helps to quickly identify process upsets without going into process details that may otherwise remain unnoticed at their incipient stage. This software was implemented in the ethylene glycol plant and successfully diagnoses process upsets and abnormalities and leads to formulating early a troubleshooting plan. This generalized intelligent software can be useful and extended to any other process plant.

Introduction. Monitoring performance and detecting faults is an integral part of the successful operation of any process. Performance can be monitored by comparing the actual results to the predictions from a mechanistic model, or by using statistical process control (SPC) charts (e.g., Shewart charts, CUSUM charts or EWMA charts to compare the current process state against “normal operating conditions.” The challenge facing process monitoring is the enormous amount of correlated data being collected from a multitude of sensors every few seconds. This data overload and lack of appropriate analytical tools have meant that very little is being done to utilize this wealth of information. The biggest drawback to using a mechanistic approach is the need for a detailed model. Even if a detailed mechanistic model is available its parameters are uncertain, and often they need to be updated in real time. Using the established statistical control charting methods has the advantage that they need no model, but rather use the operational data directly. The major drawback to these control charts is that they were developed for monitoring univariate problems or sets of independent variables, and the expansion to handle the case of many highly correlated variables is difficult. These methods are still being used on a one-variable-at-a-time basis on multivariate processes, either formally using Shewart charts or informally by operators monitoring key variables. Generally, this approach has been adequate, although extremely inefficient; however, if the variables are correlated this approach can lead to erroneous results.

This article presents a different and more efficient approach to process monitoring based on multivariable statistical methods of PCA. These methods are particularly suited to analyzing large sets of correlated data. In the general problem process measurements are collected from the plant and arranged in an n x k matrix, X, consisting of n observations on k variables. The objectives of a multivariate SPC scheme would be to monitor the process and product quality using these observations and detect process upsets, equipment malfunctions or other special events. The final step in the procedure would be to find and remove the assignable causes for these events, thus improving process performance.

**FIG. 1** Data in three dimension (a) and (b) two dimensions.
Given the current process control computer systems, on-stream analyzers and automated quality control labs, it is not uncommon to measure hundreds of process variables on line every few seconds or minutes, and tens of product variables every few minutes or hours. Although a large number of variables may be measured, they are almost never independent; rather, they are usually very highly correlated. The true dimension of the space in which the process moves is almost always much lower than the number of measurements.

In some situations this is due to underlying fundamental relationships among the variables. For example, in the hypothetical reaction of \( A + B \rightarrow C \) where \( A \) and \( B \) are fed to the reactor in a specified ratio, although the concentrations of \( A \), \( B \) and \( C \) are being measured (three-dimensional measurement space), the actual problem is univariate (the stoichiometric relationship and the fixed feed ratio each eliminate a degree of freedom). In other situations the placement of the measurements and the nature of the process make the measurements highly correlated. Consider a distillation column where only three variables change independently: reflux, reboil and feed composition. Originally, measurements are being made of the temperature profile using every fourth tray temperature. If the number of measurements is increased to every tray temperature to obtain a more detailed temperature profile, the dimension of the measured variable space has been greatly increased, but the actual dimension of the problem has not changed. As a final illustration consider another situation where measurements on many different variables are made, but the nature of the process and the disturbances are such that they only allow the variables to move in a much lower dimensional space. For example, in the manufacture of synthetic fibers it is not uncommon to measure more than 10 quality variables such as denier, elongation under different loads, breaking strength, dye depths, etc. The physical meaning of these measurements guarantees that the process is only capable of making fibers with certain combinations of properties, and disturbances to the process will affect many of these variables in a highly correlated manner. For example, fibers with very small deniers (weight/unit length) cannot be made with very high breaking strengths, and disturbances that lead to a reduction in denier lead to a reduction in breaking strength.

As discussed, fortunately in data sets with many variables, groups of variables often move together because more than one variable may be measuring the same driving principle governing the system behavior. In many petrochemical systems there are only a few such driving forces. But an abundance of instrumentation allows us to measure dozens of system variables.

![Fig. 2](image1.png) A three-dimensional image displayed in two dimensions.

![Fig. 3](image2.png) Projection of data in the direction of maximum variance.

![Fig. 4](image3.png) Plot of first vs. second compressor principal component.

![Fig. 5](image4.png) Plot of second vs. third compressor principal component.

![Fig. 6](image5.png) Plot of first vs. third compressor principal component.
When this happens, we can take advantage of this information redundancy. We can simplify our problem by replacing a group of variables with a single new variable.

PCA is a quantitatively rigorous method for achieving this simplification. The method generates a new set of variables, called principal components. Each principal component is a linear combination of the original variables. All the principal components are orthogonal to each other so there is no redundant information. The principal components as a whole form an orthogonal basis for the space of the data. PCA was originally developed by Pearson and is a standard multivariate statistical method described in many textbooks (e.g., Anderson, Mardia et al., and S. Wold et al.).

Principal component analysis. We live in a multivariable world but we can only visualize three dimensions. Consider the three-dimensional picture (Fig. 1a) when observe from two dimensions (Fig. 1b). It is obvious that two dimensions may not be enough to observe a three-dimensional relationship. However, we can observe this relationship in two dimensions (Fig. 2) if we can identify two linear combinations of $x$, $y$, and $z$ such that most of the variation in these three variables is captured. These linear combinations of variables are called latent variables.

PCA is a data transformation method that rotates data such that the principal axis of the data is in the direction of maximum variation (Fig. 3). We can view the rotated data on the new principal axes. The “coordinates” of the data in this new “coordinate system” are known as principal component scores. These are essentially projections of the data onto the principal axes. The principal axes (components) are essentially vectors in the original variable space. These “vectors” are known as principal component loadings.

Why do we need to rotate the data? Although a data set may contain many variables (i.e., “n” dimensions), variation is often limited to a few key directions. By reorienting our coordinate system to align with these key (multivariable) directions we can often find that some of the directions perpendicular to this space contain very limited variation and can, therefore, be ignored. Hence, by reorienting the way we view the data we can squeeze as much information as possible into the three key principal directions.

How do we generate principal components? The principal components represent the selection of a new coordinate 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.

Principal components should have the following properties:

- They should be orthogonal (i.e., independent).
- The first principal component should point in the direction of maximum variance in the data.

To guarantee the properties, the columns of the original data must be orthonormal (normalized).

We can normalize a data set $X$ by the formula: $X = X_d \times D$ where the “mean-centered” matrix $X_d$ can be obtained by subtracting the respective mean from each element of the matrix: $X_d = X - \overline{X}$.

$D$ and $S_{dij}$ are defined as:

Continued
It can be shown that for a normalized data matrix $X$ (i.e., $X^TX = 1$) the eigenvector of $X^TX$ (the covariance matrix) with the largest eigenvalue will point in the direction of maximum variance in the data. In fact, the variance of the data along each eigenvector is equal to the eigenvalue of that eigenvector.

The proof also shows that eigenvectors are, by definition, orthogonal to each other. Hence, the eigenvectors of the covariance matrix are the principal components of the data.

**Steps to calculating principal components:**

- Consider a normalized data matrix $X$ (each column has zero mean and unit standard deviation) of size $n$ rows and $m$ columns ($n$ by $m$). The covariance of $X = X^TX$. 

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• Calculate all eigenvectors and eigenvalues of $X^TX$.

• Place the eigenvectors in order of decreasing eigenvalue. This matrix is called the loadings matrix, $P$ (m by m).

• To calculate the principal component scores (i.e., the projections of original normalized data onto this new eigenvector basis) multiply the normalized matrix $X$ by $P$. The scores matrix will be $T = XP$ (n by m).

The loading vectors, $P$, 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.

**Case study 1: Monitoring a reciprocating reclaim compressor.** In the ethylene glycol plant, a reciprocating compressor was used to pressurize reclaim process gas from 0.1 barg to 20.2 barg for ethylene recovery. The reclaim compressor is a three-stage reciprocating compressor with intermediate cooler and separator at each stage. The loader valves used in this compressor are prone to damage (usual life is one year only) if slight moisture carryover or condensation takes place from process gas. While the compressor is running, it is very difficult to identify the loader valves’ performance deterioration in spite of its effect seen on the interstage discharge temperature. If the loader valve abnormalities were not detected then...
at their incipient stage, the sudden compressor shutdown will cause substantial process upsets. The purpose of using a multivariate process monitoring system on this compressor is to diagnose the loader valve problems at their incipient stage so that their maintenance can be planned and an emergency compressor trip and subsequent process upset can be avoided.

To develop a monitoring system based on PCA, 2,162 hr of historical data were collected from process computers for all the process parameters (a total of 29 parameters like suction, discharge and interstage temperature and pressure, interstage separator level and 10 vibration indications positioned at different compressor locations) available in the DCS related to this compressor. Hourly average data projections (after gross outliers were removed) into the plane defined by the first three principal components are shown in Figs. 4, 5 and 6 for this reclaim compressor. The data points appear to cluster into two distinct regions that correspond to different operating conditions. Simply examining the individual process variable plots would be confusing, time consuming and would not reveal such information. To help diagnose the reasons for these shifts in process operation, one can interrogate the underlying multivariate model and display the process variable contributions to these shifts. After detailed investigation of the process data it was concluded that the green cluster corresponds to normal compressor operation and the red cluster corresponds to loader valve malfunction and subsequent compressor performance deterioration.

After detecting the different clusters, all the data that correspond to normal operation (green cluster) are separated and PCA was done to identify the normal operating zone range in the first three principal component planes.

Fig. 7 gives an historical trend plot of a first principal component with time (i.e., record number). A marked increase of the first principal component represents the transition from the normal to abnormal operating zones due to loader valve malfunction.

A “Scree” plot (Fig. 8) is a Pareto plot of the percent variability explained by each principal component. We can see that the first three principal components explain roughly two thirds of the total variability in the data. Thus, it can be concluded that instead of monitoring 29 compressor parameters, one can only monitor the first three principal components and be able to get enough information about whether the compressor is running normal or not. After establishing the normal and abnormal operating zone from historic data, we make the plots 4, 5, 6 and 7 on line in an exaquantum interface. On the computer screen only one point is plotted for every minute and from the location of that point one can identify easily whether the
compressor is in the green (normal) or red (abnormal) zones. The locus of the point can indicate if the compressor is moving slowly outside the normal operating zone when the loader valves start deteriorating. Thus, it is possible to diagnose the fault in the system at its incipient stage.

Case study 2: Monitoring and fault diagnosis of carbon dioxide removal unit. A carbon dioxide removal unit (CRU) is an integral part of an ethylene glycol (EG) plant where carbon dioxide is removed from cycle gas (contains ethylene, oxygen, methane carbon dioxide and traces of ethylene oxide) by absorbing carbon dioxide with hot potassium carbonate solution in an absorber (called contactor, Fig. 9). Rich carbonate solution coming from the bottom of the contactor contains unreacted carbonate and potassium. Bicarbonate and water are flashed in two low-pressure flash drums to remove dissolved ethylene and methane. After that rich carbonate solution is fed to the regenerator where heat is applied to remove CO₂ by converting bicarbonate to carbonate. The lean carbonate solution from the regenerator bottom is heated in a process–heat exchanger and again recycled back to the contactor for fresh absorption. Stable and efficient CRU operation is important in EG plant operation since it has a long-term effect on the EO catalyst and overall plant economics.

One of the biggest problems EG plants normally face in the CRU is the formation of glycol in the carbonate solution and subsequent deterioration of carbon dioxide removal capacity by carbonate. Sometimes especially in summer, the inlet cycle gas contains more ethylene oxide than permissible due to poor performance upstream the EO scrubber and this ethylene oxide reacts with water in the contactor and forms glycol. Once formed, this glycol is accumulated in the system and very difficult to remove. If glycol content in the carbonate solution exceeds 10%, it causes rapid foaming in the contactor and, in extreme cases, causes plant shutdown. The main problem in detecting glycol in carbonate solution is that its formation and accumulation are very slow (takes one month to build up) and its effects on process parameters are not so conclusive for detection.

Monitoring system development. The primary purpose of using a multivariate process monitoring system on this CRU section is to diagnose the problems of glycol formation at its incipient stage so that corrective action can be planned and subsequent process upsets due to severe foaming can be avoided.

To develop the fault diagnosis system, the CRU system was closely studied and eight process parameters (Fig. 9) were identified based on process experience and knowledge. Approximately seven months of hourly average historical data were collected for these eight tags and PCA was performed. The projections of hourly average data (after gross outliers were removed) into the plane defined by the first three principal components are shown in Figs. 10 and 11. Again, the data points appear to cluster into two distinct regions that correspond to different operating conditions. Again, the green cluster corresponds to the normal operating zone and the red corresponds to the abnormal operating zone due to high glycol content in the carbonate solution. The slow rise of the first principal component in Fig. 12 (as opposed to the reclaim compressor case where the rise is very stiff) indicates that the glycol accumulation is slow and the process moves very slowly from the normal to abnormal zone. Fig. 13 represents Hotelling’s T², a statistical measure of the multivariate distance of each observation from the center of the data set. This is an analytical way to find the most extreme points in the data. So instead of monitoring all the parameters one can monitor simply this Hotelling plot and conclude if the process is normal or abnormal.

After establishing the normal and abnormal zones from historical data, plots 10, 11 and 12 were made on line (same as reclaim compressor case) to provide real-time plots. The locus of the point inside the plots was closely monitored and the process parameters were adjusted when this live point started moving from the normal to the abnormal zone.

When the point is lying inside the red cluster, the panel operator receives an early indication of possible foaming in the system. Thus, he becomes prepared to fight against foaming with antifoam addition. Also, a graphical interface was developed to point out the process parameters that are out of their normal operating window and make the process abnormal by detecting which parameter causes the variation of principal components. Thus, this graphical interface enables the process engineer or panel operator to detect quickly the faults at their incipient stage and guides him through the cause-and-effect relationship.

LITERATURE CITED
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