SAS Interface for Run-to-Run Batch Process Monitoring Using Real-Time Data

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Abstract

The statistical methods for statistical process control using real-time data in batch processes require intensive computation on large amounts of data. The real-time data from a batch process consists of frequent measurements on several different variables during the batch operation time. In the example in this paper, 588 measurements are taken on eleven different variables during a single batch run. Using SAS/AF® and SAS/SCL® the RTPM Pro system has been developed to implement the statistical methods for real-time process monitoring. RTPM Pro menus have been designed to walk the user through: (1) using multivariate techniques to compute summary scores from the highly correlated real-time data, (2) form a multivariate regression model relating batch inputs and initial conditions to form expected summary scores, (3) compute process monitoring statistics which compare the deviation between the expected summary scores and the observed summary scores, and (4) provide diagnostic tools which identify patterns in the real-time variable(s) for batch runs with out-of-control signals.

Key words and phrases: Automatic process control, control charts, multivariate control charts, statistical process control.

Introduction

Many industries such as the semiconductor and chemical manufacturing industries use batch processes to form products. Processes that use batch or semi-batch processing include wafer planerization, wafer etching, injection molding processes, polymer manufacturing, pharmaceuticals, and biochemical to name a few. In most cases batch processes produce or manufacture large amounts of product. Therefore monitoring these processes is necessary to ensure that high quality products are consistently produced. A good method for monitoring batch processes is through the use of real-time process monitoring (RTPM). This paper will not cover the methods used to develop real-time process monitoring rather only illustrate their use. The interested reader is referred to the references at the end of this paper for more detailed discussion on real-time process monitoring.

Real-time process monitoring consists of two steps: process modeling and process monitoring. Both steps can be computationally intensive because of the large amount of data often collected during batch runs. In addition the variables are often highly correlated indicating that dimension reduction methods such as principle components analysis are valuable in focusing only on the real-time data containing information on process operation.

Historically real-time process monitoring computations have been done using SAS macros. This proved to be both laborious and time consuming. RTPM Pro is a system designed to provide a user-friendly graphical environment to perform real-time process monitoring. RTPM Pro was developed using SAS/AF and SAS/SCL.

This paper will use a Reactive Ion Etcher (RIE) as an example batch process where real-time process monitoring can be implemented. Etching is the process of transferring a pattern to a silicon wafer by removal of material, usually silicon (Si) or silicon dioxide (SiO_2). This is done by subjecting a gas (CF_4 in this case) to a high voltage causing a chemical reaction which creates an active mixture of electrons, ions, and free radicals. Through a self voltage bias, these ions and free radicals accelerate toward the surface of the wafer reacting with and removing the silicon surface.

Process Modeling

Process Modeling can be divided into the following four steps; data selection, data standardization, dimension reduction, and summary score modeling.
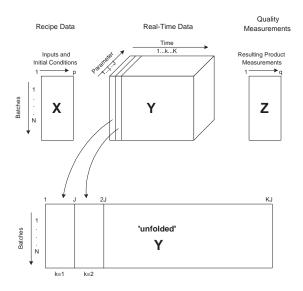
Figure 1: Data Structure of $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$.

Each of these steps is briefly explained along with its software implementation.

Data Selection

There are three types of data that may be collected from each run of a batch process. They include the following:

- the inputs or initial conditions which are referred to as the *recipe* or the $\mathbf{X}$ data.

- the real-time data on process variables know as *parameters* or $\mathbf{Y}$ data.

- the measurements on the resulting product, which are referred to as the *product quality measurements* or $\mathbf{Z}$ data.

For example with the RIE process the recipe or $\mathbf{X}$ data are the set points for chamber power and pressure. The parameters or $\mathbf{Y}$ data are those monitored during the process such as throttle position for gas outlet, flow rate of CF_4, voltage bias from wafer to ground, etc. The product quality measurements or $\mathbf{Z}$ data are uniformity, anisotropy, and etch depth.

When data is taken in real-time every few seconds or several times a second a database can quickly grow to be very large. Figure 1 shows the structure of the data. The $\mathbf{X}$ matrix containing the batch recipes is a matrix whose n rows represent the different runs and p columns contain the different recipe variables. The $\mathbf{Z}$ matrix containing the product quality measures is a matrix whose n rows represent the different runs and q columns contain

the different product quality variables. The data that pose the biggest problem are the $\mathbf{Y}$ data which Nomikos and MacGregor (1994) suggest organizing as a three dimensional array. The n rows correspond to the different runs, K columns correspond to the real-time measurements taken for a given run and the third dimension (depth) is the J different parameters. A problem with the high dimensionality of the $\mathbf{Y}$ data occurs with SAS® datasets storage and when multivariate statistical methods are used. Multivariate statistical methods require that the $\mathbf{Y}$ data be a matrix and not a three dimensional array. To deal with this problem the $\mathbf{Y}$ data is 'unfolded' so that the n rows represent the different runs and JK columns are arranged such that columns 1 through J contain the first real-time sampling point observations on the J different parameters, the $J + 1$ to $2J$ columns contain the second real-time sampling point observations on the J different parameters, and so on until the $(k - 1)J + 1$ to JK columns contain the last or Kth real-time sampling point observations on the different parameters. The bottom half of Figure 1 contains a graphical representation of how the $\mathbf{Y}$ matrix is 'unfolded'. This is how the data is used in real-time process monitoring and how it is stored in a SAS dataset. The advantage of grouping the observations by sampling points rather than by parameters is that in real-time when the data are being collected, vectors of observations can be added to the matrix at each sampling point. All further uses of the $\mathbf{Y}$ data will be referring to the 'unfolded' $\mathbf{Y}$ matrix.

This operation of 'unfolding' the $\mathbf{Y}$ matrix becomes very simple in the RTPM Pro system. As can be seen from Figure 2 the user selects which runs are to be used as training runs to build the model, which runs are to be used as test runs to cross-validate the model and which runs should be omitted. Likewise $\mathbf{X}$, $\mathbf{Y}$ and $\mathbf{Z}$ variables can either be selected or omitted. After the user has chosen the runs and variables to be used in model building the software automatically takes care of creating and storing the 'unfolded' $\mathbf{Y}$ matrix

Data Standardization

Data standardization entails centering and scaling the data in the $\mathbf{Y}$ matrix. It removes the non-linear characteristics of the parameters and also ensures high magnitude variables do not drown out variables that are measured in smaller units.

Depending on the kind of data that is available for model building, different estimates of the mean and
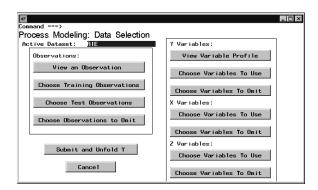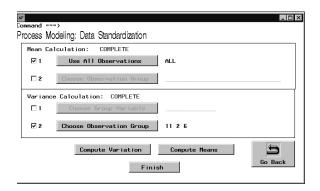
Figure 2: RTPM Pro Data Selection screen

Figure 3: RTPM Pro Data Standardization screen

Figure 4: RTPM Pro Dimension Reduction Screen

variance can be used. Figure 3 shows that the mean can be computed by using all the training runs or a group of runs can be chosen from which to compute variable means. Likewise with the estimate of variance except that a group variable can also be chosen. Figure 3 shows how the RIE data was standardized. Since the data came from a central composite design (11 data points) all the data was used to compute the means. However in computing the variance the only pure replication exists at the three center points of the design (runs 2, 6 and 11) and therefore these points were used to compute the variances. In this case other methods could be used to obtain the mean and variance estimates. RTPM Pro allows a user to try different methods and compare.

Dimension Reduction

The overwhelming dimension of parameter profile data in $\mathbf{Y}$ requires the use of dimension reduction tools. Remember that the $\mathbf{Y}$ matrix dimensions are N by JK, where J is the number of parameters and K is the number of sampling points in the batch process. For example, in the RIE process there are
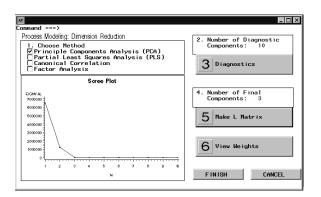
eleven parameters, each measured 588 times during the batch process. This yields a $\mathbf{Y}$ matrix with 6468 columns. The high correlation among these measurements due to their real-time nature implies that each element does not represent a unique piece of information. Rather, much of the information in a set of historical runs can be reduced to a few underlying dimensions or *summary scores*. As Nomikos and MacGregor (1995a) demonstrated, a useful monitoring method must capitalize on this feature.

The RTPM Pro system permits the analyst to investigate many different methods of data reduction. For example, principal components, partial least squares, factor analysis and canonical correlation are all candidates for forming summary scores depending on the types of batch process data available. There does not appear to be a single optimal method for each situation, so the RTPM Pro system provides an analyst with a simple interface which permits comparison of different methods of dimension reduction.

The interface includes a window which displays a diagnostic plot for the chosen dimension reduction method. Figure 4 shows that if principle components is used then the diagnostic plot is a scree plot which is used to select the final number of components to use. Likewise for each dimension reduction method RTPM Pro has a corresponding diagnostic plot.

Summary Score Modeling

To perform SPC, expected summary scores must first be established. Nomikos and MacGregor (1994, 1995a, 1995b) use historical parameter data to establish empirical models for parameter profiles and summary scores. Grimshaw, Shellman and Hurwitz (1996) take it a step further and use the recipe data ($\mathbf{X}$) to construct expected parameter profiles and
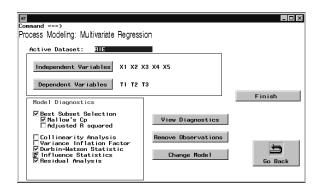
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Figure 5: RTPM Pro Summary Score Modeling Screen

Figure 6: RTPM Pro With-in Run Statistics Screen

summary scores. Using multivariate regression a relationship is established between the recipe data ($\mathbf{X}$) and the process parameters ($\mathbf{Y}$). The rationale being that recipe data will have an effect on the behavior of process parameters. This multivariate relationship can then be used to determine expected parameter profiles for different recipe data.

Using the RTPM Pro system multivariate regression becomes an easy step. An illustration of how simple and powerful SAS/AF and SAS/SCL are can be seen in the diagnostic *check boxes* of Figure 5. Each of these check boxes represents a diagnostic available in PROC REG and is represented as a SAS/SCL variable for that window. If the box is checked then the option is include in the submitted SAS code. If the box is not checked then that particular option is not included in the submitted SAS code.

Process Monitoring

The main function of RTPM Pro is as an off-line model building tool to support an on-line monitoring system. However process monitoring capabilities have been included as a means of model comparison. In addition RTPM Pro can be used as an off-line monitoring system.

Once the data has been entered into the system the off-line process monitoring is a fairly simple task using the RTPM Pro system. While the computations are not simple the system does all the messy work in the background and then presents descriptive statistics in a simple graphical manner. The system first uses the $\mathbf{X}$ data to compute the expected summary scores for the given run. This translates into an expected parameter profile for each real-time variable. Next the summary score are computed from the actual real-time data. Using
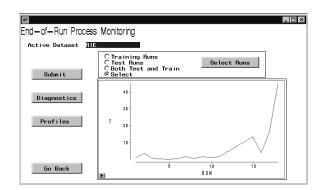
the expected summary scores and the observed summary scores two statistics, a Hotelling T^2 and a Q statistic, are computed for each run. Each statistic is believed to have unique strengths and weaknesses. These statistics are plotted in SAS/GRAPH® and imported directly into the RTPM Pro system as is shown in Figure 6. Notice that with the RTPM Pro system, statistics can be produced for different groups of runs by selecting a given *radio box*. The window contains a graph of the Hotelling T^2 statistics for the 11 training runs and a few test runs. From this chart a quick conclusion can be made that run 18 is out-of-control.

Once an out-of-control run is identified, diagnostics trace the out-of-control signal back to a variable or group of variables that caused the problem. This diagnostic check is done with a Pareto chart where a bar graph shows the contribution of each variable to the out of control signal. In the RIE process for run 18 voltage bias from wafer to ground was identified as the highest contributor to the out-of-control signal.

From there, the profile plot (similar to a time series plot) of the problem variable can be plotted to show the predicted profile versus the actual profile with an appropriate confidence interval. Figure 7 shows that voltage bias from wafer to ground was slightly lower than the expected profile at the given recipe. Different variables from the same run or from different runs can also be inspected by clicking on the *icon* buttons and selecting them from a pop-up screen list.

While these plots do not explicitly show the cause of an out-of-control event, they do show how the real-time variables were affected by it. This information could then be used by an operator or engineer to gain more knowledge of how a process is affected by different situations, possibly allowing preventative measures to be identified.
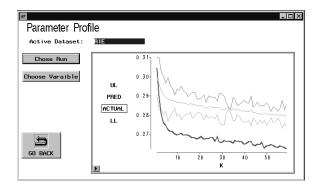
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Figure 7: RTPM Pro Parameter Profile Screen

Conclusions

Real-time process monitoring is a very valuable tool for monitoring batch processes. One of the most important steps in any monitoring system is working with a good model of the process. Having the right tool to explore and compare different models for the same process enhances a researchers ability to find a 'best' model.

The development of the RTPM Pro system in SAS/AF and SAS/SCL has greatly added the ability to explore model building for real-time process monitoring. Five specific advantages are: First, the time that it takes to analyze a data set has gone from a day and a half using SAS macros to a couple of hours. Second additional models for a given data set are very easy to create allowing model comparison. Third, the graphical menu-driven interface is a friendly environment to work in. The user does not need to memorize process variables or run numbers as these are provided in pop-up list menus. Fourth, RTPM Pro has the ability to analyze real-time process data off-line. This gives operators and engineers a tool to help them better understand a process. Finally, modification to the RTPM Pro system can easily be made using SAS/AF and SAS/SCL which allows for new methods to be integrated into the system.

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