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A METHOD FOR LOCATION CONTROL OF A MULTIVARIATE GAUSSIAN PROCESS

by

Shih-Jen Li

A Dissertation Submitted in Partial Fulfillment of the Requirements for the Degree of

Doctor of Philosophy

in

Engineering

at

The University of Wisconsin-Milwaukee

May 1998

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Graduate School Approval

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The University of Wisconsin-Milwaukee, 1998 Under the Supervision of Professor Tsong-how Chang

ABSTRACT

The Shewhart control charts, developed by Walter A. Shewhart in the 1920's are for the detection of process changes in a univariate process. When a process is monitored by two or more quality characteristics, the use of Shewhart control charts can incorrectly identify a process in or out of control. Thus, it is essential to have some control charts that are capable of controlling several quality characteristics simultaneously. In 1947, Hotelling introduced the T^2 -statistic to monitor a process with two correlated variables for bombsight tests. Ever since, a great number of methods have been developed either as a supplement to T^2 chart to extract more detailed information contained in the sample T^2 , or for the design of entirely different schemes for multivariate control. These methods, however, are not widely used because they are not sufficiently informative to be useful in practice.

In this research, a new method for multivariate process control, called major element control charts, is developed to detect any possible changes and identify their nature of change in each of the process means under assumed stability in the associated variances and covariances. The major element control charts for a p-variate process are consisted of p individual control charts one for each of the p major elements. Each major element is a statistical function of an element on the major diagonal of an inverted $p \times p$ sample variance-covariance matrix, and follows a χ^2 distribution. The control limits for the major elements can be easily calculated using the χ^2 distribution at a selected significant level. The construction and performance of the major element control charts are discussed and evaluated with simulated trivariate normal process data. Demonstrated by simulation data of various processes, the control charts for major elements are not only effective, but also informative for the control of multivariate Gaussian process means. A step-by-step procedure for actual application is recommended for the set-up and interpretation of the major element control charts. Issues related to sampling strategy, chart interpretation, and the stability of process variances and covariances are also discussed with some suggestions.

Song how (Rem

Professor Tsong-How Chang

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ACKNOWLEDGEMENTS

I would like to express my deepest and sincerest gratitude to my academic advisor, Dr. Tsong-how Chang, whose insight and comprehensive knowledge in Quality Engineering led me to the statistical applications for process control. His invaluable encouragement and tremendous patience allowed me to grow and learn gradually, and complete the research work without giving up on myself. I thank him for his cooperation and excellent guidance to finish my dissertation.

My special thanks go to Dr. Niranjani H. Patel, without her immense support, valuable discussion and review of my thesis; this research work would not even be close to finish. Her positive thinking and spiritual moral support took me through many sleepless nights and overcome the most difficult part of this research. A thank you to Dr. Timothy Haas for his kindness to serve as my minor professor and suggestion to study the Bootstrap method; Dr. Hamid K. Seifoddini and Dr. Darrell Radson, who offered their encouragement during the research.

A debt of gratitude goes to my parents, Pei-Yui Li and Yen-Hua Yen, for their unconditional support and endless encouragement through all my life. Specifically in the past seven years, they were suppose to enjoy their life after retirement, however, they still worked to support me financially and morally because of their belief in me. Without their faith and love, I can not come this far. My thanks also go to my brother who is now studying in Germany for his understanding that I was unreachable for so many years. Finally, a thank you to my dear friends, Su-Huey Jou and Barry Yang, and their little girl, Sofie, for all the meal they provided to me during the very last few months and offering me a place to go to when I felt down. I also thank Ms. Betty Warras and Dana Root for putting their time in editing my writing.

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Chapter 1

INTRODUCTION

One half century ago, Harold Hotelling (1947) introduced the use of a T^2 statistic for multivariate process control. Although statistically efficient and effective, the T^2 control chart has not been widely used in practice. One major drawback of a T^2 chart is its inability to reveal the specific nature of the underlying process changes whenever the chart shows out of control. Information regarding any specific causes is extremely valuable to the process engineer in his/her investigation and diagnostic analysis for corrective actions. Such was recognized early on by many statisticians.

Since the mid-sixties, a great number of methods have been developed either as a supplementary analysis to extract more detailed information contained in the sample T^2 , or for the design of entirely different schemes for multivariate control. These research efforts of the last three decades, however, have not significantly advanced the multivariate control technology to the point that would satisfy the engineers to actually apply it in their work. Recently, the rapid growth of data-acquisition technology and the use of online computer for process monitoring have rekindled the interest in multivariate process control. The new interest, however, demands a method that is not

only effective in detecting out-of-controls, but also informative and easily understandable for routine applications in multivariate manufacturing process control.

1.1 Motivation for Research

Unlike in univariate controls by, for example, Shewhart \overline{X} and R charts where any out-of-control signal itself also indicates the direction of change in the process parameter being monitored, the T^2 for multivariate control is a statistic that summarizes all the sample variation from each of the variables in the group. Whether an out-ofcontrol may have been caused by changes in one or more of the variables with shifts in the means, the variances, and/or covariances, they all tend to increase the sample T^2 values to exceed a control limit. This makes T^2 statistic highly efficient in signaling outof-controls, but utterly helpless in the attempt to diagnose the nature of the possible assignable causes.

The methods that have been developed in recent years either as a supplement to a T^2 chart or as a separate multivariate analysis of the data after an out-of-control signal is identified are all designed to learn more about why a sample T^2 goes out of control. These include the use of principal components, decomposition of T^2 , and additional univariate control charts. There are also some new control charts that chart cumulative residuals from regression, sample principal components and other statistics, without T^2 . Nevertheless, there remains a definite need of a multivariate process control procedure

that is efficient, effective and informative. More specifically, Hubbele (1989) states that a multivariate control procedure should possess the following capabilities:

- 1. Correct (and rapid) detection of an out-of-control state.
- 2. Identification of the variables, among the correlated variables, that caused the problem.
- 3. Determination of the magnitude and direction of the adjustments required to bring the process back to control.

1.2 Research Objectives

This research is aimed at developing a method of charting time-ordered, independent samples of data for the control of a multivariate Gaussian process with the capability listed above. Specifically, the primary objective is to develop a multivariate control scheme for the detection and identification of possible changes in each of the process means, under assumed stability in the associated variance and covariances.

1.3 Research Results

The proposed method consists of a set of p control charts, called major element control charts, one for each of the p correlated normal random variables. The p major elements are statistical functions of the elements on the major diagonal of an inverted sample covariance matrix of size $p \times p$. Since each sample major element follows a χ^2 distribution, control limits can be easily calculated at a given significance level. Each of the p control charts is reviewed for signals of out-of-control whenever a sample becomes available. Jointly, all observable out-of-control signals from the p chart are analyzed to determine the specific nature of the shifts in process means. By computer simulation of a trivariate normal process, these major element control charts appear to be very effective and informative as originally expected. When compared against several recently developed multivariate control charts, again by simulated trivariate process data, the proposed major element charts show improvements in their uniqueness and sensitivity of out-of-control signals. Finally, the major element control charts are not only capable of displaying signals of each out-of-control variable, but also its direction of shift in the mean.

1.4 An Outline

Chapter 2 presents a review of important and relevant literature in the development of multivariate control charts over the past 50 years. It is noted that most of the developments are in the control of means with an assumed or implied constant variance-covariance structure in control.

The underlying methodology of the proposed control charts for statistical control of the means of a multivariate Gaussian process is presented in Chapter 3. The methodology is primarily based on the unconditional decomposition of the quadratic form, Q, of a multivariate normal distribution. Each of the first p sample major elements is expected to have a bias when its corresponding process mean is being shifted.

The proposed methodology is evaluated in Chapter 4 by using the simulated process sample data. The structures of data simulation are designed to examine the robustness of the proposed control charts when they are applied to monitor the processes of all kinds. Additionally, a step-by-step construction procedure of the major element control charts is also presented in this chapter.

Chapter 5 presents a comparative study among several well-known multivariate process control techniques and the newly developed major element control chart. It reveals the strength and weakness of each technique based on its ability in displaying the distributional out-of-control patterns.

A five-phase application procedure for the major element control charts is outlined in Chapter 6. The five phases include: define the process, collect the data, analyze the data, interpret and identify out-of-control signals, and formulate, and implement follow up actions. Chapter 7 is a summary of the methodology, and a discussion of areas for the future research.

Chapter 2

LITERATURE REVIEW

Multivariate process control techniques have been around, ever since Hotelling applied multivariate control analysis on bombsight data in 1947. The multivariate control chart was not used widely like Shewhart Control Chart until recently because of the unavailability of fast computing technology and the complexity of implementing procedure. During past ten to fifteen years, many statisticians and quality engineers put their efforts either to develop new multivariate process control techniques, or to improve current available techniques. The objectives of these research efforts primarily were to provide more information about the out-of-control states in a process that can assist engineers to easily identify the assignable causes and to formulate correct actions more efficiently. Much of this is the result of the growth of advanced information technology, and the understanding of the relationship among quality characteristics of the process.

A literature review of the development of control charts for a multivariate Gaussian process is given focusing on their applications and performance in a manufacturing environment. In Section 2.1, the control charts designed to monitor multivariate process means are discussed. In most cases, the multivariate control charts for the process means are constructed under the assumption that the process stability in associated process variances and covariances is in-control. Several currently available multivariate control procedures for checking process variability are reviewed in Section 2.2. In the last section, several important issues of the development of multivariate process control charts are discussed.

2.1 Control Charts for Multivariate Mean

Research efforts in the development of the process control for multivariate means are directed in three main streams. The first stream makes its efforts of improving the performance of T^2 control charts by improving the sensitivity of control limits and obtaining better estimations of the process parameters. The second stream acts on designing the supplementary charts to enhance the interpretation of out-of-control signals that are detected by T^2 control chart. The last stream of the research efforts intend to develop multivariate statistical process control charts that are able to provide diagnostic information about the change in the process means without depending on T^2 control chart to signal the out-of-control states. In this section, the fundamentals of traditional T^2 control chart will be reviewed first. Then, each of the three main streams is discussed.

2.1.1 T² Control Chart (Hotelling, 1947)

The T^2 statistics derived by Hotelling at 1947, which is used for the overall control of the process, is a generalization of the t-test, and for single observation, this takes the form:

$$T^{2} = (\mathbf{X} - \mu_{0})^{T} \mathbf{S}^{-1} (\mathbf{X} - \mu_{0}), \qquad (2.1)$$

where X is a column vector, and Σ and μ_0 are the process variance-covariance matrix and process means, respectively. Derived by Hotelling, T^2 is a statistic related to F distribution with adjustment factor involving the number of samples (k) and number of variables (p) as $T_{p,k,\alpha}^2 = \frac{kp}{k-p+1}F_{p,k-p+1,\alpha}$, which is used to set up the upper control limit for T^2 at the significant level of 1000%. If the number of samples is large enough, T^2 may be approximated by the χ^2 distribution with p degrees of freedom.

Although T^2 control charts are statistically efficient and simple, they are not very informative for diagnostic analysis of out-of-control signals as to the nature of their assignable causes. The T^2 control chart also suffers three major drawbacks. It loses its optimality property against more specific shifts in mean, it confounds location shifts with scale shifts, and its signals are not associated with any particular shift or variable but must be diagnosed after the fact (Hawkins, 1991). In addition, Matrangelo, Runger, and Montgomery (1996) have also pointed out that Hotelling T^2 is based entirely on the most recent observations and consequently the procedure signals only when a relatively large shift in the mean vector occurs.

2.1.2 Improving T^2 Chart

Alt (1984) introduced two-phase procedure to apply T^2 statistics in controlling the multivariate process means. Phase I consists of using the charts for retrospectively testing if the process is in control. Control charts in Phase II are used to monitor the future process. To improve the capability of analyzing the data in Phase I for determining the status of a process, Wierda (1994) and Sullivan et al (1996) both evaluate the methods that are commonly used to estimate the process variance-covariance matrix.

When only one observation of each sample is collected in Phase I, all the observations are pooled to estimate the mean vectors and covariance matrix. Sullivan and Woodall (1996) have found that T^2 control procedure is not effective in detecting a shift in the mean vector because the covariance matrix is badly estimated. To improve the estimate of the process variance-covariance matrix for multivariate individual observations, Sullivan et al. (1996) suggest using concept of moving range method in the univariate case. The procedure uses the vector difference between successive observations to estimate the in-control covariance matrix for the process.

For a process with multiple observations of each sample, average of sample variance-covariance matrices is used to estimate the process variance-covariance matrix. This estimator is a reflection of the 'within sample dispersion'. It can not be affected by special causes of variation, which is an appropriate application for detecting the shifts in the mean vectors. To apply this method, the relationship among sample size (n), number of samples, and the number of variable has to satisfy $k(n-1) \ge p$. (Wierda, 1994)

Lowery et al. (1995) summarized a procedure to establish the most efficient control limits for T^2 control chart at Phases II, which assumed that trial control limits of Phase I for use in online statistical process control, has been established. The upper control limits should be calculated exactly as a function of F distribution. Using individual observation at Phase II, Σ and μ_0 are usually estimated by the pooled sample variance-covariance matrix, S, and average of all observation vectors, $\overline{\mathbf{X}}$. The T^2 statistics used instead of Eq. 2.1 is $T^2 = (\mathbf{X} - \overline{\mathbf{X}})^T \mathbf{S}^{-1} (\mathbf{X} - \overline{\mathbf{X}})$ with the exact upper control limits as $\frac{p(k+1)(k-1)}{k(k-p)}F_{\alpha,p,k-p}$ that were defined by Ryan (1989). However, Jackson (1985) suggests that for large k ($k \ge 100$) the LICL of $\frac{p(k-1)}{k(k-1)}F_{\alpha,p,k-p}$ would be a fair

(1985) suggests that for large k (k>100), the UCL of $\frac{p(k-1)}{(k-p)}F_{\alpha,p,k-p}$ would be a fair approximation.

For charts constructed using sample size, n > 1, the average of sample variancecovariance (\overline{S}) and average of sample mean vector (\overline{X}) are used to estimate Σ and μ respectively. The Hotelling T^2 statistics in Phase II is defined as $n(\overline{X} - \overline{X})^T \overline{S}^{-1}(\overline{X} - \overline{X})$, and the upper control limit is defined as $UCL = \frac{p(k+1)(k-1)}{kn-k-p+1}F_{\alpha,p,kn-k-p+1}$. Number of samples (k) and the sample size (n) play an important role in the procedure of estimating the control limits. For detail discussion, Tracy et al. (1992) had discussed how the number of samples affects the determination of control limits for the individual observation case. In addition, Lowry et al (1995) had shown in their evaluations of the effects of the number of samples when interacted with two different levels of sample size and six levels of number of variables.

2.1.3 Supplementary Control Chart for T^2 Control Chart

One of the major drawbacks of the T^2 control chart procedure is that it does not directly provide the diagnostic information of the out-of-control signals such as which variable causes the problems, and how the variable has been changed. In order to address appropriately these drawbacks of T^2 control chart, a number of methods have been proposed in the past twenty years. The similarity of these procedures is that the first step of them requires checking the out-of-control signals or evaluating the overall performance of T^2 control chart. Then, each of these methods will be applied to interpret the status of the process according to the signals given by T^2 statistics.

One of these procedures, named Multivariate Profile (MP) charts, is proposed by Fuch and Benjamoni (1994). Its concept is relatively simple. MP chart plots a set of bar chart along with T^2 statistics. The bar charts consist of a horizontal base line that is plotted at the value of T^2 and p bars for a p-variate process. The size of each bar is determined by the difference between sample mean and the process mean, and the standard deviation of each variable. To interpret the MP chart, first find the highest T^2 value, and then paint each bar with different color. The gray color is the variable that exceeds two standard deviations, and the black bar indicates this variable exceeds three standard deviations.

Kourti and McGregor (1996) provides a set of plots based on Principal Component Analysis to detect the variables' contribution to the out-of-control signal

which was identified from the T^2 control chart. There are three steps to establish the charts.

- 1. Detect the out-of-control signal from a sample observation vector, X, whose T^2 value is above the control limit.
- 2. Check normalized scores of the sample observation, X, based upon Principal Components Analysis, find scores with highest values. (Bonferroni limits could be used on the score chart as rough guides.)
- 3. Calculate the variable contributions for these high scores; investigate the variables with high contribution.

Based on the total contribution of the variables, one can point out a variable or a group of variables that caused the out-of-control signal in T^2 control charts. These variables need to be investigated to assign the causes.

Many researchers have suggested using decomposition techniques for identifying the particular subset of quality characteristics that cause an out-of-control signal. These procedures basically decompose the T^2 statistics into independent parts, each of which is based on a subset of the p quality characteristics with similar properties. The decomposed parts are known as T^2 variates that are used to determine which variables are causing out-of-control states.

This approach first is brought up by Murphy (1987) to partition the p quality characteristics into two subsets. One of the two subsets must be the subset that is

intuitively suspected to be directly related to the cause of the out-of-control signal. There are a couple of disadvantages for this method. First, the number of possible selections of each subset is large for the process with large number of variables, and the second, choice of the subset depends on user's intuition, which introduces the risk of misidentifying the true assignable causes.

Mason, Tracy, and Yong (1995, 1997) decompose T^2 of a *p*-variate process into *p* independent components, each of which provides information on the variables that significantly contribute to an out-of-control signal. Wierda (1994) suggests a step-down procedure that is based on the priori knowledge of the ordering among subsets of the variables. According to the ordering, the procedure partitions the mean vector into *q* sub-vectors and correspondingly *q* sub-hypotheses to test that one of the sub-vectors of the mean does not shift. For each of the *q* sub-hypotheses, a control chart is plotted. It is not necessary to examine all variables while applying this approach. However, it is very difficult to select an appropriate order of all the variables.

Timm (1996) proposed an alternative step-down method to use finite intersection tests (FIT). Both Wierda's step-down procedure and the FIT procedure are based on conditional distributions to make a choice of ordering the original variables. Timm (1996) states that the FIT method is uniformly and more powerful than the step-down procedure.

2.1.4 Multivariate Control Charts Based on Data Transformation Techniques

Several important data transformation techniques have been used to develop new multivariate control charts for detecting the mean shifts. The principal component analysis and regression-adjustment of process variables are two major techniques that have been proposed in the literature and they do not rely on T^2 statistic to signal the out-of-control states. In this section, both the principal component (PC) analysis and regression-adjustment techniques are discussed in a great length.

2.1.4.1 Principal Component Charts

Jackson (1985) proposed and demonstrated the details of the transformation of the original variables into Principal Components (PC) and monitoring these new orthogonal variables with the original variable simultaneously on control charts. The applications of Jackson's proposal had the following potential problems. The control charts of the transformed variables are a set of univariate control charts; each principal component is a combination of each of the original variables. While the out-of-control signals are identified from the sample data of principal components, it is difficult to interpret which original variables cause the signals. Unless the application can either establish a set of pattern to identify the shifts in process means, or set up another set of charts to help identify the contribution of each original variable such as Jackson's original proposal or the normalized score plots proposed by Kourti (1996). Otherwise, the principal components analysis on multivariate process control is difficult to apply. Chang (1991) have found a unique pattern for monitoring a bivariate process by plotting the Principal Components (PC) of the original sample data. Design of this procedure seems to have an advantage over T^2 control chart. The patterns of principal components based on the process mean shifts are summarized from the simulated data provide the information on the sources of assignable causes (Chang, 1991). The distribution pattern for the bivariate process control is as shown in Figure 2.1.



Figure 2. 1 Distribution Patterns of Out-Of-Control Signals for Bivaraite Control (Reproduced from Chang's 1991 paper)

In Chang's (1991) study, it is also found to extract a unique pattern for multivariate process control chart by using Principal Components becomes too complicate as the number of variables gets large. Although the sample principal components that are calculated from a simulated trivariate process sample data do show a distributional pattern, which the patterns do not agree with twenty-six out-of-control states based on simulated shift combination directly.

2.1.4.2 Regression Adjustment of Variables

Hawkins (1991, 1993) has suggested that regression adjustment of variables may be an effective alternative to classical multivariate control chart. Hawkins combined regression control chart (Mandel, 1969), with a result due to Healy (1987) and proposed to regress the variable X_l on a subset of (p-1) variables X_m such that $l \neq m$, depending on the natural order of the process. Let H_l be the l^{th} variable of **H**, where

$$\mathbf{H} = \operatorname{diag}[\operatorname{diag}(\Sigma^{-1})]^{-1/2} \Sigma^{-1} (\mathbf{X} - \mu_0). \qquad (2.2)$$

 H_l is the regression residual when variable l is regressed on all other variables, standardized by unit variance. This can be used to test the null hypothesis that the l^{h} component of the mean vector did not shift. To chart the H value of each variable, Hawkins (1991) proposed to make a univariate CuSum chart. For a *p*-variate process, *p* CuSum charts are plotted.

In order to evaluate the performance of the regression-adjusted sample data, Hawkins plots the simulated H_i on both the CuSum chart and traditional $\overline{X} - R$ chart. The results turn out to be that both charts can detect the simulated change. Obviously, it is possible to use a classical control chart for the H_i instead of a CuSum control chart. It also can be concluded that Hawkins's method performed well if the shifts occurred in a single component, or in a pair of lower correlated components. (Wierda, 1994) Besides, Hawkins does not show how sensitive the method would be if change in the standard deviation and shift in mean both occurred in the same variable.

2.1.5 Multivariate Techniques for Detecting Small Shifts

Because the design of T^2 control chart is based on the most recent observations, it becomes relatively insensitive to small and moderate shifts in mean vector. Several researches extend the concepts that are used in the univariate case such as the CuSum Control chart and Exponentially Weighted Moving Average (EWMA) procedure to improve the traditional T^2 control charts to detect the small shifts. The advantages of these procedures are that they not only use the most recent observations, but also use the observations collected in the past.

Two major multivariate CuSum control charts are developed based on the sequential probability ratio test (SPRT) by Healy (1987) and Alwan (1986). Essentially both methods are the extension of the univariate CuSum approach, however, Alwan's procedure is not based on the sequence of original variable, but rather on a sequence of transformed T^2 variables.

Lowry et al. (1992) proposed Multivariate Exponentially Weighted Moving Average (MEWMA) control chart which is a natural extension of univariate EWMA control procedure. Both multivariate CuSum and MEWMA methods have been shown that they are relatively sensitive to the small shift in the multivariate process means, however, they still cannot provide the information regarding the nature of the change. In addition, a design procedure for those control chart and guidance for chosen parameters are also needed for practical applications.

2.2 Control Charts for Multivariate Process Variability

As discussed earlier, it is not sufficient to monitor only the means of the quality characteristics associated with the product, but measures of the process variability should be controlled as well. In the univariate case, the sample range is often used as a measure of process dispersion, thus the R-chart is the established control chart to monitor dispersion of the process. The variability of a multivariate process is summarized by the variance-covariance matrix, Σ_{pxp} . An analogous procedure would be very much helpful to monitor the dispersion of a multivariate normal process. However, often problems are encountered within the industrial realm where it is essential to examine possible change in the relationship among related variables.

In many instances, the change in process variances and covariances went undetected while the correlation between two variables changed. Although checking the process variability is such a critical issues for the multivariate process control, unfortunately, only very limited research efforts have been devoted on developing the multivariate control charts for controlling process dispersion. In this section, most of the available control charts for multivariate process variability will be discussed.

2.2.1 Control Charts for S

In extension of the idea of range control chart, Alt (1985) proposes two control charts to monitor process variability. The first control chart is a direct extension of the univariate S^2 control chart. The procedure is based on the repeated tests of significance
of the hypothesis that the sample variance-covariance matrix, S, is equal to a specific population variance-covariance matrix, Σ . To apply this approach, the following statistic for the i^{th} sample is plotted on the control chart

$$W_{i} = -pn + pn\ln(n) - n\ln\left(\frac{|A_{i}|}{|\Sigma|}\right) + tr(\Sigma^{-1}A_{i}), \qquad (2.3)$$

where $A_i = (n-1)S_i$, S_i is the sample variance-covariance matrix for sample *i*, *i*= 1, 2,...,n, and *tr* is the trace operator. If the value of W_i plots above the upper control limit UCL = $\chi^2_{\alpha,\rho(\rho+1)/2}$, the process is identified as out of control. The second control chart is constructed to monitor the sample generalized variance-covariance, using the determinant of S, |S|. The method treats the determinant of sample variance-covariance, |S|, as a variable, and use the mean and variance of |S| to construct the control limits. Let E(|S|) and V(|S|) be the mean and variance of |S|.

Use the property that the probability distribution of most |S| is contained within the interval of $E(S) \pm 3\sqrt{V(|S|)}$ to construct the control limits of |S|. In addition, if the variance-covariance matrix is estimated by sample variance-covariance matrix, $|\Sigma|$ should be replaced by $|S|/b_1$ which is an unbiased estimator of $|\Sigma|$ and b_1 is a constant determined by sample size and number of variables. Furthermore, as part of this procedure, Montgomery (1991) suggest that it will be a good idea to use univariate control charts for variability in conjunction with the control charts for |S|. Chang (1991) proposed to use $\log|S|$ in stead of |S|, since it had been shown theoretically that the statistic of |S| has more normality in its logarithm. To construct control chart of $\log|S|$, first, calculate the determinant of each sample variance-covariance matrix for the in-control process. Then, find mean and variance of $\log|S|$. A control chart with $100(1-\alpha)$ % probability limits is constructed as $\overline{\log|S|} \pm Z_{\alpha/2}(\sqrt{\operatorname{var}(\log|S|)})$, where $\overline{\log|S|}$ is the mean of $\log|S|$, and $Z_{\alpha/2}$ is $\alpha/2$ percentage point of the standard normal density.

In addition, Bonferroni confidence intervals are proposed to graphically interpret and identify the nature of out-of-control conditions that do occur on the $\log|S|$ control chart. A common problem with control charts developed using |S| or $\log|S|$ is that different matrices can have the same determinants. For example, consider the three 3×3 variance covariance matrices:

$$S_{1} = \begin{bmatrix} 2.56 & 1.536 & 1.080 \\ 1.536 & 1.44 & 1.613 \\ 1.080 & 1.613 & 0.81 \end{bmatrix}, S_{2} = \begin{bmatrix} 5.76 & 0.921 & 2.70 \\ 0.921 & 0.23 & 0.604 \\ 2.70 & 0.604 & 2.25 \end{bmatrix}, S_{3} = \begin{bmatrix} 1.44 & 1.843 & 0.675 \\ 1.843 & 3.686 & 1.210 \\ 0.675 & 1.210 & 0.563 \end{bmatrix}$$

Now, $|S_1| = |S_2| = |S_3| = 0.298$, yet these three matrices convey considerably different information about the process correlation among three variables and process variability among the samples. Therefore, Alt and Smith (1988), and Montgomery (1991) suggested that the appropriate univariate procedures to monitor the individual variances are necessary while the control charts based on |S| are applied. Chang (1991)

proposed a new chart, namely Z^{**} , to monitor the change of process's correlation coefficient along with the control chart of $\log |S|$ for controlling process variability. Here Z^{**} is a measure based on the Hotelling's investigation of Fisher's transformation of correlation coefficient between two variables.

2.2.2 Generalized T^2 Statistics

Another line of approach is due to Hotelling (1947) called Generalized T^2 statistic. Jackson (1985, 1991) proposed to use three statistics available from Hotelling T^2 to monitor the process means, variances and covariances simultaneously. Three statistics are: T_o^2 , a measure of overall variability, T_M^2 , a measure of the distance between the mean of sample observations and the target mean, and T_D^2 , a generalized measure of the dispersion of the sample around its own mean. Among them, T_D^2 of each sample is a measure for controlling the dispersion of the process. The relationship among these three statistics can be written as in Eq. 2.4.

$$T_O^2 = T_M^2 + T_D^2$$
(2.4)

Based on Jackson (1985), it suggests that T_M^2 and T_D^2 for multivariate process can be used as average and range chart for the univariate case for statistical process control. There are cases where, because of cost, time, the nature of the test or whatever, it is not practical or possible to use averages for short-range process control. This is true whether the control procedure is univariate or multivariate. However, in the multivariate case, the three T^2 statistics may be useful as summary statistics to evaluate the process performance. It is relatively difficult to apply them as a chart to monitor the process variability.

There have two main concerns of the proposed control chart reviewed in this section. First, the statistics and/ or the control limits depend on the estimates of process variance-covariance, however in general, the process variances and covariances are unknown. Second, the control scheme for process variability only signaled the out-of-control state without further information to present the nature of change in the process variances and covariances.

Because of the similar concerns discussed above, Wierda (1994) presents and evaluates four methods to test the hypothesis that an unknown process variancecovariance matrix is constant in-control. The four methods include Likelihood Ratio Test (LRT) statistics, the Nagao's test statistic, Quotient of the generalized variance, and univariate test statistic. Furthermore, he also proposes a hierarchical procedure with LRT testing that could signal the change in the variance-covariance matrix. The complexity of Wierda's procedure might improve its performance if user understood underlying statistics. It is still very far from the possibility of practical application even though the high-speed computers are available. Indeed, the other methods mentioned in this section are relatively simple and have easily understandable statistics.

2.3 Some Issues on Multivariate Process Monitoring

• Data transformation or standardization tend to lose potential important information in the original data.

A lot of information will be lost or altered when the data transformation and standardization are applied. We usually do not know what has been missed, and no one really pay much attention to it. It is necessary to make sure the techniques can preserve the information as much as possible. Moreover, we should make sure at least that the information is not modified.

• Certain process data are inherently autocorrelated in time or in space, many, however, are time independent

If process data are dependent on time, the data should be treated with time concern. It is not easy to assure that a given process is always dependent on time. Because any data collected from process, all of them can be fitted with time series model. Then, one will try to use control chart with autocorrelation concern, which might be totally misleading. When the data is modeled by time series, it is assumed that the residuals are independent which might model the error into it. Because of the concerns, many researchers focus on the process, which has timed autocorrelation concern that only applied to process industry. (Montgomery et al., 1993).

• Most multivariate control charts for the process means heavily rely on two assumptions. First, the sample data are always well behaved following a multivariate

normal distribution. The second one assumes that the process variance-covariance matrices of the samples are well maintained as a constant that can be estimated by the sample data.

Most multivariate control scheme developed without even considering the evaluation of the stability of a process. They assume that the multivariate process is stable and in-control. However, to improve the current multivariate techniques for process mean, one thing for sure needs to be emphasized on is to develop a effective, efficient, and easy to apply multivariate control chart for checking the stability of a process.

• Many techniques are developed to interpret the out-of-control signal that was identified from T^2 control chart. What if T^2 misidentify the signal or it just simply is not able to show the process mean has been shifted?

In a recent assessment of multivariate control charts, Mason et al. (1997) had concluded that two aspects must be considered of evaluating the out-of-control signals from T^2 control chart. First, the overall significance level of the simultaneous use of *p*univariate control chart must be calculated and is known to difficult to determine it. Second, not necessary only one quality characteristic causes the out-of-control situation at one time. Therefore, many other techniques are more efficient and effective than the application of T^2 control chart.

Chapter 3

METHODOLOGY

This chapter presents the underlying methodology of the proposed control charts for statistical control of the means of a multivariate Gaussian process. It is assumed that the process variances and covariances are not subject to change or in statistical control. The methodology itself is quite straight forward in that it is a decomposition of the familiar quadratic form of a multivariate normal distribution, $Q = (\mathbf{X} - \mu)\Sigma^{-1}(\mathbf{X} - \mu)$, or the classical Hotelling's T^2 . Unlike many of the earlier work with the T^2 as discussed in Chapter 2, this research proposes the use of a certain portion of the decomposed elements of the quadratic form including the inverted variance associated with each variable. These are to be called the major elements of Q. Since the Q is also a measure of the distance between two vectors \mathbf{X} and μ , each major element of Q containing $(\mathbf{X}_t - \mu_t)$ expresses the distribution of \mathbf{X}_t centered at μ_t . All the major elements of a pvariate process are independent of each other; therefore, they can be analyzed individually.

When applied for multivariate process control of the means, each such sample major element serves as an indicator of the state of its mean independent of the states of the other means. Together, the p sample major elements are capable of characterizing

simultaneously the states of all the p means of a process. What follows in this chapter is to propose a decomposition of the Q such that it allows for the selection of pindependent major elements, each of which follows a chi-square distribution with one degree of freedom. Based on the χ^2 distributions, control charts of sample major elements, one for each of the p means, may be constructed for multivariate statistical process control. Additionally, a complete set of distributional patterns of various out-ofcontrol signals of a trivariate process will be developed as an aid in chart interpretation.

This chapter is organized as follows. The multivariate normal distribution will be reviewed in section 3.1. Section 3.2 will present the method of decomposition of a Qand define the major and minor elements of a *p*-variate Gaussian process. Section 3.3 describes the estimation of process parameters from sample data and the calculation of sample major elements. Section 3.4 presents the χ^2 distribution for the sample major elements, which provides the basis for the proposed control charts. In Section 3.5, the expected sample distribution patterns of each major element control chart of a trivariate Guassian process is developed with illustrations. It is also shown in this section that all 26 possible combinations of shifts in the three means have unique distributional out-ofcontrol signals to be displayed on the three major element control charts.

3.1 Multivariate Normal Distributions

The multivariate normal density function is a generalization of that of a univariate normal with mean μ and variance σ^2 ,

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}, \quad -\infty < x < \infty$$
(3.1)

The term in the exponent of the univariate normal density function of Eq. 3.1 may be written as

$$\left(\frac{x-\mu}{\sigma}\right)^2 = (x-\mu)(\sigma^2)^{-1}(x-\mu)$$
(3.2)

which measures the squared distance from x to μ in terms of the standard deviation.

For a p-variate normal process, Eq. 3.1 can be generalized to

$$f(\mathbf{X}) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} e^{-\frac{1}{2} \left(\mathbf{X} - \mu\right)^r \Sigma^{-1} \left(\mathbf{X} - \mu\right)}, \quad -\infty < x_l < \infty, \quad l = 1, 2, \dots, p, \quad (3.3)$$

where μ is a $p \times 1$ vector of the mean values of a normal random vector X and Σ^{-1} is the inverse of the variance-covariance matrix of X.

$$\Sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1p} \\ \sigma_{12} & \sigma_{22} & \cdots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1p} & \sigma_{2p} & \cdots & \sigma_{pp} \end{bmatrix}, \text{ and } \Sigma^{-1} = \begin{bmatrix} \sigma^{11} & \sigma^{12} & \cdots & \sigma^{1p} \\ \sigma^{12} & \sigma^{22} & \cdots & \sigma^{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma^{1p} & \sigma^{2p} & \cdots & \sigma^{pp} \end{bmatrix}.$$

The symmetrical covariance matrix Σ is positive definite, so the squared distance from X to μ is given by (Johnson and Wichern, 1992)

$$Q = (\mathbf{X} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{X} - \boldsymbol{\mu}), \qquad (3.4)$$

which is also known as the quadratic form of a multivariate normal.

3.2 Decomposition of A Quadratic Form

Suppose a process is characterized by a $p \times 1$ random vector $\mathbf{X}' = [x_1, x_2, ..., x_p]$ following a *p*-variate normal distribution as defined in Eq. 3.3. The quadratic form, $(\mathbf{X} - \mu)^T \Sigma^{-1} (\mathbf{X} - \mu)$ of Eq. 3.4, can be expressed as

$$Q = \begin{cases} (x_1 - \mu_1)^2 \sigma^{11} + (x_2 - \mu_2)^2 \sigma^{22} + \dots + (x_p - \mu_p)^2 \sigma^{pp} + \\ 2[(x_1 - \mu_1)(x_2 - \mu_2)\sigma^{12} + (x_1 - \mu_1)(x_3 - \mu_3)\sigma^{13} + \dots + (x_{p-1} - \mu_{p-1})(x_p - \mu_p)\sigma^{(p-1),p}] \end{cases},$$

or as

$$Q = \sum_{l=1}^{p} (\mathbf{x}_{l} - \mu_{l})^{2} \sigma^{ll} + 2 \sum_{l=1}^{p-1} \sum_{m=l+1}^{p} (\mathbf{x}_{l} - \mu_{l}) (\mathbf{x}_{m} - \mu_{m}) \sigma^{lm}, \quad l, m = 1, 2, \dots, p; \quad (3.5)$$

which is a linear combination of two types of terms. The first type of terms in Eq. 3.5, $\sum (x_i - \mu_i)^2 \sigma''$, is the sum of functions of squared distances from the means, one for each X_i . The second type of terms involves cross products of the distances between two variables.

For control chart applications, it is important to employ the sample statistics that are sensitive to any changes in the process parameter being monitored. In multivariate process control, it is also desirable that each sample statistic to be charted is capable of clearly reflecting one specific change in only one variable with no influence of changes in other variables. It is seen in Eq. 3.5 that only the first type of terms appears to have the Now, the major and minor elements of a Q are defined as follows:

3.2.1 Major Elements

The p terms of the first type of elements in the distance function of Eq. 3.5 are defined as major elements to be denoted by M_{μ} .

$$M_{ll} = (x_l - \mu_l)^2 \sigma^{ll}, \quad l = 1, 2, \dots, p.$$
(3.6)

3.2.2 Minor Elements

The p(p - 1) cross-product terms of the second type in Eq. 3.5 are called the minor elements to be denoted by M_{lm} .

$$M_{lm} = (x_l - \mu_l)(x_m - \mu_m)\sigma^{lm}, \quad l, m = 1, 2, ..., p, l \neq m.$$
(3.7)

The value of a sample minor element M_{lm} will change if either or both μ_l and μ_m are shifted to $\mu_l + \Delta \mu_l$ and $\mu_m + \Delta \mu_m$. However, the value of major element M_{ll} will change only when μ_l is shifted to $\mu_l + \Delta \mu_l$ and will not be affected by any shifts in the other μ 's. Thus only the sample major elements need to be charted, one for each of the *p* variables, to monitor each of the *p* process means. Being a squared distance between a sample value from the mean, each sample major element should be a highly sensitive statistic in detecting a shift in the mean. It is reminded that such major element control charts will be effective provided that the process covariance structure remains in statistical control.

3.3 Sample Major Elements

In practical applications, the process mean vector μ and covariance matrix Σ are generally unknown or unspecified, they are estimated respectively by a sample mean vector $\overline{\overline{X}}$ and a sample covariance matrix S.

Suppose that k samples of size n each are collected from a process while it is in statistical control. The j^{th} observation of sample *i* on variable *l* is denoted as $x_{ij,l}$. For the i^{th} sample, its sample mean vector and sample variance-covariance matrix, respectively denoted by $\overline{\mathbf{X}}_i$ and \mathbf{S}_i ,

$$\overline{\mathbf{X}}_{i} = \begin{bmatrix} \overline{X}_{i,l} \\ \overline{X}_{i,2} \\ \vdots \\ \overline{X}_{i,p} \end{bmatrix} = \begin{bmatrix} \overline{X}_{i,l} \end{bmatrix}_{p \times 1}, \ \mathbf{S}_{i} = \begin{bmatrix} s_{i,11} & s_{i,12} & \cdots & s_{i,1p} \\ s_{i,12} & s_{i,22} & \cdots & s_{i,2p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{i,1p} & s_{i,2p} & \cdots & s_{i,pp} \end{bmatrix} = \begin{bmatrix} s_{i,lm} \end{bmatrix}_{p \times p}$$
(3.8)

are obtained by

$$\overline{X}_{i,l} = \frac{\sum_{j=1}^{n} x_{ij,l}}{n}, \text{ and } s_{i,lm} = \frac{1}{n-1} \sum_{j=1}^{n} \left(x_{ij,l} - \overline{x}_{i,l} \right) \left(x_{ij,m} - \overline{x}_{i,m} \right)^{\mathrm{T}} \qquad l,m = 1, 2, \dots, p.$$

Then, the process mean vector, μ , and the process variance-covariance matrix,

$$\Sigma$$
, may be estimated by $\overline{\overline{\mathbf{X}}} = \frac{\sum_{i=1}^{k} \overline{\mathbf{X}}_{i}}{k}$, and $\mathbf{S} = \frac{\sum_{i=1}^{k} \mathbf{S}_{i}}{k} = [s_{lm}]_{p \times p}$ respectively. The inverse

matrix, S^{-1} , of the sample variance-covariance matrix S is calculated by

$$\mathbf{S}^{-1} = \left[s^{lm} \right]_{p \times p} = \left[\left(-1 \right)^{l+m} \frac{\left| \mathbf{S}_{lm} \right|}{\left| \mathbf{S} \right|} \right]_{p \times p}$$
(3.9)

where S_{lm} is the matrix obtained from S by deleting l^{th} row and m^{th} column and "| |" is the determinant of a matrix.

Let the $p \times p$ population correlation matrix ρ be estimated by its corresponding sample correlation matrix **R**, which may be obtained from the sample variancecovariance matrix as follows:

$$\mathbf{R} = \begin{bmatrix} \frac{s_{11}}{\sqrt{s_{11}s_{11}}} & \frac{s_{12}}{\sqrt{s_{11}s_{22}}} & \cdots & \frac{s_{1p}}{\sqrt{s_{11}s_{pp}}} \\ \frac{s_{12}}{\sqrt{s_{11}s_{22}}} & \frac{s_{22}}{\sqrt{s_{22}s_{22}}} & \cdots & \frac{s_{2p}}{\sqrt{s_{22}s_{pp}}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{s_{1p}}{\sqrt{s_{11}s_{pp}}} & \frac{s_{2p}}{\sqrt{s_{22}s_{pp}}} & \cdots & \frac{s_{pp}}{\sqrt{s_{pp}s_{pp}}} \end{bmatrix} = \begin{bmatrix} 1 & r_{12} & \cdots & r_{1p} \\ r_{12} & 1 & \cdots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{1p} & r_{2p} & \cdots & 1 \end{bmatrix}$$
(3.10)

where the r_{lm} 's are sample correlations between variable l and m for l,m=1,2,...,p.

Now, let the *pxp* sample standard deviation matrix, $\mathbf{V}^{\frac{1}{2}}$, be

$$\mathbf{V}^{\nu_{2}} = \begin{bmatrix} \sqrt{s_{11}} & 0 & 0 & \cdots & 0\\ 0 & \sqrt{s_{22}} & 0 & \cdots & 0\\ 0 & 0 & \ddots & & \vdots\\ \vdots & \vdots & & \ddots & 0\\ 0 & 0 & \cdots & 0 & \sqrt{s_{pp}} \end{bmatrix}$$
(3.11)

Then, S can be obtained from $\mathbf{V}^{\frac{1}{2}}$ and **R** by

$$\mathbf{S} = \mathbf{V}^{\frac{1}{2}} \mathbf{R} \mathbf{V}^{\frac{1}{2}},\tag{3.12}$$

and the determinant of S by

$$\begin{aligned} |\mathbf{S}| &= \left| \mathbf{V}^{\frac{1}{2}} \mathbf{R} \mathbf{V}^{\frac{1}{2}} \right| \\ &= \left| \mathbf{V}^{\frac{1}{2}} \right| \cdot \left| \mathbf{R} \right| \cdot \left| \mathbf{V}^{\frac{1}{2}} \right| \end{aligned}$$

With $|\mathbf{V}_{2}| = \sqrt{s_{11}} \cdot \sqrt{s_{22}} \cdots \sqrt{s_{pp}}$, it is also true that

$$|\mathbf{S}| = \left(\sqrt{s_{11}s_{22}\cdots s_{pp}}\right)^2 |\mathbf{R}|$$

= $s_{11}s_{22}\cdots s_{pp}|\mathbf{R}|$. (3.13)
= $\left(\prod_{l=1}^p s_{ll}\right) |\mathbf{R}|$

Let R_{lm} be the matrix obtained from R by deleting l^{th} row and m^{th} column, and $\mathbf{V}^{\frac{1}{2}}$ be the matrix obtained from $\mathbf{V}^{\frac{1}{2}}$ by deleting l^{th} row and l^{th} column. Similarly, \mathbf{S}_{lm} can be obtained by $\mathbf{S}_{lm} = \mathbf{V}_{l}^{\frac{1}{2}} \mathbf{R}_{lm} \mathbf{V}_{m}^{\frac{1}{2}}$ and the determinant of \mathbf{S}_{lm} by the following expression,

$$\left|\mathbf{S}_{lm}\right| = \left|\mathbf{V}_{l}^{\mathscr{Y}_{2}}\mathbf{R}_{lm}\mathbf{V}_{m}^{\mathscr{Y}_{2}}\right| = \left|\mathbf{V}_{l}^{\mathscr{Y}_{2}}\right| \cdot \left|\mathbf{R}_{lm}\right| \cdot \left|\mathbf{V}_{m}^{\mathscr{Y}_{2}}\right|, \quad l,m = 1,2,...,p.$$
(3.14)

From Eqs. 3.13 and 3.14, the elements of S^{-1} , s^{lm} , can be written as

$$s^{lm} = (-1)^{l+m} \frac{\left|\mathbf{V}_{l}^{\mathcal{V}_{l}}\right| \cdot \left|\mathbf{R}_{lm}\right| \cdot \left|\mathbf{V}_{m}^{\mathcal{V}_{l}}\right|}{\left(\prod_{l=1}^{p} s_{ll}\right) \left|\mathbf{R}\right|}, \qquad l,m = 1,2,...,p.$$
(3.15)

Thus the i^{th} sample major element, $M_{i,ll}$, is

$$M_{i,ll} = \left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)^{2} s^{ll}, \ l = 1, 2, \dots, p$$
(3.16)

where

$$s^{\prime\prime} = (-1)^{l+l} \frac{\left(\prod_{q=1, q\neq l}^{p} S_{qq}\right) |\mathbf{R}_{ll}|}{\left(\prod_{q=1}^{p} S_{qq}\right) |\mathbf{R}|} = \frac{|\mathbf{R}_{ll}|}{s_{ll} |\mathbf{R}|}, \quad l = 1, 2, ..., p,$$
(3.17)

since $\left|\mathbf{V}_{l}^{\mathcal{H}}\right| \cdot \left|\mathbf{R}_{ll}\right| \cdot \left|\mathbf{V}_{l}^{\mathcal{H}}\right| = \left(\prod_{q=1, q\neq l}^{p} s_{qq}\right) \left|\mathbf{R}_{ll}\right|.$

Finally, the sample major elements may be expressed as

$$M_{i,ll} = \left(\frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|}\right) \frac{\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)^{2}}{s_{ll}}, \qquad l = 1, 2, \dots, p,$$
(3.18)

which shows that each sample major element is simply a squared standardized normal deviate, modified by a correlation factor $\left(\frac{|\mathbf{R}_{\parallel}|}{|\mathbf{R}|}\right)$ of a *p*-variate process.

3.4 Sampling Distribution of Major Elements

The sample major element M_{II} of Eq. 3.18 is a function of $(\overline{X}_{i,I} - \overline{\overline{X}}_{I})$ which is a normal random variable with the expected value and variance given by

$$E\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right) = E\left(\overline{X}_{i,l}\right) - E\left(\overline{\overline{X}}_{l}\right) = \frac{n\mu}{n} - \mu = 0, \ l = 1, 2, ..., p,$$
(3.19)

$$\sigma_{\overline{X}_{i,l}-\overline{X}_{l}}^{2} = \operatorname{var}\left(\overline{X}_{i,l}-\overline{X}_{l}\right)$$

$$= \operatorname{var}\left(\overline{X}_{i,l}\right) - 2\operatorname{cov}\left(\overline{X}_{i,l}, \frac{\sum_{i=1}^{k} \overline{X}_{i,l}}{k}\right) + \operatorname{var}\left(\overline{\overline{X}}_{i,l}\right)$$

$$= \frac{\sigma_{ll}}{n} - \left(\frac{2}{k}\right)\left(\frac{\sigma_{ll}}{n}\right) + \left(\frac{\sigma_{ll}}{kn}\right)$$

$$= \left(\frac{k-1}{kn}\right)\sigma_{ll}$$
(3.20)

Thus, $\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)$ is a $N\left(0, \frac{k-1}{kn}\sigma_{ll}\right)$ distribution. Let Z_{l} be the standardized

normal variable of $\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)$. Then

$$Z_{l} = \frac{\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right) - 0}{\sqrt{\frac{k-1}{kn}\sigma_{ll}}} \sim N(0,1), \quad l = 1,2,...,p.$$
(3.21)

Subsequently, Z_l^2 follows a Chi-square distribution with one degree of freedom, that is

$$Z_{l}^{2} = \frac{\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)^{2}}{\frac{k-1}{kn}\sigma_{ll}} \sim \chi_{1}^{2}, \qquad l = 1, 2, ..., p.$$
(3.22)

And

$$\frac{\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)^{2}}{\sigma_{ll}} \sim \left(\frac{k-1}{kn}\right) \chi_{1}^{2}, \qquad l = 1, 2, \dots, p.$$
(3.23)

With a large number of samples (k>50, say), the practice of control charts has been to simply substitute σ_{ll} by s_{ll} in Eq. 3.23. Then, approximately,

$$\frac{\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)^{2}}{s_{ll}} \sim \frac{k-1}{nk} \chi_{1}^{2} , \qquad l = 1, 2, ..., p.$$
(3.24)

On multiplying Eq. 3.24 by $\left(\frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|}\right)$, it then follows that the sample major element has

the adjusted chi-square distribution with one degree of freedom. That is,

$$M_{i,ll} = \left(\frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|}\right) \frac{\left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)^{2}}{S_{ll}} \sim \left(\frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|}\right) \left(\frac{k-1}{nk}\right) \chi_{1}^{2}, \quad l = 1, 2, ..., p, \quad (3.25)$$

which provides the basis for control limit calculations and the interpretation of each of the p control charts of sample major elements.

3.5 Expected Out-Of-Control Patterns of A Trivariate Process

In Section 3.2, it was speculated that the sample major elements should be highly sensitive and unique to any shifts in the process means, individually for each mean and simultaneously for all p means. To demonstrate how the sample major elements distribute themselves on their respective control charts when the process is out of control because one or more shifts in the process means, a trivariate process is analyzed in this section.

Consider a trivariate Gaussian process, p=3, with a mean vector μ and a covariance matrix Σ . Let $h\delta$ be a vector $[h_1\delta_1, h_2\delta_2, h_3\delta_3]^T$ of the shifts in the mean vector, μ , where each of the h_l may have values [-1,0,1] denoting respectively a downward shift, no shift or an upward shift of size δ_l in the process mean of X_l . For each sample, a sample mean vector $\overline{X} = [\overline{x}_1, \overline{x}_2, \overline{x}_3]^T$ is analyzed for possible signals of any one or more shifts in the means. Since the process is subject to any shifts in the means at any time, the process variables may be written as $\mathbf{Y} = \mathbf{X} + h\delta$ for the following analysis. The sample mean vector of \mathbf{Y} is

$$\overline{\mathbf{Y}} = \overline{\mathbf{X}} + h\delta \,. \tag{3.26}$$

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The expected difference between \overline{Y} and the grand mean $\overline{\overline{X}}$ is

$$E\left(\overline{\mathbf{Y}} - \overline{\overline{\mathbf{X}}}\right) = E\left(\overline{\mathbf{X}} + h\delta - \overline{\overline{\mathbf{X}}}\right) = E\left(\overline{\mathbf{X}} - \overline{\overline{\mathbf{X}}} + h\delta\right) = E\left(\overline{\mathbf{X}} - \overline{\overline{\mathbf{X}}}\right) + h\delta$$

Since $E\left(\overline{\mathbf{X}} - \overline{\overline{\mathbf{X}}}\right) = 0$,

$$E\left(\overline{\mathbf{Y}} - \overline{\overline{\mathbf{X}}}\right) = h\delta.$$
(3.27)

The value of the expected sample major element associated with X_l is given as follows.

$$E[M_{ll}] = E\left[\left(\overline{\mathbf{y}}_{l} - \overline{\overline{\mathbf{x}}}_{l}\right)^{2} s^{ll}\right], \text{ for } l = 1, \dots, p.$$

$$= E\left[\frac{\left(\overline{\mathbf{y}}_{l} - \overline{\overline{\mathbf{x}}}_{l}\right)^{2}}{s_{ll}} \cdot \frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|}\right],$$
(3.28)

where \overline{y}_l is the sample mean of Y_l

When the process variance-covariance is stable and in-control, $\left(\frac{|\mathbf{R}_u|}{|\mathbf{R}|}\right)$ may be

treated as a constant. Therefore,

$$\mathbf{E}[M_{ll}] = \frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|} E\left[\frac{(\overline{\mathbf{y}}_{l} - \overline{\mathbf{x}}_{l})^{2}}{s_{ll}}\right], \quad l = 1, 2, \dots, p.$$
(3.29)

From Eq. 3.24 and $E(\chi_1^2) = 1$, the following result can be obtained.

$$E\left[\frac{\left(\overline{\mathbf{y}}-\overline{\mathbf{x}}\right)^{2}}{s_{ll}}\right] = E\left[\frac{\left(\overline{\mathbf{x}}_{l}-\overline{\mathbf{x}}_{l}+h_{l}\delta_{l}\right)^{2}}{s_{ll}}\right]$$
$$= E\left[\frac{\left(\overline{\mathbf{x}}_{l}-\overline{\mathbf{x}}_{l}\right)^{2}+2h\delta\frac{\left(\overline{\mathbf{x}}_{l}-\overline{\mathbf{x}}_{l}\right)}{s_{ll}}+\frac{\left(h_{l}\delta_{l}\right)^{2}}{s_{ll}}\right]$$
$$= E\left[\frac{\left(\overline{\mathbf{x}}_{l}-\overline{\mathbf{x}}_{l}\right)^{2}}{s_{ll}}\right]+2h\delta E\left(\frac{\overline{\mathbf{x}}_{l}-\overline{\mathbf{x}}_{l}}{s_{ll}}\right)+E\left[\frac{\left(h_{l}\delta_{l}\right)^{2}}{s_{ll}}\right]$$
$$= \frac{k-1}{nk}+\frac{\left(h_{l}\delta_{l}\right)^{2}}{s_{ll}}$$
(3.30)

Accordingly, the expected value of M_{ll} is given by

$$E(M_{ll}) = \frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|} \left[\frac{k-1}{nk} + \frac{(h_l \delta_l)^2}{s_{ll}} \right], \qquad l = 1, 2, ..., p. \qquad (3.31)$$
$$= \frac{k-1}{nk} \left(\frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|} \right) + (h_l \delta_l)^2 \sigma^{ll}$$

Eq. 3.31 shows that the expected value of a sample major element will be very large if a shift actually occurs, because the amount of the shift is squared in the expression of M_{II} .

3.5.1 Shift Combinations

When a process is monitored for three process variables, there are a total of $3^3=27$ possible states of the three process means, including the one with no shifts in any of the means, as shown in Table 3.1. The shift size δ_l will be expressed, as usual, in terms of the standard deviation of X_l .

|--|

Variable	Shifts	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
Xt	_h,	-	-	-	-	-	-	-	-	-	0	0	0	0	0	0	0	0	0	+	+	+	+	+	+	+	+	+
X ₂	h ₂	t	-	1	0	0	0	+	+	+	-	1	1	0	0	0	+	+	+	1	ţ	-	0	0	0	+	+	+
X3	h ₃	-	0	+	-	0	+	-	0	+	-	0	+	-	0	+	-	0	+	-	0	+	-	0	+	-	0	+

+ : the shift is upward, or an increase in the mean.

0 : no shift

- : the shift is downward, or a decrease in the mean.

For any multivariate control charts to be informative for the identification of the specific nature of shifts in each of the p means, when a process is judged to be out of control, the out-of-control signals of all the p control charts must exhibit unique patterns, one for each possible combination of the shifts.

3.5.2 Possible Correlation Structures of A Trivariate Process

In practical applications, correlation coefficients are often used to represent the dependency relationships among the variables. Out of a total of eight, mathematically possible, pair-wise combinations of the three correlations, there are only four such combinations that can exist physically in a real process. These are listed in Table 3.2. For example, if ρ_{12} is positive, then ρ_{13} and ρ_{23} must have the same sign to be physically meaningful.

 Table 3.2
 Possible Correlation Coefficient Combinations

	ρ_{12}	ρ ₁₃	ρ ₂₃
1	+	+	+
2	+	-	-
3	-	+	-
4	-	_	+

Moreover, in statistical analysis, we only need to consider the following two distinct types of correlation structure need to be considered:

(a) All Positive Correlations
$$\Rightarrow \left[\rho_{12} > 0, \ \rho_{13} > 0, \ \rho_{23} > 0\right]$$

(b) Two Negative and one Positive Correlations $\Rightarrow \left[\rho_{12} < 0, \ \rho_{13} > 0, \ \rho_{23} < 0\right]$

The expected out-of-control patterns of the sample major elements will be different between the two processes with different correlation structures.

3.5.3 An Example of Expected Patterns of Major Element Distributions

To demonstrate the expected out-of control patterns corresponding to each possible combination of the shifts in the three means, a trivariate process where all three correlations are positive has been analyzed as presented in Figure 3.1. Part (a) of Figure 3.1 gives the data about the process which includes correlation and variance-covariance matrices, a mean vector, and the type and size of the shift in each mean. A stacked bar chart in Part (b) presents the expected sample major elements, according to the shift combinations listed in Part (a). The various lengths of the stacked bars in Figure 3.1 reflect the expected magnitude of the changes in the respective sample elements.

It can be seen that the plots of the expected sample major elements of Figure. 3.1 clearly indicate which of the three process means may have been shifted. This is definitely an advantage over most conventional multivariate control charts. However, there are only seven unique patterns of the three sample major elements for all twentysix possible shifts in the three process means. In other words, these sample major elements can only display whether the possible shifts are in any one, two or all three variables, but can not reveal the specific nature of each of the 26 shift combinations. For instance, shift combinations #2, #8, #20 and #26 all have the same expected out-of-control pattern, although each of which involves a different kind of upward and downward shifts in the means of X_1 and X_2 .



Figure 3.1 Process Information and Major Element Plots

When the plots of the three sample major elements are supplemented with the sample minor element plots, together they would be capable of displaying thirteen distinguishable patters. For example, with the help of sample minor elements, combinations #2 and #8 would have different expected patterns. So would have combinations #20 and #26. But the expected pattern of (#2, #26) would be still the same, and so would be (#8, #20). It would be a great improvement in chart interpretation if plots of sample minor elements were also employed in addition to the major elements.

That, however, would be achieved at the extra and added complexity expense. An alternative approach that utilizes only the major element charts presented in the next section has been tried with good results.

3.5.4 Detecting the Direction of Shifts in the Means

As discussed earlier, the sample major element plots can not reveal the specific nature of each and every combination of shifts in the means. In order to achieve such a capability, the following modification of the sample major element calculations is proposed to produce all the twenty-six expected patterns one for each specific combination of shifts in the three process means.

Let
$$\Delta_{i,j} = \overline{X}_{i,j} - \overline{\overline{X}}_{i}$$
 and compute $\frac{\Delta_{i,j}}{|\Delta_{i,j}|}$ for each sample *i* so that the sample major

element now carries a "sign" clearly indicating the direction of the observed sample deviation. Each signed or directional sample major element when deviating a great deal from their expected value is more likely a reflection of the direction of the shift, up or down. Furthermore, the expected value, $E(M_{il}), l = 1, 2, 3$, of the modified sample element will indicate the sign of the underlying shift. These modified sample major elements, denoted by M'_{il} , are defined as follows.

$$M'_{ij} = \begin{cases} \frac{\Delta_{ij}}{|\Delta_{ij}|} M_{ijl}, \Delta_{ij} \neq 0. \\ 0, \Delta_{ij} = 0 \end{cases}, \quad l = 1, 2, ..., p.$$
(3.32)

Figure 3.2 is a plot of the expected patterns, $E(M'_{i,l})$'s, corresponding to each of the twenty-six combinations of shifts in the means of the same example trivariate process discussed in the last section. The direction of each $E(M'_{i,l})$ is clearly displayed by the stacked bars in Figure 3.2. The twenty-six distinctly unique patterns are clearly identifiable for each specific combination of the shifts.

A table of out-of-control patterns such as the one shown in Figure 3.2 will be very helpful in practice for diagnostic analysis of multivariate control charts.



Figure 3.2 Modified Major Element Plots (M'_{iJ})

It is noted that by adding the "sign", indicating the direction of a shift, each of the p major element control charts can be analyzed individually, one for each variable. Such makes the analysis of a multivariate process control very simple and easy.

3.5.5 Control Limits for Major Elements

It was shown in Section 3.4 that the sample major element is distributed as a function of a chi-square variable having one degree of freedom. For control chart construction, the upper and lower control limits of the sample major elements may be set at a significance level α as follows:

$$UCL_{1-\alpha/2} \text{ of } M_{i,ll} = \left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi^2_{1,1-\alpha/2}$$

$$LCL_{\alpha/2} \text{ of } M_{i,ll} = \left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi^2_{1,\alpha/2} \cong 0$$
(3.33)

In the application of the major element control charts, the lower control limit of each of the major element charts may be set to zero for simplicity. The reason for this is that any shift in the mean will lead to a big increase in the sample major element, while the magnitude of LCL becomes relative very small. The sample major elements, however, are sensitive not only to shifts in the process means but also to changes in the variance-covariance matrix. It is therefore a prerequisite that the variances and covariances of the process are in statistical control before meaningful analysis of the major element control charts can be conducted

When control charts are to be constructed for the modified sample major elements, both upper and lower control limits must be calculated. Since the modifier, $\frac{\Delta_{ij}}{|\Delta_{ij}|}$, can only be either +1 or -1, the upper and lower control limits will have the same

absolute value. With negligible error, it is recommended to set the center line at zero such that one two-sided control chart is used for each sample major element with symmetrical control limits as follows:

$$UCL = \left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi_{1,1-\alpha/2}^{2}$$

$$CL = 0 , \qquad l = 1,2,3...,p. \qquad (3.34)$$

$$LCL = -\left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi_{1,1-\alpha/2}^{2}$$

3.5.6 Expected Direction Pattern for p-variate Process

For a general *p*-variate process with p>3, each shift combination of the *p* variables is also expected to exhibit a unique directional pattern. Since each variable of a *p*-variate process can only be in one of the three states: shifts upward, downward or no shift, there are 3^{p} -1 types of shift combinations. For example, a four-variate process has 81 states with 80 unique out-of-control patterns to be expected for the sample major elements. Such unique out-of-control patterns of a 4-variate process are displayed in Figure 3.3.

The number of the shift combinations will increase drastically even for moderately large p vales such as five or six. Theoretically, it seems that no matter how many variables are being controlled, changes in the process means can be identified by similar charts with upward and downward stack bars. However, as p increases, it will become more difficult to read a large number of sample major element charts with reference stack-bar charts.



Chapter 4

MAJOR ELEMENT CONTROL CHARTS BY SIMULATION

The methodology of Chapter 3 is developed for the control of the means of a multivariate Gaussian process. It was shown that the sample p major elements could be analyzed individually for statistical signals of possible upward or downward shifts in each of the process means. This chapter demonstrates how these major element control charts are applied, using simulated sample data of a number of trivariate processes with different process means and covariance matrices. In the estimation of the process parameters needed for initial chart constructions, the sample size effect on estimation errors is discussed with simulated demonstrations. The programs that were employed for data simulation are written in SAS IML language and executed on UNIX computers. They are listed in Appendix I.

This chapter begins with a description of the algorithm for computer simulation of a trivariate normal process in section 4.1. Section 4.2 presents the design of various sets of parameter and shift combinations for the simulations to exhibit the out-of-control patterns of sample major elements. In Section 4.3, a step-by-step computation and charting procedure of the three major element control charts is discussed. An example of a simulated trivariate process is described with illustrations in Section 4.4. The estimation of process parameters for control limit calculations and the distributional patterns of the directional major element control charts are discussed in Section 4.5. Some results on the sample size effects on parameter estimation and on the general effectiveness of the proposed major element control charts are given in Section 4.6 and some summarized results in the final section.

4.1 Simulation of A Trivariate Normal Process

Consider a trivariate normal process characterized by a random vector $\mathbf{X} = [X_1, X_2, X_3]^T$ with a mean vector μ , a variance-covariance matrix Σ and a correlation matrix ρ as

$$\rho = \begin{bmatrix} 1 & \rho_{12} & \rho_{13} \\ \rho_{12} & 1 & \rho_{23} \\ \rho_{13} & \rho_{23} & 1 \end{bmatrix}.$$

4.1.1 Input Process Parameters

The simulation of a *p*-variate normal process requires certain process parameters as input data. The specific parameter inputs are determined according to the method or algorithm selected for simulation. The method of Cholesky's Factorization, which decomposes the process variance-covariance matrix, Σ , was employed for data simulation in this research. Similar to Eq. 3.12, the method uses the expression, $\Sigma = v^{\frac{N}{2}}\rho v^{\frac{N}{2}}$, where

$$v^{1/2} = \begin{bmatrix} \sqrt{\sigma_{11}} & 0 & 0 \\ 0 & \sqrt{\sigma_{22}} & 0 \\ 0 & 0 & \sqrt{\sigma_{33}} \end{bmatrix}.$$

As a result, the input parameters required for simulating a trivariate normal process include the means (μ_1, μ_2, μ_3) , the standard deviations $(\sigma_1, \sigma_2, \sigma_3)$ and the correlations $(\rho_{12}, \rho_{13}, \rho_{23})$.

4.1.2 Cholesky Decomposition of Variance-Covariance Matrix

Since the variance-covariance matrix Σ is positive definite, there exists a unique lower triangular matrix L ($l_{ij} = 0, i < j$) with positive diagonal elements such that (Anderson, 1984)

$$\Sigma = \mathbf{L}\mathbf{L}^T \,. \tag{4.1}$$

The first step of the Cholesky simulation is to generate a data matrix Y of three correlatedd normal vectors with variance-covariance matrix Σ and 0 mean vector,

$$\mathbf{Y} = \mathbf{Z}\mathbf{L}\,,\tag{4.2}$$

where

$$\mathbf{Z} = \left[Z_1, Z_2, Z_3 \right]_{a \times 3}$$

is an $(a \times 3)$ matrix of three vectors of an independent, standardized normal deviates, N(0, I) where I is an identity matrix of order 3. So

$$\mathbf{Y} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}). \tag{4.3}$$

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Then, the simulated sample data of size a of the trivariate X is obtained by

$$\mathbf{X} = \boldsymbol{\mu} + \mathbf{Y} = \boldsymbol{\mu} + \mathbf{Z}\mathbf{L} \,. \tag{4.4}$$

4.2 Simulation Design of Mean Shifts

A design of the simulation runs is described in detail in this section. In order to demonstrate that certain distributional patterns of the sample major elements do exist while the process means are shifted, shifts of different sizes and directions were simulated for the analysis. Simulated data sets were also generated from different processes of various process means, standard deviations and correlation structures. Results from these various simulated data allow for the evaluation of the performance effectiveness of the major element control charts.

Each of the three process means may be in one of three states, (-, 0, +) which denote respectively "a downward shift", "no shifts", and "an upward shift". There are a total of $3^3 = 27$ possible states of the process at any time, as shown in Table 4.1. Four different sizes of the shifts, 0.25 σ , 0.5 σ , 1.0 σ and 1.5 σ , in the process means were simulated to observe their effects on the distributional patterns of sample major elements on each of the three control charts. Table 4.1 lists all the 27 states under each of the 4 sizes of shift, where h_l and δ_l denote the direction and size of a shift in the mean of variable *l*.

In order to ascertain the possible effects on the sample distribution patterns of the major elements due to various types and degrees of correlation among the three variables, a total of ten different correlation matrices were used in data generation. Five of which, with various degrees of correlation, were simulated for all positive correlations and another five for cases with two negative correlations. Table 4.2 summarizes the parameter values for all the simulation runs of the base data when the process is in control.

Shifts		μıδ	ıσı			h₂δ	2 ^σ 2		h ₃ ŏ ₃ σ ₃				
1	$-0.25\sigma_{1}$	-0.5 ₀	-1.0σ ₁	$-1.5\sigma_{1}$	-0.25o2	-0.5œ	-1.0o2	-1.50 <u>-</u>	-0.25o3	-0.5o3	-1.0 0 3	-1.5 ₀	
2	-0.25σ _ι	-0.5σ ₁	-1.0σ _ι	-1.5σ ₁	-0.25oz	-0.5œ	-1.0 <u>0</u> 2	-1.502		·	0		
3	-0.25σ _ι	-0.5σ _ι	-1.0σι	-1.5σ _ι	-0.25 <u>0</u>	-0.5o2	-1.0 <u>5</u>	-1.5o2	+0.25σ3	+0.5 ₃	+1.003	+1.503	
4	$-0.25\sigma_{1}$	-0.5σ ₁	$-1.0\sigma_1$	-1.5σ ₁		()		-0.25 ₃	-0.5 0 3	-1.0σ3	-1.5σ3	
5	$-0.25\sigma_{1}$	-0.5σ ₁	-1.0σ _l	-1.5σ ₁)				0	·	
6	-0.25σ _ι	-0.5σ ₁	-1.0σ _ι	-1.5σ ₁	<u> </u>	()		+0.25 ₃	+0.5ơ3	+1.003	+1.503	
7	-0.25 ₀₁	-0.5σ _ι	-1.001	-1.5σ _ι	+0.25o2	+0.502	+1.0o2	+1.502	-0.25o3	-0.5 0 3	-1.0o3	-1.5 0 3	
8	$-0.25\sigma_{1}$	-0.5ơ _l	$-1.0\sigma_1$	-1.5σ ₁	+0.25o2	+0.502	+1.002	+1.502			0	·	
9	-0.25o ₁	-0.5σ ₁	-1.0σ _ι	$-1.5\sigma_1$	+0.25o2	+0.502	+1.0o2	+1.502	+0.25o3	+0.5o3	+1.0o3	+1.503	
10		C)		-0.25o2	-0.5 <u>0</u>	-1.0 <u>0</u> 2	-1.502	-0.25 ₃	-0.5σ3	-1.0 0 3	-1.503	
11		0			-0.25oz	-0.5 0 2	-1.0o2	-1.502		•	0		
12		0			-0.25o2	-0.5o2	-1.0o2	-1.502	+0.2503	+0.5 ₃	+1.0o3	+1.503	
13		0			1	()	·	-0.25o3	-0.5 o3	-1.0 0 3	-1.503	
14		0				()		0				
15		0				()		+0.25o3	+0.5 ₃	+1.00 ₃	+1.503	
16		0	·		+0.25o2	+0.5o2	+1.0 <u>0</u>	+1.502	-0.25 ₃	-0.5σ3	-1.0 0 3	-1.503	
17		0	, <u> </u>		+0.25o2	+0.5og	+1.0o2	+1.502			0		
18		0			+0.25o2	+0.502	+1.0o2	+1.502	+0.25σ3	+0.5σ3	+1.0 ₃	+1.503	
19	$+0.25\sigma_{i}$	+0.5σ ₁	+1.0σ _ι	+1.5σ _ι	-0.25o2	-0.5 <u>0</u>	-1.0σ <u>-</u>	-1.502	-0.25 0 3	-0.5 ₃	-1.003	-1.5 0 3	
20	+0.25σ ₁	+0.5σ _i	+1.0σ ₁	+1.5 0 1	-0.25σ <u>2</u>	-0.5œ	-1.0o2	-1.502			0		
21	+0.25 ₀ 1	+0.5σ ₁	+1.0σ _ι	+1.5σ ₁	-0.25o2	-0.5 <u>0</u>	$-1.0\sigma_{2}$	-1.502	$+0.25\sigma_{3}$	+0.5σ3	+1.0og	+1.503	
22	+0.25σ ₁	+0.5σ ₁	+1.0σ ₁	+1.5σ _ι		()		-0.25o3	-0.5 0 3	-1.0 0 3	-1.503	
23	+0.25σ ₁	+0.5σ _i	+1.0σ ₁	+1.5σ ₁		()		0				
24	+0.25ơ ₁	+0.5σ _l	+1.001	+1.5σ _ι		()		+0.25 ₃	+0.5σ ₃	+1.0 0 3	+1.503	
25	+0.25σ _ι	+0.5σ ₁	+1.0σ _ι	+1.5σ ₁	+0.25o2	+0.5o2	+1.0og	+1.5o2	-0.25σ ₃	-0.5σ3	-1.0 0 3	-1.5 0 3	
26	+0.25 ₀ 1	+0.5σ ₁	+1.0σ ₁	+1.5σ ₁	+0.25o ₂	+0.55	+1.0o2	+1.5 <u>5</u>			0		
27	+0.25 ₀₁	+0.5σ ₁	+1.0σ ₁	+1.5σ _ι	+0.2502	+0.5o2	+1.0o2	+1.5o2	+0.25 ₃	+0.5σ3	+1.0o3	+1.5σ3	

Table 4.1 Simulated Shifts among the Three Variables

The order of a simulation run is denoted by a 2- or 3-digit 'run no' as listed in Table 4.2. It is noted that the even numbers, Run 00 to Run 100, indicate those runs with all positive correlations, while the odd numbers, Run 01 to Run 101, with two negative and one positive correlations. In addition, each simulation run contains four different sets of sample data, one for each of the four shift sizes in the means.

	E(X)			lard Dev	viation	Simultion	All Posi C	itive Con Defficien	relation t	Simultion	Two Negative and One Positive Correlation Coefficient				
X1	X ₂	X3	St	\$2	\$ ₃	Run No.	۲ ₁₂	۲ ₁₃	ſ ₂₃	Run No.	Γ12	r ₁₃	۲ ₂₃		
	1			1.2		00	0.7	0.9	0.6	01	-0.7	0.9	-0.6		
ł						10	0.2	0.1	0.15	11	-0.2	0.1	-0.15		
3	15	9	1.6		0.9	20	0.3	0.8	0.35	21	-0.3	0.8	-0.35		
						30	0.85	0.4	0.8	31	-0.85	0.4	-0.8		
						40	0.95	0.9	0.875	41	-0.95	0.9	-0.875		
2	15	9	0.06	0.012	0.00	50	0.7	0.9	0.6	51	-0.7	0.9	-0.6		
~	13		0.00		0.09	60	0.2	0.1	0.15	61	-0.2	0.1	-0.15		
0.5	0.65	0.25	1.6	1.2	0.9	70	0.7	0.9	0.6	71	-0.7	0.9	-0.6		
0.5	0.00	0.20				80	0.2	0.1	0.15	81	-0.2	0.1	-0.15		
0.5	0.65	0.25	0.06	0.012	0.09	90	0.7	0.9	0.6	91	-0.7	0.9	-0.6		
0.5 0.6	0.00	0.25	0.00	0.012		100	0.2	0.1	0.15	101	-0.2	0.1	-0.15		

 Table 4.2
 Summary of the Parameters Used in Simulation

Another twelve more runs were also simulated for relatively very small values for the process means and standard deviations using the correlation structures in Run 00 & 01 and Run 10 & 11.

For each simulation run, the computer generated 13500 of 3×1 vectors. Every set of ten vectors was taken as one sample. There are 50 samples for each shift combination. The sequence of samples from sample no.651 to no.700 (shift no. 14 in Table 4.1) of each run represents the in-control state without shifts. These in-control data were used to calculate the sample means, the sample standard deviations, the sample correlation matrix, and the sample variance-covariance matrix. These sample statistics were used to construct the major element control charts.

All the simulated sample data including input process parameters are documented in Appendix II.

4.3 Setting-Up Major Element Control Charts

Upon completion of each simulation of an input process, the simulated sample data is used to calculate the sample major elements and the control limits for each chart. A step-by-step procedure for the construction of the major element control charts will be explained in this section. In addition, programs for all the computations were written in SAS IML and are listed in Appendix I.

According to the methods described in Chapter 3, the following is a step-by-step procedure for the construction of the major element control charts.

 For each sample of n simulated observations, the sample means and sample variances and covariances are calculated.

$$\overline{X}_{i,l} = \frac{\sum_{j=1}^{n} x_{ij,l}}{n}$$

$$s_{i,lm} = \frac{1}{n-1} \sum_{j=1}^{n} \left(x_{ij,l} - \bar{x}_{i,l} \right) \left(x_{ij,m} - \bar{x}_{i,m} \right)^{\mathrm{T}} \qquad l,m = 1, 2, 3.$$
(4.5)

where $x_{ij,l}$ is the j^{th} observation, j=1,2,...,n, in the i^{th} sample of variable l and $S_{i,lm}$ is the i^{th} sample covariance of variables l and m. When l=m, $S_{i,ll}$ is the i^{th} sample variance of variable l. The sample variance-covariance matrix can be written as

$$\mathbf{S}_{i} = \begin{bmatrix} s_{i,11} & s_{i,12} & s_{i,13} \\ s_{i,12} & s_{i,22} & s_{i,23} \\ s_{i,13} & s_{i,23} & s_{i,33} \end{bmatrix}, i = 1, 2, \dots, k$$
(4.6)

where k is the number of samples.

2. The grand sample mean, $\overline{\mathbf{X}}$, and variance-covariance matrix, S, are respectively the arithmetic average of all the k sample means and k sample variances and covariances.

$$\overline{\overline{\mathbf{X}}} = \frac{\sum_{i=1}^{k} \overline{X}_{i}}{k}, \text{ and } \overline{\mathbf{S}} = \frac{\sum_{i=1}^{k} S_{i}}{k} = \left[\frac{\sum_{i=1}^{k} S_{i,lm}}{k}\right]_{3\times 3}.$$
 (4.7)

3. The inverted sample variance-covariance matrix (S^{-1}) is then calculated.

$$\mathbf{S}^{-1} = \left[s^{lm} \right]_{P \times P} = \left[\left(-1 \right)^{l+m} \frac{|\mathbf{S}_{lm}|}{|\mathbf{S}|} \right]_{P \times P}$$
(4.8)

where S_{lm} is the matrix obtained from S by deleting l^{th} row and m^{th} column and "| |" is the determinant of a matrix.

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4. The sample major element of each variable l is calculated as follows:

$$M_{i,ll} = \left(\overline{X}_{i,l} - \overline{\overline{X}}_l\right)^2 s^{ll}, l = 1, 2, \dots, p.$$

5. The directional sample major element with $\overline{X}_{i,l} - \overline{\overline{X}}_{l} = \Delta_{i,l}$ may be calculated by

$$M'_{i,J} = \begin{cases} \frac{\Delta_{i,J}}{|\Delta_{i,J}|} M_{i,JI}, \Delta_{i,J} \neq 0\\ 0, \Delta_{i,J} = 0 \end{cases}$$
(4.9)

- 6. The value of $\frac{|\mathbf{R}_{ll}|}{|\mathbf{R}|}$ is calculated for each process variable, where the value of \mathbf{R}_{ll} is the matrix obtained from the sample correlation matrix **R** by deleting l^{th} row and l^{th} column, l = 1, 2, ..., p.
- 7. The control limits and centerlines for the major element control charts are obtained by Eq. 3.34 as follows.

$$UCL_{l} = \left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi^{2}_{1,1-\alpha/2}$$
$$CL_{l} = 0$$
$$LCL_{l} = -\left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi^{2}_{1,1-\alpha/2}$$

where k is the number of samples, and n is the sample size.

4.4 A Simulated Trivariate Process - Run 00

A simulation run is a set of 1,350 simulated samples of size 10 with each 50 samples generated under one of the 27 states of a trivariate process including an incontrol state. Each of the other 26 states is an out-of-control state having a particular combination of the shifts in the three means. In this section, the construction and interpretation of the major element control charts for a trivariate process will be illustrated using the simulated data Run 00, where the shift is one standard deviation in size. The control limits, based on the 50 simulated samples of size 10 (Data Nos. 651 to 700) while all three means are in control, are calculated at a significance level $\alpha/2 = 0.00275$ for chart analysis. The input parameters for generating the data of run 00 are given in Table 4.3.

	μ	Std.Dev.	C	on	
X ₁	3	1.6	1	0.7	0.9
X ₂	15	1.2	0.7	1	0.6
X ₃	9	0.9	0.9	0.6	1

Table 4.3 Simulation Input Parameters for Run 00

Run 00 data are simulated for a process with relatively high correlations among the three variables. All relevant sample statistics calculated from the in-control data (Parameter estimates and sample statistics) are given in Tables 4.4 and 4.5.

		Run 00													
	$\overline{\overline{X}}_{l}$	\overline{X}_{l} s _l R S							S ⁻¹						
X ₁	3.028	1.662	1	0.709	0.910	2.761	1.415	1.448	2.791	0.853	-3.803				
X ₂	15.038	1.200	0.709	1	0.626	1.415	1.440	0.720	0.853	1.402	0.209				
X ₃	9.035	0.958	0.910	0.626	1	1.448	0.720	0.917	-3.803	0.209	7.213				

Table 4.4 In-Control Process Statistics of Run 00

The following are the control limits at $\alpha/2 = 0.275\%$ for the three control charts. From Table 4.4,

$$|R| = 0.08512$$
; $|R_{11}| = 0.6081$; $|R_{22}| = 0.1719$; $|R_{33}| = 0.4973$.

With n=10, k=50 and $\chi^2_{1,1-0.275\%}$ = 8.9665, the control limits and centerline are:

$$UCL_{1} = \left(\frac{0.6081}{0.08512}\right) \left(\frac{50-1}{10\times50}\right) (8.9665) = 6.2777; CL_{1} = 0; LCL_{1} = -6.2777$$
$$UCL_{2} = \left(\frac{0.1719}{0.08512}\right) \left(\frac{50-1}{10\times50}\right) (8.9665) = 1.7745; CL_{2} = 0; LCL_{2} = -1.7745$$
$$UCL_{3} = \left(\frac{0.4973}{0.08512}\right) \left(\frac{50-1}{10\times50}\right) (8.9665) = 5.1398; CL_{3} = 0; LCL_{3} = -5.1398$$

The sample major elements and their corresponding control charts are plotted as shown in Figure 4.1. All three major element charts show the process in good statistical control. Five sets of 10 samples, each with one kind of shift combinations, are listed in Table 4.6 and plotted on the control charts as shown in Figure 4.2.

Subgroup (i)	$\overline{X}_{i,\mathrm{I}}$	$\overline{X}_{i,2}$	$\overline{\overline{X}}_{i,3}$	$M'_{i,1}$	<i>M</i> ′ _{<i>i</i>,2}	$M'_{i,3}$
1	3.049	15.179	8.951	0.001	0.028	-0.051
2	2.980	15.129	8.832	-0.006	0.012	-0.296
3	1.998	14.678	8.335	-2.963	-0.182	-3,529
4	3.164	15.466	9.054	0.052	0.256	0.003
5	2.772	14.866	8.828	-0.182	-0.041	-0.309
6	3.376	15.619	9.112	0.337	0.473	0.042
7	2.741	14.975	9.000	-0.231	-0.006	-0.009
8	2.493	14.904	8.894	-0.799	-0.025	-0.143
9	3.017	14.881	8.928	0.000	-0.034	-0.083
10	2.570	14.862	8.632	-0.585	-0.043	-1.171
11	3,309	15.514	9.066	0.220	0.318	0.007
12	2.245	14.426	8.877	-1.709	-0.525	-0.180
13	3 502	15 008	9 257	0.628	-0.001	0 354
14	2 631	14 984	8 915	-0 440	-0.004	-0.103
15	3 038	15 641	8 868	0.000	0 509	-0.200
16	2 965	14 959	9.243	-0.011	-0.009	0 312
17	2 490	14 847	8 887	-0.809	-0.054	-0.157
18	3 416	15 113	8.951	0.421	0.008	-0.051
19	2 407	14 438	8 801	-1 075	-0.505	-0.395
20	3 758	15 387	9 401	1 487	0.165	0.968
20	2 955	15.013	9 130	-0.015	-0.001	0.766
21	4 100	15 879	9 536	3 204	0.877	1 807
22	3 004	13.827	8 898	_0.002	-0.094	.0 135
2.5	2 753	14 815	8 870	-0.002	-0.074	-0.197
27	2.755	15 597	9350	0.211	0.070	0.11
20	3,009	13.507	8 875	-0.001	.0 194	0.715
20	2 863	14.000	8 886	-0.001	-0.174	-0.160
27	3 985	15 558	9.607	2 554	0.140	2 360
20	2.205	14 750	8 6 3 9	-1 542	0.00	1 129
20	2.205	15 205	0.000	1 010	0.110	-1.127 2 100
30	3.037	15.075	0.070	0.056	0.005	2.100
31	2 275	15.030	9.0/2	0.030	0.001	0.010
32	2.2/2	15.014	0.70/	1.425	-0.001	-0.033
33	2.313	13.030	0./ 4/	-1.423	0.000	-0.377
24	2.373	15 52/	0.000	-1.124	-0.127	-0.303
35	2.433	12.226	7.1/1	1.000	0.340	0.133
20	2.403	15 202	0.717	-1.082	-0.10/	-0.077
37	2./8/	15.303	7.431	1.609	0.077	1.248
38 70	2.780	14.713	7.30/	2.361	-0.022	0./75
39	3.1/8	14.0/4	7.281	1.020	-0.038	0.436
40	2.197	15.514	8.305	-1.929	0.107	-2.029
41	3.533	15.154	9.254	0./11	0.015	0.54/
42	2.220	14.415	0.07/ 0.07/	-1.823	-0.344	-0.823
45	2.3/3	14./47	8.7/6	-0.008	-0.11/	-0.026
44	5.584	15.465	9.418	0.862	0.255	1.061
45	3.101	14.900	9.251	0.015	-0.027	0.338
46	3.220	14.535	9.135	0.103	-0.354	0.0/2
47	3.084	15.237	9.516	0.009	0.056	0.570
48	2.903	15.180	· 8.894	-0.043	0.028	-0.143
49	5.16/	14.918	9.190	0.054	-0.020	0.1/2
50	5.164	14.605	9.102	0.052	-0.263	0.033

Table 4.550 Simulated Samples of A Process In-Control



Figure 4.1 Control Charts of the 50 Sample Major Elements in Table 4.5.

Subgroup	\overline{X}	\overline{X}	\overline{X}	<i>M</i> '.	M's	M'.,
(i)	²¹ i,1	11 1,2	21 i,3		1,2	1,3
()						
51	1.692	13.805	8.461	-4.9/8	-2.132	-2.3/4
52	0.5/9	13.518	7./14	-16./45	-3.241	-12.390
53	0.352	13.06/	7.460	-19.982	-5.445	-17.894
54	0.973	13.600	8.088	-11./88	-2.900	-6.469
55	1.588	14.056	8.139	-5./84	-1.351	-5./89
56	0./49	13.816	/.482	-14.496	-2.093	-17.404
57	1.933	13./5/	8.312	-3.345	-2.299	-3./66
58	1.292	13.972	/.989	-8.410	-1.594	-/.876
59	1.410	14.044	8.188	-7.308	-1.386	-5.1/3
60	1.625	15.935	8.188	-5.491	-1./13	-5.1/2
61	0.957	15.268	9.705	-11.972	0.074	3.236
62	0.921	14.797	9.531	-12.390	-0.082	1.774
63	1.401	14.761	10.022	-7.391	-0.108	7.020
64	1.020	14.784	9.720	-11.250	-0.091	3.388
65	1.739	15.598	9.996	-4.635	0.440	6.656
66	1.853	14.916	10.106	-3.853	-0.021	8.270
67	2.106	15.845	10.440	-2.371	0.912	14.231
68	1.737	15.289	10.127	-4.651	0.088	8.603
69	1.635	15.230	9.840	-5.413	0.052	4.670
70	1.482	15.123	9.846	-6.673	0.010	4./40
71	2.958	13.948	8.060	-0.014	-1.666	-6.857
72	2.317	13.205	7.459	-1.411	-4.712	-17.923
73	3.200	13.939	8.393	0.082	-1.694	-2.974
74	3.375	14.091	8.097	0.336	-1.258	-6.353
75	3.537	13.923	8.431	0.724	-1.742	-2.627
76	2.302	13.417	7.640	-1.469	-3.684	-14.034
77	3.272	13.669	8.320	0.166	-2.627	-3.686
78	2.827	13.569	8.147	-0.113	-3.024	-5.690
79	3.142	13.745	8.417	0.036	-2.343	-2.753
80	3.715	13.696	8.729	1.318	-2.526	<u>-0.675</u>
81	4.342	16.436	8.746	4.817	2.739	-0.602
82	4.821	15.760	9.119	8.974	0.730	0.051
83	3.942	15.511	8.605	2.333	0.313	-1.336
84	3.727	15.746	8.450	1.365	0.702	-2.469
85	4.452	16.074	9.044	5.662	1.504	0.001
86	5.509	16.421	9.229	17.186	2.683	0.272
87	4.213	16.294	8.896	3.918	2.212	-0.140
88	4.581	16.471	9.109	6.732	2.880	0.039
89	4.544	15.854	9.285	6.414	0.933	0.449
90	5.342	16.161	9.310	14.950	1.769	0.546
91	4.358	13.867	9.611	4.940	-1.923	2.396
92	4.805	14.014	10.093	8.810	-1.470	8.074
93	5.119	13.679	10.031	12.206	-2.588	7.159
94	4.577	13.601	9.920	6.698	-2.896	5.643
95	4.903	13.605	9.980	9.817	-2.877	6.439
96	4.317	13.387	9.799	4.636	-3.821	4.212
97	4.856	13.286	10.006	9.326	-4.302	6.807
98	4.232	13.539	9.614	4.048	-3.148	2.418
99	4.438	14.053	9.890	5.551	-1.361	5.269
100	4.782	14.651	10.119	8.582	-0.210	8.469

 Table 4.6
 Samples of Five Different Shift Combinations



Figure 4.2 Continuation of the Major Element Control Charts for Samples 51 to 100

The 50 sample major elements of Figure 4.2 clearly show 5 different out-ofcontrol patterns, one for each kind of shifts in the means. These are summarized in Table 4.7.

Variable	Sample No.				
	51 - 60	61 - 70	71 - 80	81 - 90	91 - 100
X ₁	Downward	Downward	No shift	Upward	Upward
X_2	Downward	No Shift	Downward	Upward	Downward
Χ,	Downward	Upward	Downward	No shift	Upward

Table 4.7Shift Patterns of Samples 51 to 100

4.5 Evaluation of the Major Element Control Charts

For a control chart to be effective in general applications, it should have a high degree of sensitivity to detect small shifts in the process parameter(s) being monitored. In the case of univariate controls, the detection sensitivity depends simply on the amount of common-cause variability in the process. With multivariate controls, however, the factors that can affect such sensitivity are many and become rather complex. The process parameters such as the means and variances of a p-variate process may have widely different values among the p variables. Furthermore, the p!/2!(p-2)! pair-wise correlations may differ a great deal from one another.

For the purpose of evaluating the effectiveness of the proposed major element control charts, a total of 22 simulation runs were generated each with a different set of parameter values, correlations, and sizes of the shifts. Details of the input process parameters and simulated results including all the control charts for sample major elements are listed under each run number in Appendix III.

All the 22 sets of major element control charts in Appendix III are constructed by the parameter estimates using only the data simulated for a trivariate process in control. The various out-of-control patterns exhibited on these charts are summarized below in terms of the effects of process parameter values, shift sizes and correlation structures.

4.5.1 Effects of Correlation Structures

The control charts for sample major elements of a trivariate process in Appendix III are arranged in the order of simulation runs. For each simulation run, there are four sets of three control charts of sample major elements generated according to four different sizes of shift in the means. The control charts are numbered by III-*a.b*, where *a* is the Run # and *b* denotes either one of the two types of correlations. As shown in Table 4.2, there are 11 runs under each type of the correlations. Since the first 10 runs (00, 01, 10, 11, 20, 21, 30, 31, 40 and 41) are samples generated from a process with various correlation structures all having a same set of means and variances, the corresponding control charts for these samples should reveal the correlation effects, if any, on the distributional patterns of out-of-control.

A careful examination of this group of 120 major element control charts does not seem to show any noticeable variations in the out-of-control patterns of the sample major

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elements under different correlation structure. Due to the fact that the value of $\frac{|\mathbf{R}_u|}{|\mathbf{R}|}$ varies greatly under different **R**, however, the numerical scales of the major element control charts vary a great deal with different correlation structures.

4.5.2 Effects of Process Means and Process Standard Deviations

In order to find any possible effects on the out-of-control sample patterns due to varying magnitudes of process means and variances, three different sets of means and variances were simulated each under four representative correlation structures (high and low positive correlations, and high and low negative correlations.) These are identified as Runs 50, 51, 60, 61, 70, 71 80, 81, 90, 91, 100 and 101. Together with the one in the first group having the same correlations (Runs 00, 01, 10 or 11,) any deviations in the out-ofcontrol sample patterns among the four different means and/or variances may be examined. As shown by the simulated control charts of Appendix III, there are no apparent changes in the sample patterns when either or both the process means and variances vary. Also, between the two correlation structures which produce very different scales for the major element control charts, the pair-wise sample patterns of the four sets of process means and/or variances are not distinguishable.

The above analysis through selected simulation data, although limited, seems to show the robustness of the proposed major element control charts in their capability of signaling the root cause(s) of a trivariate process out-of-control.

4.5.3 Effects of The Size of Mean Shifts

Although the patterns of all simulation runs do not seem to change while the process parameters are varied, the size of the shifts in the means does appear to have an effect in the degree of clarity of the out-of-control patterns under all different process correlations and parameters. Among the four different shift sizes (0.25 σ to 1.5 σ) that were simulated, it is obvious that the identification of the sample patterns under various shift combinations become less clear when the size of the shift is as small as 0.25 σ . Since a chart's sensitivity in detecting shifts of a certain size increases as the variance of the sample mean decreases, an increased sample size will improve the sensitivity in the detection of very small shifts.

4.6 Deciding On Sample Sizes and Sampling Frequency

Routine operations of control charts often are constrained by time and costs of sampling. Moreover, smaller samples are more likely to produce the information about one and only one state of the process, whether it be in control or out of control. Therefore, it is desirable to take small samples for process control in practice. Then the question is how small should a sample be to satisfy a reasonable degree of confidence in statistical estimation.

Another concern in sampling design is to determine the frequency of sampling. Samples should be taken more frequently if the process is subject to frequent occurrences of assignable causes and/or critical consequences of delayed detection of those causes. Economically, both the sample size and sampling frequency must be considered together. These practical issues are not discussed further as they are beyond the scope of this research. It is important, however, to analyze the effects of sample size and the number of samples on the statistical properties of the proposed major element control charts during their initial construction. While it is recognized that no exact solutions can be expected, a simulation experiment on a trivariate normal process is presented in this section to help illustrate the effects on chart construction and interpretation by varying the sampling plans. For initial construction of the control charts, the errors between the calculated control limits and their corresponding true values, called bias, are evaluated to provide some basis for the design of sampling plans. The computation program of this simulation experiment is documented in Appendix II.

4.6.1 Estimation Errors of Various Sampling Plans

The total amount of sample data to be used for initial chart construction is the product of the number of samples k and the sample size n. In order to evaluate their effects on the estimation errors of the control limits, the following simulation experiment was conducted.

A trivariate process is characterized by a total of nine parameters that include three means, three variances, and three covariances, the sample size required for their estimations must be greater than 3 and preferably greater than 9. In this experiment, the simulated data of nine different numbers of samples (k=25, 35, 50, 75, 100, 250, 500, 750 and 1000) and four sample sizes (n=6, 8, 10, and 15) were chosen for the analysis. Increasing either the sample size or the number of samples should increase the accuracy of the estimates. It was expected, however, the effects of k may behave differently from those of n.

A full size simulation, consisting of all possible combinations of these two factors, k and n, was conducted at each of the five correlation structures with the same process means and standard deviations as shown in Table 4.8.

Table 4.8 Process Parameters of the Simulation Experiment for the Study of the Effects of Sample Size and Number of Samples

Simultion	E(X)			ultion E(X) Standard Devi				viation	Corre	lation Coe	fficient
Run No.	Χ ₁	X ₂	X ₃	S ₁	Sz	S ₃	Ρ12	ρ ₁₃	ρ ₂₃		
110							0.7	0.9	0.6		
120						Ì	0.2	0.1	0.15		
130	3	15	9	1.6	1.2	0.9	0.3	0.8	0.35		
140							0.85	0.4	0.8		
150							0.95	0.9	0.875		

Twenty-five simulated replications of each run with each sampling plan (k, n)were generated. The sample statistics, calculated from each simulated replicate, were used as estimates of their corresponding process parameters for control limit calculations. All upper control limits have a significance $\alpha = 0.01$. Thus, there are 25 estimates of a control limit for each run with one sampling plan. Since the lower control limit of a major element control chart is obtained by multiplying the upper control limit by -1, only the upper control limits are evaluated in all cases. Corresponding to each set of the 25 estimated or simulated control limit UCL_{sim}, a true control limit, UCL_{true}, is computed according to the process parameters that were used as inputs to generate the replicated data. As a measure of the estimation error of each UCL_{sim} , the following is defined for subsequent analysis.

$$Bias_{\text{Re}\,\rho}(\%) = \frac{|UCL_{true} - UCL_{sim}|}{UCL_{true}} \times 100\%, \text{Rep} = 1, 2, ..., 25.$$

The mean, standard deviation, and range of the 25 $\operatorname{Bias}_{\operatorname{Rep}}(\%)$ of each simulation were calculated and given in Appendix IV. Figure 4.3 and Figure 4.4 summarize the results by plots of the percentage of bias for each of the three major element charts, grouped respectively by sample size (n) and by the number of samples (k). Each plot also contains five lines, each of which represents the changing behavior of the average Bias_{Rep}(%) of a correlation structure.

4.6.2 Effects of the Sample Size (n)

As can be seen from the plots of Figures 4.3, increasing sample size tend to increase the accuracy (smaller Bias) of the control limit estimates. When the sample size is equal to 6, the accuracy gradually improves as the number of samples is increased. However, the rate of improvement varies quite a lot among the different structures of correlation. For sample sizes of 8 and 10, the rates of improvement are very comparable and less influenced by the correlations. In most cases, the percentage of bias is reduced to less than 2% with 50 samples or more. When the sample size is increased to 15, even with very small number of samples at 25, the bias error is 3% or less. It is interesting to observe that the bias is uniformly small for data of Run 120 even with small k. This is

the case where the three variables are only slightly correlated ($\rho_{12} = 0.2$, $\rho_{13} = 0.1$, $\rho_{23} = 0.15$). Thus, a much larger number of samples and/or large sample sizes are needed for more accurate control limit estimations when the variables are highly correlated.

4.6.3 Effect of the Number of Samples (k)

Comparing with the effects of sample sizes, the plots of Figure 4.4 show that the number of samples has relatively minimal effect on the estimation errors when it is greater than 50. In most cases, with relatively larger sample sizes, 35 samples may be sufficient for practical applications. However, even when 1000 samples are used to construct the control charts, the bias is still about 1% in most cases.



Figure 4.3 Average of Bias_{Rep} (%) Grouped by Sample Size (n)



4.7 Summary of Simulation Results

Through simulated sample data of a trivariate process with various parameters, this chapter has demonstrated the construction of the control charts for sample major elements for practical multivariate process control. More important, the analysis of many simulated control charts for sample major elements does confirm the existence of unique distributional patterns of all 26 types of out-of-control, as expected from the methodology developed in Chapter 3.

The similarity in the sample patterns of the wide range of simulation runs can be seen on all the major element control charts. However, for processes subject to very small shifts, e.g. 0.25σ , a much larger sample size, say 15, may be needed in order to improve the clarity of the sample distributional patterns for more speedy identification.

Overall, the major element control charts have been demonstrated to be effective in the detection of every possible combination of the shifts in means.

For most applications, it may be adequate to have about 50 samples of size 10 as initial data base to establish the three control charts for a trivariate process. When the number of correlated variables increases, a larger sample size and perhaps more samples are needed for adequate chart constructions. It is suggested that a preliminary simulation analysis similar to the ones described in this chapter may be conducted to find the appropriate sampling plan for each special situation. More on the questions about sample size and the number of samples will be discussed in Chapter 6.

Chapter 5

COMPARATIVE STUDY OF VARIOUS CONTROL CHARTS

The control charts for sample major elements have been developed with the objective to improve the effectiveness and information content for statistical control of the means of a multivariate Gaussian process. It has been demonstrated in Chapters 3 and 4 that the proposed sample major elements are efficient, effective and informative statistics capable of representing or reflecting each and every one of the 3^p-1 states of a *p*-variate normal process. It is, therefore, interesting to make some comparative analysis between the major element control charts and some of the other multivariate control charts developed in recent years. This chapter presents a summarized report on such a comparative study using simulated data.

As reviewed in Chapter 2, several alternative multivariate control charts have been introduced during this decade. Three of these control charts were selected for the comparative study. These are: the multivariate profile control charts (Fuch et al, 1994); the regression adjusted control charts (Hawkins, 1993); and the principal component control charts (Chang, 1991). Common to all of these control charts, including the major element control charts, is the idea of using independent sample statistics for charting. The methods that are employed for producing independent sample information of each variable, however, are quite different. The independent principal components are obtained by rotating a correlated p-dimensional space into p orthogonal coordinates. The regression-adjusted variables are the results of adjusting each of the p variables for its associated covariates. The

multivariate profile consists of p individual bar plots of the standardized normal deviates that are examined for out-of-controls only when the corresponding T^2 goes out of control. The sample major elements are only certain selected elements of a T^2 as discussed in Chapter 3. Since transformation and adjustment are likely to lose or alter some of the covariation in each sample, none of the above methods could be expected to be perfect for multivariate control. It is, therefore, their relative merits and shortcomings that are important to evaluate for applications. The following comparative analysis was conducted to do just that.

For this study, the simulated data sets of Run #00 and Run #10 with the process parameter values listed in Table 5.1 are used. As can be seen from Table 5.1, the two trivariate processes selected for the simulation study have very different correlation structures, high and low. These were selected for the purpose of ascertaining any correlation effects on the respective merits of each type of the control charts. According to each of the four methods, the required sample statistics were calculated and charted for comparison analysis. Each data set includes 26 combinations of shifts in the means. The control charts by each method are examined for (1) the uniqueness and clarity of out-of-control sample patterns and (2) the agreement (or departures) between the unique sample patterns, if exist, and the expected patterns from theory for each of the 26 possible out-of-control states.

Table 5. 1Process Parameters for Simulation Run 00 and Run 10

μ_l	σι		R _{Run 00}			R _{Run 10}	
3	1.6	1	0.7	0.9	1	0.2	0.1
15	1.2	0.7	1	0.6	0.2	1	0.15
9	0.9	0.9	0.6	1	0.1	0.15	1

This chapter is organized as follows. Section 5.1 summarizes the simulated data sets by the sample estimates of the process means, process standard deviations and covariances and process correlation coefficients. The computation and plotting of the sample statistics and control limits for the T^2 chart and for each type of the control charts are presented Section 5.2. The last section presents some of the important findings from the simulated comparative study of the four types of multivariate control charts.

5.1 Summarized Information of The Simulated Data

For the estimation of process parameters and the construction of control charts, it is essential to use only the data collected from a process in-control. As described earlier in Chapter 4, Case #14 of each simulation run represents the process in control. The 50 samples of size 10 in Case #14 of each simulation run are used as the initial database for the calculation of all needed parameter estimates. By Eqs. 4.5 to 4.7, the results are listed in Table 5.2 and Table 5.3 for Run #00 and Run #10 respectively.

l	$\overline{\overline{x}}_{l}$	S _l		R			S	
1	3.03	1.49	1	0.65	0.89	2.22	1.16	1.14
2	15.01	1.20	0.65	1	0.53	1.16	1.43	0.55
3	8.99	0.86	0.89	0.53	1	1.14	0.55	0.75

 Table 5.2
 Estimated Process Parameters for Run 00

Table 5.3 Estimated Process Parameters for Run 10

l	$\overline{\overline{\mathbf{x}}}_{l}$	S _l		R			S	
1	2.94	1.54	1	0.26	0.09	2.37	0.47	0.12
2	15.00	1.18	0.26	1	0.23	0.47	1.40	0.24
3	8.99	0.88	0.09	0.23	1	0.12	0.24	0.78

5.2 Simulated Control Charts of Four Multivariate Methods

Since T^2 control charts is of such a basic interest and importance and for use together with the multivariate profile charts, two T^2 control charts, one for each simulation run, are shown in Figure 5.1. In the remainder of this section, all the calculation of the sample statistics and control limits are presented for each of the four multivariate control methods. Accordingly, a set of three control charts following each of the four methods,

- 1. Multivariate Profile Control Charts
- 2. Principal Component Control Charts
- 3. Regression-Adjusted Control Charts
- 4. Major Element Control Charts

are plotted for each simulation run as shown in Figures 5.2, 5.3, 5,4 and 5.5.

5.2.1 T^2 Control Chart

To compute sample T^2 statistics, inverses of process variance-covariance matrices for Run #00 and Run #10 are obtained by using Eq. 3.9 and listed as:

$$\mathbf{S}_{Run\,00}^{-1} = \begin{bmatrix} s^{11} & s^{12} & s^{13} \\ s^{12} & s^{22} & s^{23} \\ s^{13} & s^{23} & s^{33} \end{bmatrix} = \begin{bmatrix} 2.67 & -0.84 & -3.45 \\ -0.84 & 1.24 & 0.37 \\ -3.45 & 0.37 & 6.34 \end{bmatrix}, \text{ and}$$

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$$S_{Run\,10}^{-1} = \begin{bmatrix} -0.67 & 0.39 & -0.52 \\ 0.39 & -0.85 & -0.10 \\ -0.40 & 0.34 & -0.85 \end{bmatrix}$$

With process means, $\overline{\overline{X}}$, and S^{-1} of both simulation runs, the T^2 value of each sample is computed by

$$T^{2} = n\left(\overline{\mathbf{X}} - \overline{\overline{\mathbf{X}}}\right)^{T} \mathbf{S}^{-1}\left(\overline{\mathbf{X}} - \overline{\overline{\mathbf{X}}}\right).$$

The upper control limits of Runs #00 and #10 at $\alpha = 0.3\%$ are:

$$UCL = \frac{p(k+1)(n-1)}{kn-k-p+1} F_{\alpha, p, kn-k-p+1}$$
$$= \frac{3(50+1)(10-1)}{50 \times 10 - 50 - 3 + 1} F_{0,3\%,3,448}$$
$$= 14.481$$

Sample T^2 values and control limits for both simulation runs are plotted in Figure 5.1. From Figure 5.1, the sample T^2 statistics of both simulation runs have shown patterns for the twenty-six simulated out-of-control states. The patterns of Run #00 are much clearer than the patterns presented in Run #10. Correspondingly, the behavior of the patterns is altered when the correlation structure has been changed. Eventually, there are cases simulated as all three process means are shifted upward or downward, the sample T^2 value are around the control limits which indicates the out-of-control signals are very possible to be misidentified. Such as

Cases #1, #4, #11, #17, #24, and #27 in Run 00, and Cases #1, #2, #4, #5, #6, #10, #11, #13, and so on.



Figure 5. 1 T^2 Control Charts for Run 00 and Run 10 with Control Limits at $\alpha = 0.3\%$

5.2.2 Multivariate Profile (MP) Control Charts

To construct multivariate profile chart, first one needs to establish T^2 control chart that was shown in the previous section. Then, compute and plot the standardized normal

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variates, $d_{i,l} = \frac{\overline{X}_{i,l} - m_l}{S_l}$, for each variable with T^2 simultaneously. Here m_l is a target value for the process variables, and it is estimated by $\overline{\overline{X}}_l$.

The sample multivariate profile data are plotted in Figure 5.2 as three individual plots are for each variable. The MP charts indeed are shown clear patterns that agree with twentysix states of shift combinations. Additionally, the patterns are not changed when the process correlation structures are different. However, the patterns can not be very useful if T^2 is not able to correctly signal the out-of-control states.

5.2.3 Principal Component Control Charts

To establish a set of principal component control charts for the standardized variables, the eignenvalues and eigenvectors of correlation matrix must be obtained first. They are listed below for both simulation runs. For simulation Run #00 and #10, the eigenvalues (λ), and eigenvectors (e) are listed below:

$$\lambda_{Run 00} = [\lambda_1 \ \lambda_2 \ \lambda_3] = [2.39 \ 0.51 \ 0.10], \text{ and}$$

$$\mathbf{e}_{Run\,00} = \begin{bmatrix} e_{11} & e_{21} & e_{31} \end{bmatrix} = \begin{bmatrix} -0.62 & 0.23 & 0.75 \\ -0.52 & -0.84 & -0.17 \\ -0.59 & 0.49 & -0.64 \end{bmatrix}.$$

$$\mathbf{e}_{Run\,10} = \begin{bmatrix} 0.55 & 0.65 & -0.52 \\ 0.66 & 0.04 & 0.72 \\ 0.51 & -0.76 & -0.41 \end{bmatrix}$$

The independent sample principal components $Y_{i,i}$ for standardized variables $Z_{i,i}$ are obtained through the following equation,

$$Y_{i,l} = e_{i,l} Z_{i,1} + e_{i,2} Z_{i,2} + e_{i,3} Z_{i,3}.$$

Principal components, Y_{iJ} , are plotted in Figure 5.3. The principal component plots are displaying the patterns in both simulation Run #00 and Run #10. However, the patterns for both simulation runs are not identical, which means the uniqueness of the distributional pattern for principal components does not exist between two different correlation structures. Further, the patterns do not directly correspond to the shift combinations. To interpret the nature of mean shifts according to the pattern becomes very difficult, especially as the number of variables increases.

5.2.4 Regression-Adjusted Control Charts

To apply the standardized data on the regression-adjustment procedure, Eq. 2.3 has to be rewritten as following:

$$H = \operatorname{diag}\left[\operatorname{diag}\left(\mathbf{R}^{-1}\right)\right]^{-1/2}\mathbf{R}^{-1}\mathbf{Z},$$

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where Z is the standardized sample data of X, R^{-1} is the inverse of the sample correlation matrix. The R^{-1} of both the simulation runs are computed and listed as follows:

For the simulation Run 00,

$$R_{Run\,00}^{-1} = \begin{bmatrix} 5.92 & -1.50 & -4.45 \\ -1.50 & 1.77 & 0.38 \\ -4.45 & 0.38 & 4.74 \end{bmatrix}, \text{ and}$$

Simulation Run 10,

$$R_{Rum10}^{-1} = \begin{bmatrix} 1.07 & -0.27 & -0.03 \\ -0.27 & 1.12 & -0.23 \\ -0.03 & -0.23 & 1.06 \end{bmatrix}$$

Hawkins (1991) in his research suggested to plot the regression adjusted data by either traditional Shewhart control charts or CuSum control charts. In this study, the regression-adjusted data, H_1 , where l = 1, 2, 3, are plotted as three individual charts without any further transformation by CuSum procedure. These three charts are shown in Figure 5.4. The regression-adjusted sample statistics are presenting clear patterns in both Run #00 and #10. Nevertheless, only the patterns in Run #10 agree with the 26 out-of-control states. In Figure 5.4, H_1 of Run #10 indicates variable x_1 shifted down from case #1 to #9, no shift from case #10 to #18, and shift upward between case #19 to #27. Similar interpretation can be concluded on both variable x_2 and x_3 . Unfortunately, the patterns in Run #00 do not

correspond to the expected out-of-control states. Based upon the observations, it can be conclude the patterns of sample regression-adjusted variable are not unique at least when the correlation structure is different between two processes.

5.2.5 Major Element Control Charts

The computational procedure and the interpretation of the major element control charts have been illustrated in detail in Chapter 4. Figure 5.5 displays the major element control charts for both simulation runs. The sample major elements of both runs have shown the unique directional patterns for all twenty-six out-of-control states. In addition, each pattern of the three process means can be interpreted as the direction of the simulated shift in process means.

5.3 Conclusions

 T^2 control charts can effectively signal most of the out-of-control states, however, it is very sensitive to the process correlation coefficient structure change. Sample T^2 statistics for each process have shown its own distributional patterns with respect to the corresponding shifts in process means. That is, different correlation structure shows different pattern, indicating that the pattern is not unique. Surprisingly even with one standard deviation, T^2 becomes very insensitive when the process variables are with correlation structures.

Multivariate Profile charts are established based the signals from T^2 control chart. Therefore, it automatically loses its power to reveal the nature of the process mean shifts if the out-of-control status is not reflected by T^2 . Although patterns of MP sample data agree with the corresponding the 26 out-of-control states, the patterns will become unclear when the changes in process means are small.

Use the principal component analysis and regression adjustment to transform multivariate sample data that have shown the relatively similar results. Such that both of the control charts are shown some patterns, however, the patterns are not unique to each of the out-of-control states and do not agree with the simulated shift combinations

The three major element control charts for three variables displays twenty-six unique patterns that are free of the change in the process correlation structures. Furthermore, the patterns are directly corresponding to each combination of the process mean shifts. Therefore, we can conclude that the major element control charts overcome several deficiencies unlike the other multivariate control charts that include the classical T² control charts. It is also really easy and simple to apply. The shortcoming of the major element control chart as discussed in Chapter 4, is that the patterns will become less clear when the size of change in process means get smaller. The following chapters presents practical application procedure, and discusses how the major element control charts can be used more efficiently and effectively.

In this study, the trivariate process sample data of two simulation runs are used to construct four types of multivariate control charts. The results of comparative analysis have shown that only the multivariate profile control charts and the major element control charts have show their sample statistics consist of unique patterns for each of 26 out-of-control states. The other multivariate control charts including the T^2 control charts have shown the patterns, however, the patterns are not unique to the out-of-control state when the correlation structures of the both processes are different from each other. To further verify these findings, it is necessary to apply more runs of simulated data with different combinations of process parameters (e.g. positive correlation vs. negative correlation structure) to show whether the correlation structure is the only factor to affect the clarity and uniqueness of the patterns of the sample statistics.



Figure 5. 2 Multivariate Profile Data Plots for Run 00 and Run 10



Figure 5. 3 Principal Components Control Charts for Run 00 and Run 10





Figure 5. 5 Major Element Control Charts for Run 00 and Run 10

Chapter 6

A PROCEDURE FOR PRACTICAL APPLICATIONS

A set of multivariate control charts, named major element control charts, is now available to monitor the changes in process means. There are two fundamental functions that the major element control charts can usually provide.

- To detect an out-of-control state, and identify the variable among those correlated variables that caused the changes in the process means.
- To provide information about the direction of the changes in the process means.

In order to establish control charts for the major elements, it is desirable to follow a set procedure. A five-phase procedure is outlined to appropriately set up the major element control charts and successfully serve their fundamental functions. Phases of the procedure includes:

- Define the process,
- Collect the data,
- Analyze the data,
- Interpret and identify out-of-control signals, and
- Formulate, implement, and follow up corrective actions.

An overview of the procedure is presented in the succeeding section. Each phase of the procedure will be reviewed, however, some of the important issues will be further discussed in detail the remainder of this chapter.

6.1 Overview

Define the process

The process must be understood in terms of its relationship to other operations and users both upstream and down stream, and in terms of the process elements (people, equipment, material, measurement, method, and environment) that affect it at each stage. To achieve the best understandings of the process, the following questions need to be answered while any techniques are applied to analyze the process. (AIAG, 1992) The questions are:

- 1. What should the process be doing?
- 2. What can go wrong?
- 3. What is the process doing?

Many techniques such as the histogram, the cause-and-effect diagram, and the process flow diagram help answer these questions. Furthermore, they can make the relationships among the process elements visible and allow the pooling of experience from people who understand different aspects of the process.
• Collect the Data

There are two important aspects of the data collection procedure. First, the procedure has to decide what quality characteristics to be observed and how to observe them. Then, a sampling procedure need to be planned which is concerned with the selections of sample size, sampling frequency, and number of samples. The details of the sampling procedure will be discussed in detail later in section 6.2.

To determine what quality characteristics should be observed over time, first one should look into the current and potential problem area of a process. Considering existing evidence of waste or poor performance (e.g. scrap, rework, excessive overtime) and area of risk (e.g., upcoming changes to the design of the product, or to any elements of the process). Sometimes, review of the process's history or construct a Failure Mode and Effects Analysis (FMEA) would help to identify the most important quality characteristics.

In many manufacturing environments, there are a large number of variables to make up a process. It is another concern that how many quality characteristics should be observed at the same time. Although a multivariate process control scheme is designed to observe multiple quality characteristics of a process simultaneously, it usually will become very tedious and inefficient as the number of variables gets larger. Therefore, study efforts should be focused on those characteristics that are most promising for process improvement, and can be proved that there is a need to control them simultaneously.

The correlation coefficient among the variables can help a great deal in determining how many variables need to be monitored by the multivariate control charts. Correlation

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coefficient between two quality characteristics is bounded between -1 and +1. If it is extremely high, say 0.95, two variables can be treated as one, or if it is very low, say 0.1, then these two variables should be probably treated as two independent variables. There is no specific range of correlation coefficient for which pairs of variables should be monitored by the multivariate control scheme. Nevertheless, it is a good measure to assess what the multivariate control charts is for two possibly related variables.

• Analyze the Data

The procedure of analyzing data is planned to ensure that the process is in a state of statistical control. The major element control charts are designed to test how the process means change over time. To establish the control limits for the major elements, it is very important to assure variations among the variables are maintained at a constant level. However, the methods of evaluating the dispersion of a multivariate process are very limited as was discussed in Chapter 2. Control charts for Z^* and $\log|S|$ proposed by Chang (1991) are easier to understand and to implement than the other charts. Therefore, to examine the stability of a multivariate process, this research suggests applying control charts for Z^* and $\log|S|$ which is the most complete procedure introduced by Chang (1992) to look over correlation and variance-covariance among variables respectively.

After process variability is examined to be in-control, the sample means of variables have to be investigated with control limits calculated from the process means and process variance-covariance matrix, which are estimated by average of sample means and average of sample variances-covariances. The detailed procedure will be discussed in section 6.3

Interpret and Identify Out-of-control Signals

Once the control limits for the major elements are established, the sample data should be continuously collected from the process and plotted against the control limits. The major element control charts would show the out-of-control signal once the process means are shifted. To detect the out-of-control signals and relate the signal to physical evidence of the process will assist to eliminate assignable causes of the process. In this research, a set of zone rules modified from the univariate case is introduced to enhance the capability of detecting the out-of-control signals while apply the sample major elements control charts. Moreover, a program written in Microsoft Excel is provided to assist user to recognize expected pattern for all kinds of shift in process means. Both of the procedures will be discussed in details in Section 6.4.

Formulate, Implement, and Follow up Corrective Actions

Up to this point, the major element control charts provide the information to identify the special causes, an act on eliminating the causes will be the immediate solution to redeem the problems. However, a cosmetic solution will not result in any real, long-term process improvement. It is very important to find the underlying root causes and formulate the corrective actions to attack the problems. Therefore, an off-line analysis of the major elements should be conducted. Furthermore, developing a serious plan of implementation and follow up of the corrective actions will be an essential component of an effective multivariate statistical process control.

6.2 Sampling Plan for Major Element Control Charts

An essential idea of using control charts is to collect sample data according to what Shewhart called the rational subgroups or samples concept. Generally speaking, it means that samples should be collected from a system whose variation is only subjected to common causes. In other words, the samples should be selected so that if assignable causes are present, the chance for differences between samples will be maximized, while the chance for differences due to these assignable causes within a sample will be minimized. Whether or not the objectives of the rational sample are achieved, they will determine the effectiveness and efficiency of the control charts. Assume that the sample data are collected rationally from a trivariate process. By appropriately selecting the other factors such as the size, frequency, and number of samples would enhance the capability of detecting abnormal shifts in process means while the major element control charts are used.

6.2.1 Selection of Size, Frequency, and Number of Samples

The major element control charts are developed from measurements of a set of particular quality characteristics of a multivariate process output. These data are reported in small number of samples of constant size, usually from 6 to 10 consecutive pieces for a multivariate process that monitors three variables, with samples taken periodically. A data gathering plan must be developed and used as the basis for collecting, recording and plotting the data on the major element control charts.

6.2.1.1 Samples Size

The samples should be chosen such that opportunities for variation among the units within a sample are small. If the variation within a sample represent the piece-to-piece variability over a very short period of time, then any unusual variation between samples would reflect changes in the process that should be investigated for appropriate action.

Based on the studies in Section 4.4, the sample should typically contain 8 to 10 pieces consecutively during the initial study of a trivariate process. Also, produced pieces must represent only a single process. The intention is that the pieces within each sample would all be produced under very similar production conditions over a very short time interval with no other systematic relationship to each other. Further, the sample size must remain constant for all samples while plotting the major element control charts.

6.2.1.2 Number of samples

From a process standpoint, enough samples should be gathered to assure that the major sources of variation have had an opportunity to appear. Determination of the number of samples very often depends on the production rate. Although large number of samples would provide a sufficient amount of data for accurate computation of the control limits, it would delay the use of control charts if the production of samples takes too long to complete. From the simulation study in Chapter 4, a minimum of 35 samples or more containing about 400 or more individual readings of each variable collection gives a good indication of the process's stability. If the process is stable, good estimates of the process location and spread can be obtained.

6.2.1.3 Frequency of Sampling

As with any control charts, the frequency of samples is a function of the production rate, the cost of inspection, the failure rate, and the cost of failures. Yet, the goal of the major element control charts is to detect the changes in the process over time. Samples should be collected often enough, and at appropriate times, that they can reflect the potential opportunities for change. Such potential causes of change could be due to work-shift changes, unskilled operators, warm up trend, or new raw material lots, etc.

During an initial process study, the samples themselves are often taken consecutively or at a short interval, to avoid any factors that can contribute to the instability of the process over a brief period. As the process demonstrates stability (or process improvements are made), the time between samples can be increased. Sample frequencies for ongoing production monitoring could be twice per shift, hourly, or some other feasible rate.

6.2.2 Supplementary Tool - Bootstrap Percentile Control limits for Major Elements

In some practical applications, it is unable for us to follow the sampling plan suggested in the previous section due to the manufacturing conditions. Moreover, the sampling frequencies are limited because of concerns related to the production rate or the inspection cost. The total number of observations is usually limited, or it takes a long time period to collect a suitable size of sample data in the types of production environment described earlier. When the total number of observations is too small, say 150 observations for a trivariate process, it is difficult to obtain good estimates for the process parameters, and to ensure the independence between the consecutive samples. Thus, the control limits can not be appropriately estimated when the two assumptions do not hold. In such a situation the bootstrap percentile method can be used to estimate the control limits for major elements, and the procedure is introduced below.

6.2.2.1 Theoretical Background

The theoretical development of bootstrapping concept was introduced by Efron (1979) to estimate the sampling distribution of a given statistic. There are few advantages for considering the use of bootstrap. First, the bootstrap is a computer intensive resampling procedure that does not require a priori distribution assumption. Second, it was developed to find the distribution of statistic when the distribution is not known. A large body of research on and applications of the bootstrap have accumulated in 1980's and 1990's. Nevertheless, the most important work on the bootstrap applicable to process control is related to the assessment of confidence intervals. Hall (1989) gives a theoretical comparison of the different bootstrap methods that can be used to determine the confidence intervals. Related discussions are given by Efron (1987), Diciccio, and Romano (1988). Efron (1990) proposed a percentile method, with modifications, to obtain estimates of percentile of a sampling distribution. The complete works are documented in Effron and Tibshiranis (1993).

A number of articles discussing the use of the bootstrap with respect to quality have recently been published. Gunter (1991-1992), in a series of papers, discussed Efron's percentile method and considered application of the bootstrap to the assessment of process capability for hole-drilling errors and life test of a compressor. In addition, Franklin and Wasserman (1992) had discussed the use of the bootstrap lower limits on process capability. In 1992, Bajgier first proposed bootstrap approaches for assessing process control limits for a \overline{X} control chart. The Bajgier's approach assumes that the process is stable and in control, when the control limits are assessed. Recently, Seppala et al. (1995) proposed to use within group variance model for estimating process variances instead of using pooled variance estimates in Bajgier's approach when using the bootstrap to assess control limits. Furthermore, Sepala et al. (1995) has extended their applications of percentile bootstrap method to estimate the process control limits for \overline{X} control chart.

Along the development of the bootstrap method with respect to statistical process control, the bootstrap is not much discussed or considered to use for designing multivariate process control charts. Liu and Teng (1996) suggested that perhaps combining the data depth approach (Liu 1990, and Liu and Sigh 1993) and the moving blocks bootstrap method may lead to nonparametric approach for statistical control of dependent multivariate observations.

In the application of the major element control charts, the percentile bootstrap method suggested by Seppala et al. (1995) is adopted to improve estimates of control limits. Via simulation, the comparative effects of control limits estimated by the bootstrap percentile method versus the theoretical control limits are evaluated under the combinations of different level of sample size and number of samples. The application procedures of the bootstrap resampling and percentile control limits for the major elements are discussed in the successive sections.

6.2.2.2 Bootstrap Resampling Algorithm

The general bootstrap resampling algorithm (Efron, 1979) is as follows:

- 1. Initiate an iteration counter i = 1 and set B, a large number (1000-2000).
- Draw a random sample X₁^{*}, X₂^{*},..., X_n^{*} of size n from the initial sample vector X₁, X₂,..., X_n with replacement, and compute the bootstrap value for the statistic of interest, T_i^{*} = T(X₁^{*}, X₂^{*},..., X_n^{*}).
- 3. If i equals B, stop. Other, increment i to i + 1, and repeats step 2.

The bootstrap algorithm needs to be modified to take advantage of variance reduction techniques that are typically used in Monte Carlo simulations. In the general bootstrap resampling procedure, it is assumed that each observation has an equal probability of selection for a bootstrap sample. The bias will occur if there are unequal proportions of these observations in bootstrapped samples. A computer intensive procedure provided by Davison et al. (1986) guarantees equal probability of observations in the pooled bootstrap samples. The procedure, called balanced bootstrap algorithm, is modified by Seppala et al. (1995) for assessing process control limits from a series of k sample vectors of sample size n collected from an in-control process, where N is the total number of observation available for bootstrap sampling, is described as follows:

- 1. Obtain the resample size, B, by finding an integer, A, such that $B = Ak \ge 1000$ (minimum number of resamples required to obtain accurate percentile estimates).
- Replicate the original N observation vectors A times for a total of Bn observation vectors (note that balance is achieved since each observation vector occurs A times).

- 3. Randomly permute the AN observation vectors.
- Obtain n consecutive observation vectors with replacement B times from AN permuted observation vectors, B sample vectors will be drawn at the end of resampling.
- 5. For each bootstrap sample, compute the statistic of interest T_i^* , i = 1, 2, ..., B. For the application of the major element control charts, the interest T_i^* is the sample major elements.

6.2.2.3 Percentile Control Limits

After bootstrap resampling for B times, we will obtain B statistics of interest results, T_i^* . The non-parametric percentile will be used to estimate the control limits at α level. To estimate accurately, the interpolation will be used to determine the percentile control limits. Let $y(1), y(2), \ldots, y(m)$ be a set of ordered statistics for a set of *m* observations. Further, let *j* be the greatest integer that is less than or equal to (m+1)p to find the *q* value for *p* percentile. Then,

$$q_{p} = \begin{cases} y(j) + ((m+1)p - j)(y(j+1) - y(j)) & \text{if } 1 < j < m \\ y(1) & \text{if } j \le 1 \\ y(m) & \text{if } j \ge m \end{cases}$$

Thus, to find control limits, we calculate the interpolated $\alpha/2$ and $(1-\alpha/2)$ percentiles using the *m* ordered observations of the bootstrap estimate of the sampling distribution of $T(X_1, X_2, ..., X_n)$.

6.2.2.4 Simulation Results and Conclusions

This research has designed a plan of simulation to study the best resample size when the number of sample observations of an in-control trivariate process is limited between 150 and 400. The observations can be regrouped with the sample size equals to 6 and 8, and the number of samples is at 25 and 50 levels in each case. The resample size, B, used to run bootstrap resampling is chosen at four levels: 1000, 1500, 2000, and 2500.

Details of this study are presented in Appendix V that include the design and analysis of the simulation study, and the SAS program used to run the Bootstrap Resampling and to compute Percentile Control limits. The following conclusions are drawn based on the simulation results and analyses.

- For the sample size of 6 and 25 samples, 2500 resamples will give the best estimates of the control limits for the major elements which contains the smallest average of bias is between 1.5% and 2.5%, when compared with the theoretical true control limits.
- While the number of observations increased to 400 for 50 samples of size 8, 1000 resample is enough to give the estimates of the major elements control limits with average bias of 3.86%.
- Overall, for the number of samples between 25 and 50 does not make much difference between the percentile control limits and theoretical control limits. We suggest using the larger sample size (e.g. select sample size of 8 instead of sample size of 6) while the number of sample data can be collected is limited. Then, run bootstrap resampling at size between 1000 and 2000. This should give very good estimates of control limits for the major elements.

6.3 Checking Sample Data of the Initial Study

Before the major element control charts can be appropriately constructed, the sample data collected for the initial study must be examined to show the stability of the process. The procedure includes three steps. First, check the correlation coefficients among variables by plotting Z^{**} suggested in Chapter 2 for each sample correlation. Then, examining variance-covariance matrix of each sample by $\log |S|$. Finally, if both correlation and variance-covariance among sample data do not show any abnormal pattern, the control limits for major elements can be calculated. In this case, plot sample major elements to find out whether the process means have changed. When the abnormal pattern of plotted data occurs, it is necessary to identify what causes the problem. Further, make effort to remove the problem, recollect the sample data, and check them again until the stability of the process is assured. In the following section, a trivariate example will be presented to show how the necessary computation should be carried out.

6.3.1 Checking the Correlation among Variables by Z^{**}

For a trivaraite process, there are three plots for three correlation coefficients respectively. First, calculate correlation coefficient matrix of each sample data. Let $r_{i,lm}$ be the i^{th} sample correlation coefficient between variable l and m.

Then,
$$Z_{i,lm} = \frac{1}{2} \log \left(\frac{1 + r_{i,lm}}{1 - r_{i,lm}} \right)$$

where i = 1, 2, ..., k; l, m = 1, 2, 3 for a trivariate process; and $l \neq m$.

$$Z_{i,lm}^{\bullet\bullet} = Z_{i,lm} - \frac{3Z_{i,lm} + r_{i,lm}}{4N} - \frac{23Z_{i,lm} + 33r_{i,lm} - 5r_{i,lm}^3}{96N^2}, N = n - 1$$

where k is the number of samples, and n is the sample size.

Compute the control limits, $\overline{Z_{lm}^{**}} \pm A \sqrt{Var(Z_{lm}^{**})}$, as references to examine the plotting pattern of Z^{**} , where $\overline{Z^{**}}$ is the average and $Var(Z_{lm}^{**})$ is the variance of Z_{lm}^{**} . A is a preselected coefficient, say 3. The data should be randomly distributed as the plots in Figure 6.1.







Figure 6. 1 Z_{lm}^{**} plots for A Trivariate Process

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6.3.2 Checking the Variance-Covariance among Variables with $\log |S|$

To check the variance-covariance of each sample, calculate the determinant of sample variance-covariance matrix first. Let S_i be the variance-covariance matrix of i^{th} sample. Then take log of the determinant of S_i , as $\log |S_i|$. A chart with $100(1 - \alpha)$ % probability control limits is constructed as

$$UCL = \overline{\log|\mathbf{S}|} + Z_{\alpha/2} \left(\sqrt{\operatorname{var}(\log|\mathbf{S}|)} \right)$$
$$CL = \overline{\log|\mathbf{S}|}$$
$$LCL = \overline{\log|\mathbf{S}|} - Z_{\alpha/2} \left(\sqrt{\operatorname{var}(\log|\mathbf{S}|)} \right)$$

where $\log |S|$ is the mean of $\log |S_i|$, $var(\log |S|)$ is the variance of $\log |S_i|$, and $Z_{\alpha/2}$ is $\alpha/2$ percentage point of the standard normal density. The control limits here are only used as references. A set of sample data must not have an abnormal pattern, and it should be randomly distributed as in shown the Figure 6.2.



Covariance

6.3.3 Evaluating Process Means with the Major Element Control Chart

Computational procedure for the major elements had been discussed in a great detail in Chapter 4. This section simply summarizes the equations for calculation of sample major elements and construction of control limits.

$$M_{i,ll} = \left(\overline{X}_{i,l} - \overline{\overline{X}}_{l}\right)^{2} s^{ll}, l = 1, 2, ..., p.$$

 $M_{i,ll}$ is the i^{th} sample major element of variable l.

Let
$$\overline{X}_{i,l} - \overline{\overline{X}}_{l} = \Delta_{i,l}$$
, find $M'_{i,l} = \begin{cases} \frac{\Delta_{i,l}}{|\Delta_{i,l}|} M_{i,ll}, \Delta_{i,l} \neq 0\\ 0 & , \Delta_{i,l} = 0 \end{cases}$

$$UCL_{l} = \left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi^{2}_{1,1-\alpha/2}$$
$$CL_{l} = 0$$
$$LCL_{l} = -\left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi^{2}_{1,1-\alpha/2}$$

where k is the number of samples, and n is the sample size. All other notations are as defined earlier.

In the major element control charts, $M'_{i,l}$ and control limits for each variable are plotted against to each other. For a in-control process, the sample major element should be randomly distributed around the center line which equals to zero. Figure 6.3 is a sets of major element charts with their control limits.



 M'_{2} M'_{2} M'_{2} 0 1 -1 -2 0 10 20 30 40 50



Figure 6. 3 Major Element Charts for an In-control Process

If any abnormal signal shows up in the major element control charts, it should be analyzed and the assignable causes should be identified. Then, act on the special cause to improve the process. Reevaluate the process variability and process means, revise the control limits of major-element control charts.

6.4 Interpretation of Major Element Control charts

As the research attests that an expected pattern will show whenever a shift occurs in the process means. Nevertheless, the shifts must be detected as soon as it occurs in most practical application. Therefore, a set of zone rules modified from the univariate case is developed to enhance the capability of detecting out-of-control signals of the major element control charts. In addition, the expected pattern of major elements can be used as references for both on-line monitoring and off-line analysis. A user-friendly program is developed in Microsoft Excel, which is displayed in section 6.4.2 to assist user to apply the major element control chart.

6.4.1 Zone Rules for Out-of-control Signals Interpretation

Some of the tests in univariate control chart applications are referred as "zone rules" which are developed on the basis of a normal distribution of the sample statistics and their statistical independence. (DeVor et al., 1992) To set up zones for the major element charts to be able to extend the zone rules of \overline{X} control chart appropriately, the probability of each zone must first to be evaluated. Because the sample major element follows an adjusted chi-square distribution with one degree of freedom, and the upper and lower control limits of major elements are mirror image of each other, the zone probability should be calculated using chi-

square distributions. In this section, first we define and calculate the probability of the zones. Then, display examples for each zone rule and compute the risk for applying the zone rule to identify out-of-control signals. However, the zone rules explained in this section are just a theoretical proposal. The rules need to be applied in the practical field and further modified according to the practical situations.



Figure 6. 4 χ_1^2 Probability Distribution Function

6.4.1.1 Probability of Each Zone

The upper control limit for one side chi-square distribution is set at $\alpha = 0.27\%$. For applying the tests, the control chart is divided into three sections between the upper control limit and zero line. Zone C is set from zero line to probability level at 68.27% at which point is mean of the sample major elements. Zone B is from upper boundary of Zone C to probability level at 95.45% and Zone A is from upper boundary of Zone B to the upper control limit. Figure 6.4 displays the probability distribution of a chi-square variable with one degree of freedom along illustrates probability level of the three zones defined earlier.

6.4.1.2 Combined Chi-square Distribution

For the combined chi-squared distribution, we recall that the sample major element,

$$\left(\overline{X}_{i,I} - \overline{\overline{X}}_{I}\right)^{2} S''$$
, is distributed as $\left(\frac{|\mathbf{R}_{I}|}{|\mathbf{R}|}\right) \left(\frac{k-1}{nk}\right)$ times a chi-square variable having 1 degree

of freedom.

Let
$$\upsilon = \chi^2_{1,1-\alpha}$$
, then
 $P(\chi^2_1 \ge \upsilon) = \alpha$. (6.1)

Based on the theory of statistics, $P(\chi_1^2 \ge \upsilon)$ can be written as follows:

$$P(\chi_1^2 \ge \upsilon) = P((\chi_1^2 \ge \upsilon) \cap Z \ge 0) + P((\chi_1^2 \ge \upsilon) \cap Z < 0)$$
$$= P(Z \ge 0 \mid \chi_1^2 \ge \upsilon) \cdot P(\chi_1^2 \ge \upsilon) + P(Z < 0 \mid \chi_1^2 \ge \upsilon) \cdot P(\chi_1^2 \ge \upsilon)$$

Let

$$P(Z \ge 0 \mid \chi_1^2 \ge \upsilon) \cdot P(\chi_1^2 \ge \upsilon) = P(+\chi_1^2 \ge +\upsilon)$$

and,

$$P(Z < 0 \mid \chi_1^2 \ge \upsilon) \cdot P(\chi_1^2 \ge \upsilon) = P(-\chi_1^2 < -\upsilon)$$

Also
$$P(Z \ge 0 \mid \chi_1^2 \ge \upsilon) = P(Z < 0 \mid \chi_1^2 \ge \upsilon) = 0.5,$$
 (6.2)

Apply Eqs. 6. 1 and 6.2,
$$P(+\chi_1^2 \ge +\upsilon) = P(-\chi_1^2 < -\upsilon) = 0.5\alpha$$

The probability and risk of each zone while the sample major element fell in are calculated in Table 6.1 and illustrated in Figure 6.5.

		Chi-Square Distribution		Combined Chi-squared Distribution	
Zone	υ	P(² ¹ < ט)	α	$0.5P(+\chi^2_{1}, v)$ or $0.5P(-\chi^2_{1}, -v)$	$P(+\chi^{2}_{1} > v) \text{ or } P(-\chi^{2}_{1} < -v)$
C	Т	68.27%	31.731%	34.13%	15.87%
В	4	95.45%	4.550%	47.72%	2.28%
A	9	99.73%	0.270%	49.87%	0.13%

Table 6. 1Probability of Three Zones



Figure 6. 5 Probability and Zones for Major Elements Control Chart

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6.4.1.3 Zone Rules

In the previous section, we have established the upper and lower control limits, and the three zones, which will be used to identify the unnatural pattern of a sequence of sample major elements. However, before the presence of special causes can be tested on-line by applying any zone rules, the process has to be brought into a state of statistical control. Therefore, we will discuss the appearance of a process in a good statistical control first. Then, five zone rules based on the simulated data and their usage in major element control chart are summarized with graphic illustrations. These tests will provide the basis for the statistical signals, which indicates to us that the process has undergone a change in its mean level. Nevertheless, each test may as well as contain certain level of probability that provides false alarm while it is applied. Consequently, the risk of each test is calculated along with the illustrations.

Dr. Deming (1993) pointed out in "Out of the Crisis" that the rules have to be made in advance, for use in the future. Further, any rule as a practical matter, must be constructed in the absence of full information about the future. However, the more practical information about unnatural patterns will not only improve the chances of identifying the special cause, but also reduce the probability of false alarms. Afterwards, we like to suggest collecting the process information as much as possible to improve the capability of each zone rule.

Rule 0. Random Pattern

When a process is in control, there occurs a random pattern of variation, which is illustrated by control chart in the Figure 6.6. The sample results are scattered evenly around zero line. Because the sample major element with direction is distributed as the combined chi-

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square distributions, about 50% of all in-process sample results will be randomly distributed above zero line, and the other half will be below the zero line. Further, we expected certain proportion of sample major elements to fall in Zone A and Zone B.



Figure 6. 6 An Example of Major Element Control Chart for In-Control Process

Rule 1. Extreme Points

Rule 1 is applied to identify the extreme points - points beyond the 99.73% control limits. The specific rule is that while the sample result is located beyond Zone A, the risk of misidentification out-of-control signal is 0.27%. Figure 6.7 shows several such the occurrences as by identified this rule, indicating a special cause that may have caused out-of-control signals.



Figure 6.7 Examples of Extreme Points

Rule 2. Two out of three points in Zone A or beyond on one side of the center line.

 $P(+\chi_i^2 > B) = P(-\chi_i^2 < -B) = 2.28\%$

risk₊ = P((1 out of the first 2 points ≥ B) and (3rd ≥ B))
=
$$\binom{2}{1}$$
 (2.28%)²(47.72%) = 0.0496%

Similarly,

risk₋ = P((1 out of the first 2 points ≤ -B) and (3rd ≤ -B))
=
$$\binom{2}{1}$$
 (2.28%)² (47.72%) = 0.0496%

Total risk = $risk_{+} + risk_{-} = 0.0992\%$

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Figure 6.8 Two out Three Points in Zone A or Beyond

If there are two of any three successive sample results in Zone A or beyond, it signals the out-of-control condition of the process. Figure 6.8 presents several possible occurrences of Rule 2. The chance of false alarm is around 0.0992%.

Rule 3. Four out of five points in Zone B or beyond on one side of zero line.

$$P(+\chi_1^2 > C) = P(-\chi_1^2 < -C) = 15.87\%$$

risk₊ = P((3 out of the first 4 points ≥ C) and (5th ≥ C))
=
$$\binom{4}{3}$$
(15.87%)⁴(34.13%) = 0.087%

risk_ = P((3 out of the first 4 points ≤ - C) and (5th ≤ -C))
=
$$\binom{4}{3}$$
(15.87%)⁴(34.13%) = 0.087%



Figure 6.9 Four out of five points in Zone B or Beyond

Four out of five consecutive sample results in Zone B or beyond presents the out-ofcontrol condition. The probability of misidentification the out-of-control signal is about 0.174%. Figure 6.9 presents several examples for Rule 3.

Rule 4. Six out of seven points within Zone C on one side of the zero line.

$$P(C > +\chi_{1}^{2} > 0) = P(0 < -\chi_{1}^{2} < -C) = 34.13\%$$

risk₊ = P((5 out of the first 6 points $\geq C$) and (7th $\geq C$))

$$=\binom{6}{5}(34.13\%)^{5}(15.87\%) = 0.15\%$$

risk₋ = P((5 out of the first 6 points ≤ -C) and (7th ≤ -C))
=
$$\binom{6}{5}$$
(34.13%)⁵(15.87%) = 0.15%

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Figure 6. 10 Six out of Seven Points within Zone C

Six out of seven consecutive points fall within Zone C that indicates the process mean shifted upper or lower. The probability of misidentification of the out-of-control signal is about 0.30%. Figure 6.10 presents several examples for Rule 4.

Rule 5. Eight or More Successive Points run above or below Zero Line

$$P(+\chi_{i}^{2} > 0) = P(-\chi_{i}^{2} < 0) = 50\%$$

 $risk_{+} = P(All 8 \text{ points are on one side of center line})$ = (50%)⁸ = 0.391%

Total risk = $risk_{+} + risk_{-} = 0.391\% \times 2 = 0.782\%$

Rule 5 considers a long run of eight or more sample data strictly either above or below zero line. The presence of such a run indicates that the evidence is strong that the process mean has shifted from the grand mean. Figure 6.11 illustrates the run of eight points that fell above or below the zero line. The risk of this rule is 0.782%.



Figure 6. 11 Eight or More Successive Points above or below the Centerline

6.4.1.4 Probability of False Alarms Using Multiple Rules

The probability of any zone rules applied from above is a risk of false alarm. These zone rules are not all independent or mutually exclusive to each other, nevertheless, the probability of their joint occurrence is relative very small. In practice, one can approximate the total probability of false alarms of all the various zone rules as the sum of their individual risks. The following example illustrates on such estimation.

Suppose only zone rules #1 and #2 are used for the interpretation of an Major Element chart where the center line is set at zero line. Let

 $\alpha_1 = \text{risk}$ for the Zone #1 = 0.0027

 α_2 = risk for the Zone #2 = 0.000992

 $\alpha_{12} = Prob\{(\text{one of the first two} \geq B) \text{ and } (\text{ the } 3^{rd} > UCL)\} = \ 0.000029$

Thus the probability of Type I errors in this occurrence is

 $Risk = 1 - (1 - \alpha_1)(1 - \alpha_2) = 0.00369 = 0.369\%$

6.4.1.5 Probability of False Alarms for Multivariate Process

The zone rule is applied to each major element independently, however, we like to find out the probability that zone rules used in each major element are giving the false alarm. The risk can be calculated as:

Risk = P(at least one major element control chart give false alarm)

$$=1-\prod_{l=1}^{P}\left(1-\alpha_{l}\right),$$

where p is the number of variables, and α_l is the risk of applying any of the zone rule to variable *l*.

6.4.2 Reading the patterns

For the off-line analysis, the expected directional patterns of sample major elements are produced as an aid for user to identify the substantial change in process means. Based on the methodology developed in Chapter 3, Figure 6.12 and 6.13 illustrate the expected directional patterns for each possible combination of shifts in the means for the processes monitoring with three and four variables. In addition, Figures 6.12 and 6.13 are the displays of a Microsoft Excel program that generates all types pattern for different process parameters with different expected size of shifts. To interpret the pattern, follow the signs on top of the chart correspondingly. "+" indicates the process mean of the corresponding variable has shifted upward, "0" indicates there is no shifts in the corresponding process mean, and "-" implies that the shift in the corresponding variable is downward. The magnitude of each stack bar is the average of the shift size.

To use the Excel program to generate expected pattern, simply change the correlation among variables and the expected size of shifts. Note that the pattern will remain the same in each combination of the shifts. Only the size of the stack bars reflecting the change in each of the process means will be varied according to expected value of the directional major elements.



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Chapter 7

SUMMARY, DISCUSSIONS AND RECOMMENDATIONS

7.1 Summary and Discussions

The control charts for major elements, developed in this research, have shown to be not only effective, but also informative for the control of multivariate normal process means. These charts are effective because they are highly sensitive to any one or more shifts in the means. They are informative because each chart is capable of independently displaying a unique out-of-control pattern of the sample major elements that are associated with only the shifted variable in question. These results were shown by the theoretical expectations of the sample statistics and by the analysis of simulated sample data of processes with various out-of-control scenarios. Also by simulation, the sample major elements were demonstrated to be robust to a wide spectrum of variancecovariance structures. By comparison, for example, the sensitivity of the T^2 statistic was shown to depend on the levels of correlation among the variables.

For actual applications, a step-by-step procedure was recommended for the set-up and interpretation of the major element control charts. Issues related to sampling strategy, including the use of bootstrap sampling for better parameter estimation when sample database is limited during initial chart construction, were discussed with some suggestions. To aid in routine chart interpretation, a set of zone rules similar to those used in reading \overline{X} charts was developed for the analysis of each of the major element charts.

The proposed method calls for constructing and/or maintaining a set of p sample major element control charts, one for each of the p variates. To plot the control charts, the p sample major elements and their control limits are computed for each sample i by the following equations.

$$M_{i,J}' = \begin{cases} \frac{\Delta_{i,J}}{|\Delta_{i,J}|} M_{i,JI}, \Delta_{i,J} \neq 0\\ 0, \Delta_{i,J} = 0 \end{cases}$$

 $M'_{i,l}$ is the i^{th} directional sample major element of variable l, where $\Delta_{i,l} = \overline{X}_{i,l} - \overline{\overline{X}}_{l}$ and $M_{i,ll} = (\overline{X}_{i,l} - \overline{\overline{X}}_{l})^2 s^{ll}$, l = 1, 2, ..., p.

Control limits at an α level for the major element control charts are:

$$UCL_{l} = \left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi^{2}_{1,1-\alpha/2}$$
$$CL_{l} = 0$$
$$LCL_{l} = -\left(\frac{|R_{ll}|}{|R|}\right) \left(\frac{k-1}{nk}\right) \chi^{2}_{1,1-\alpha/2}$$

where k is the number of samples, and n is the sample size.

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To illustrate the application of sample major elements that are derived from the quadratic form, Q, of a multivariate normal distribution, eighty-eight simulated data sets with replicates of a trivariate normal process were analyzed in detail. The control charts of sample major elements for all cases did show clearly recognizable directional patterns for all twenty-six mean shift combinations of a trivariate normal process with many different means, variances and correlations. These sample distributional patterns were found to be in agreement with the corresponding patterns expected from theory. According to the simulation results, fifty samples of size 10 should be collected before control limits are calculated to assure a reasonable reliability in parameter estimation.

Since the proposed control charts assume that the variance-covariance structure remains in statistical control, it is essential to have each sample checked for stability of both the variances and the covariances or correlations. Two additional control charts, one for the sample variances and the other for the sample correlations were presented as a possible supplementary procedure to the construction and operation of the major element control charts. It is noted, however, these supplementary charts are not capable of making diagnostic analyses of the specific nature of out-of-controls in variances and correlations.

Lastly, one major limitation of the sample major element control charts is that they are not applicable for those processes where samples of a size greater than one can not be taken meaningfully for statistical control.

7.2 Recommendations for Future Research

Although recent work in multivariate process control has aimed mostly at improving the control charts' effectiveness for practical applications, the actual use of multivariate control still remains very sporadic at best. One possible major reason of this seemingly lack of interest could be that few practitioners, including engineers, really think of multiple variables as a set with correlations. Another important reason might be due to the general shortage of success stories with multivariate control charts. A third one that is more directly relevant to this research is that these newer control charts have become either more complicated or more difficult statistically for typical process and quality engineers. The proposed major element control charts appear to be more user friendly both in their constructions and interpretations. To further develop methodological and operational improvements in multivariate process control, some areas for future research are suggested below from both the practical and theoretical perspectives.

7.2.1 Practical Applications

Since the three reasons mentioned above are themselves inter-related, or correlated, a "multivariate" approach is needed for future research in multivariate process control. It is, therefore, suggested that research in this area must involve heavily, if not exclusively, the practicing engineers, with the statisticians serve more as advisors rather than the sole players.

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Nearly all the known methods of multivariate process control either assume, explicitly or implicitly, a constant variance-covariance structure; or allow changes/shifts in all process parameters to occur without specific identifications. In the latter case the chart(s), similar to the T^2 chart, are designed only to display a shift without regard to its nature. In either case, a better understanding of the inter-relationships of or the mutual effects between the mean vector and the covariance matrix will enhance the effectiveness of these charts in practice. Such fundamental understandings about, for instance, the physical meanings of a covariance change, are needed in order to improve the design and operation of multivariate control charts for variances and/or covariances. Another question of practical importance is how physically a change in the mean(s) will or will not affect a change in one or more of the variances and covariances, and vice versa.

7.2.2 Theoretical Development

Some areas for future research from a more theoretical perspective are suggested as follows.

 One immediate research topic to follow is in the development of an exact or approximate probability distribution for each of the minor elements. Such could enable one to utilize the complete sample information for more detail analysis of outof-control signals because of possible shifts in other process parameters in addition to the means.

- 2. The zone rules proposed for the interpretation of the major element control charts may be further improved, perhaps with experiences from actual field applications. While it is desirable to minimize the probability of false alarms, the corresponding probability of Type II errors should be considered in the design of the zone rules. Furthermore, the zone rules may be programmed for on-line, computer control and diagnosis.
- 3. To improve the sensitivity in detecting very small shifts in the means, while keeping the sample size from becoming too large, alternative statistics such as the CuSum and EWMA of sample major elements may be investigated for their advantages and disadvantages.
- 4. The variances and covariances of a process are subject to change either by themselves or by shifts in the means. Further research is needed in the development of schemes for overall controls that are more effective and/or more informative than the use of a generalized variance recommended in this research. As mentioned in (1) above, the statistical properties of sample minor elements may be studied for possible applications.
- 5. Performance evaluation of the major element control charts should be conducted in actual applications. The actual sample data may be used also for comparative analysis between the major element and other well-known multivariate control charts. One commonly used measure for the speed of signaling a process change is the Average Run Length (ARL). Some theoretical work is needed for the calculation of the ARLs

of sample major element (and possibly also sample minor elements) both when the process is in control and is out of control.

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Appendix I. SAS Program for Data Simulation and Sample Major Elements Computation

•

```
Title "Trivariate Data Simulation, Sample Major Element and Control
      Limits Computation"
proc iml;
                               /* data generator */
start data;
/* Basic Information */
do p1=1 to 1350;
                               /* Sample Index */
in=j(n,1,p1);
s no=s no//in;
end;
                               /* Size of Observations */
size=k*n;
c=cinv(alp,1);
                               /* Chi-square Value at Alpha level */
                               /* Variance Covariance Matrix /
siq=s*r*s;
                               /* Cheloski Factorization */
l=half(sig);
/* True Upper Control Limits */
dR=det(r); dR11=det(r[2:3,2:3]);dR1=dR11/dR;
dR22=det(r[{1 3}, {1 3}]);dR2=dR22/dR;
dR33=det(r[1:2,1:2]); dR3=dR33/dR;
M1 E=((k-1)/(n*k))*dR1*c;
M2^{E} = ((k-1)/(n^{k}))^{d}R2^{c};
M3 E=((k-1)/(n*k))*dR3*c;
/* Observations Generation, X~N(0,I)
                                        */
do k1=-1 to 1 by 1;
      do k2=-1 to 1 by 1;
            do k3=-1 to 1 by 1;
            xl=(normal(repeat(p,1,size)));
            x2=(normal(repeat(p+3256,1,size)));
            x3=(normal(repeat(p+103256,1,size)));
            x=x1/(x2)/(x3;
            Yt=t(1) *x;
      u1=mu1+k1*a*s[1,1];u2=mu2+k2*a*s[2,2];u3=mu3+k3*a*s[3,3];
            y1=yt[1,1:size]+repeat(u1,1,size);
            y2=yt[2,1:size]+repeat(u2,1,size);
            y3=yt[3,1:size]+repeat(u3,1,size);
            y=y1//y2//y3; z1=t(y);z=z//z1;
            end:
      end;
end;
/* Sample Covariance */
      do j=1 to k;
            v=n*(j-1)+6501; m=n*j+6500; xj=z[v:m,];
            sum=xj[+,];
            xpx=t(xj)*xj-t(sum)*sum/n;
            Sp=diag(1/sqrt(vecdiag(xpx)));
            corr=Sp*xpx*Sp;
            mean=sum/n;
            xj=xj-repeat(mean,n,1);
            ss=xj[##,];
            std=diag(sqrt(ss/(n-1)));
            covar=std*corr*std;
            cov=cov+covar;
            meanS=meanS+mean;
      end;
```

```
/* Average Sample Variance-Covariance */
      sigma=cov/k; isig=inv(sigma);
      isiql=isiq[1,1];isiq2=isiq[2,2];isiq3=isiq[3,3];
      meanX=meanS/k;
      var=vecdiag(sigma);
      v=diag(1/sqrt(vecdiag(sigma)));
      cor base=v*sigma*v;
      R=det(cor base);
      R11=det(cor base[2:3,2:3]); R1=R11/R;
      R22=det(cor_base[{1 3}, {1 3}]); R2=R22/R;
      R33=det(cor base[1:2,1:2]); R3=R33/R;
      M1 ucl=((k-1)/(k*n))*R1*c;
      M2^{ucl} = ((k-1)/(k*n)) * R2*c;
      M3 ucl=((k-1)/(k*n))*R3*c;
      Mi=M1 E||M1 ucl||M2 E||M2 ucl||M3 E||M3 ucl;
      print meanX; print cor base sigma isig;
      print Mi;
do l=1 to 1350;
      v1=n*(1-1)+1; mk=n*1; xi=z[v1:mk,];
      meani=xi[+,]/n;
      md=meani-meanX;
      ml=md[1,1]; m2=md[1,2]; m3=md[1,3];
      ml1=abs(ml)*ml*isigl;
      m22=abs(m2)*m2*isiq2;
      m33=abs(m3)*m3*isig3;
      mai=m11||m22||m33;
      mdi=mdi//mai;
end;
/* Output Directional Sample Major Elements */
filename tri 3 'md0025';
file tri 3;
do i=1 to 1350;
M1E=mdi[i,1];M2E=mdi[i,2];M3E=mdi[i,3];
put M1E 10.5 +1 M2E 10.5 +1 M3E 10.5 +1 i 4.0;
end;
closefile tri 3;
finish;
/* Input Information */
r={1 0.7 0.9,
   0.7 1 0.6,
   0.9 \ 0.6 \ 1\};
s={1.6 0 0,
   0 1.2 0,
   0 \ 0 \ 0.9;
k=50; n=10;
cov = \{0 \ 0 \ 0,
     000,
     0 \ 0 \ 0};
meanS = \{0 \ 0 \ 0\};
alp=0.9973; rep=25;
mu1=3; mu2=15; mu3=9;
a=0.25;p=125;
run data;
```

Appendix II. Tables of Input Process Parameters and Simulated Process Parameters for 22 Simulation Runs

		·····		Run: 00					Run: 01		
		All	Positive C	orrelation	Coefficier	nts	Two Neg	ative and On	e Positive Co	orrelation Coe	efficients
ຽ		μ	σ		ρ		μ	σ		ρ	
put	Shift Size for	3	1.6	1	0.7	0.9	3	1,6	1	-0.7	0.9
lul arar	Simulation	15	1.2	0.7	1	0.6	15	1.2	-0.7	1	-0,6
		9	0.9	0.9	0.6	1	9	0.9	0.9	-0.6	1
		$\overline{\overline{X}}_{i}$	S _{-x}		R		$\overline{\overline{X}}_{i}$	S _x		R	
	+/- 0.25σ	2.9960	1.6520	1	0.6885	0.9109	3.0767	1,5635	1	-0.7476	0,9017
		15.0597	1.2288	0.6885	1	0.5819	14,9506	1.1678	-0.7476	1	-0.6311
		8.9949	0.9370	0.9109	0.5819	1	9.0390	0.89907	0.9017	-0.6311	1
		$\overline{\overline{X}}_{t}$	S _x		R		$\overline{\overline{X}}_{i}$	S _r		R	
ι N	+/- 0.5σ	3.0615	1.5635	1	0.7081	0,8881	3.0325	1.6125	1	-0.6842	0.9070
esult		15.0482	1.1678	0.7081	1	0.5973	15.0274	1,2130	-0,6842	1	-0.5804
L L		9.0316	0.8991	0.8881	0.5973	1	9.0254	0.8832	0.9070	-0.5804	1
latic		$\overline{\overline{X}}_{l}$	<i>S</i> - <u></u> ,		R		$\overline{\overline{X}}_{i}$	S _ī		R	
Sim	+/- 1.0σ	3.0280	1.6629	1	0.7091	0.9101	3.1069	1.5907	1	-0.6916	0.9046
		15.0380	1.2000	0.7091	1	0.6263	14.9316	1.2207	-0.6916	1	-0.5783
		9.0350	0.9579	0.9101	0.6263	1	9.0313	0.8871	0,9046	-0.5783	1
		$\overline{\overline{X}}_{i}$	$S_{\overline{x}}$		R		$\overline{\overline{X}}_{i}$	S _x		R	
	+/- 1.5σ	3.0369	1.5428	1	0.7098	0.8949	2,9892	1.5940	1	-0.7077	0.8909
		14.9921	1.1691	0.7098	1	0.6160	15.0586	1.1978	-0.7077	1	-0.6169
		9.0057	0.8975	0.8949	0.6160	1	8,9697	0.8903	0,8909	-0.6169	1

Table II.1: Input Process Parameters and Simulated Process Parameters for Run 00 & 01

		· · · · · · · · · · · · · · · · · · ·		Run: 10					Run: 11		
·		All	Positive C	orrelation	Coefficier	nts	Two Neg	gative and On	e Positive Co	orrelation Coe	efficients
ស		μ	σ		ρ		μ	σ		ρ	
nete	Shift Size for	3	1.6	1	0,2	0,1	3	1.6	1	-0,2	0.1
	Simulation	15	1.2	0.2	1	0.15	15	1.2	-0.2	1	-0,15
Ľ.		9	0.9	0.1	0.15	_1	9	0.9	0.1	-0.15	1
		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{t}$	S _x		R	
	+/- 0 25σ	2,9582	1.5522	1	0.1917	0.1740	3.0024	1.6707	1	-0.1803	0.0031
		15,1146	1.1759	0.1917	1	0.1346	15.0096	1,1416	-0.1803	1	-0.1662
		9,0363	0.9018	0.1740	0.1346	1	8.9445	0.89764	0.0031	-0.1662	1
		$\overline{\overline{X}}_{i}$	<i>S</i> - <i>x</i>		R		$\overline{\overline{X}}_{l}$	<i>S</i> - <u></u> <i>x</i>		R	_
S	+/- 0.5g	3.0580	1.6707	1	0.2826	0.0315	2.9793	1.5925	1	-0.1401	0.1434
esult		14.8847	1,1416	0.2826	1	0.1350	15.0258	1.2000	-0,1401	1	-0.1660
n Re		8.9852	0.8976	0.0315	0.1350	1	8.9978	0.9286	0.1434	-0.1660	1
llatic		$\overline{\overline{X}}_{i}$	<i>S</i> - <i>x</i>	_	R		$\overline{\overline{X}}_{I}$	S ₋		R	
Simu	+/- 1.0σ	3.0156	1.5957	1	0.2090	0.0417	3.0049	1.6309	1	-0.1592	0.1684
		14.9505	1.1648	0.2090	1	0.2357	15.0675	1.1344	-0.1592	1	-0.2263
		8.9296	0.8862	0.0417	0.2357	1	8.9935	0.9013	0,1684	-0.2263	1
1		$\overline{\overline{X}}_{i}$	<i>S</i>		R		$\overline{\overline{X}}_{I}$	S-z		R	
	+/- 1.5σ	2.9608	1.6454	1	0.2279	0.0865	2.9514	1.6301	1	-0.2145	0.1802
		14.9811	1.1650	0.2279	1	0.0733	14.9827	1.2371	-0.2145	1	-0.1943
		8.9698	0.9167	0,0865	0.0733	1	8.9420	0.8270	0.1802	-0.1943	1

Table II.2: Input Process Parameters and Simulated Process Parameters for Run 10 & 11

				Run: 20				·····	Run: 21		
		All	Positive C	orrelation	Coefficier	nts	Two Neg	gative and Or	e Positive Co	orrelation Coe	efficients
SI		μ	σ		ρ		μ	σ		ρ	
put	Shift Size for	3	1.6	1	0.3	0.8	3	1.6	1	-0.3	0,8
Inl arar	Simulation	15	1.2	0.3	1	0.35	15	1.2	-0.3	1	-0.35
		9	0.9	0.8	0,35	1	9	0.9	0.8	-0,35	1
		$\overline{\overline{X}}_{i}$	<i>S</i> - <u></u> ,		R		$\overline{\overline{X}}_i$	S- x		R	
	+/- 0.25σ	2.8698	1.6345	1	0.3269	0.8152	3.0537	1.6475	1	-0.2492	0.7701
		14.9942	1.2313	0.3269	1	0.3579	15.0187	1.2044	-0.2492	1	-0.3246
		8.9593	0.9025	0.8152	0.3579	1	9.0183	0.92284	0.7701	-0.3246	1
		$\overline{\overline{X}}_{I}$	S _x		R		$\overline{\overline{X}}_{l}$	<i>S</i> - <u></u> <i>x</i>		R	
s l	+/- 0.5σ	2.8524	1.6475	1	0.3692	0.7999	2.9577	1.6005	1	-0.2553	0.7796
esult		15.0590	1.2044	0.3692	1	0.4372	15.0697	1.1649	-0.2553	1	-0.3587
L R		8.9563	0.9228	0.7999	0.4372	1	8.9638	0.8802	0.7796	-0.3587	1
latic		$\overline{\overline{X}}_{i}$	S _ī		R		$\overline{\overline{X}}_{t}$	S _x		R	_
Sim	+/- 1.0σ	3.1517	1.5182	1	0,3320	0,8048	2.9245	1.6066	1	-0.2844	0.7995
		15.0217	1.1405	0.3320	1	0.3799	14.8870	1.1190	-0.2844	1	-0.3393
		9.0784	0.8774	0.8048	0.3799	1	8.9995	0,9160	0.7995	-0.3393	1
		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{l}$	S _x		R	
	+/- 1.5σ	2.9337	1.6421	1	0.2774	0.8079	2.9540	1.6045	1	-0.3708	0.8136
		15.0511	1.2126	0.2774	1	0.3482	15.0563	1.2413	-0.3708	1	-0.4322
		9.0274	0.9087	0.8079	0.3482	1	9.0199	0.9137	0.8136	-0.4322	1

Table II.3: Input Process Parameters and Simulated Process Parameters for Run 20 & 21

				Run: 30					Run: 31		
		All	Positive C	orrelation	Coefficier	nts	Two Neg	gative and On	e Positive Co	prrelation Coe	efficients
្ទ		μ	σ		ρ		μ	σ		ρ	
out	Shift Size for	3	1.6	1	0.85	0.4	3	1.6	1	-0.85	0.4
aran	Simulation	15	1.2	0.85	1	0.8	15	1.2	-0.85	1	-0.8
<u> </u>		9	0.9	0.4	0.8	1	9	0.9	0.4	-0.8	1
		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{I}$	$S_{\overline{x}}$		R	
	+/- 0.25g	3.0630	1.5569	1	0.8333	0.3279	2,9443	1.6588	1	-0.8523	0.4071
		15.0324	1.1342	0.8333	1	0.7723	15.0429	1.2572	-0.8523	1	-0.8014
		8.9795	0.8565	0.3279	0.7723	1	8.9774	0.89415	0.4071	-0.8014	1
		$\overline{\bar{X}}_{i}$	<i>S</i> - <u></u>		R		$\overline{\overline{X}}_{i}$	S _x		R	
Ś	+/- 0.5 0	3.0804	1.6588	1	0.8868	0.5216	3.0647	1.5647	1	-0.8439	0.3802
esult		15.0722	1.2572	0.8868	1	0.8349	14.9250	1.1801	-0.8439	1	-0.7918
ц Ц Ц		9.0314	0.8941	0.5216	0.8349	1	9.0515	0.9013	0.3802	-0,7918	1
llatio		$\overline{\overline{X}}_{i}$	S _ž		R		$\overline{\overline{X}}_{i}$	S _x		R	
Simu	+/- 1.0σ	2.9037	1.5474	1	0.8483	0.4188	3.1231	1.6150	1	-0.8412	0.3857
		14.9492	1.1837	0.8483	1	0.8133	14.9067	1.2350	-0.8412	11	-0.8024
		9.0078	0.9011	0.4188	0.8133	1	9.0443	0.9570	0,3857	-0.8024	1
		$\overline{\overline{X}}_{I}$	S _x		R		$\overline{\overline{X}}_{I}$	S _x		R	
	+/- 1.5σ	2.9165	1,6343	1	0.8442	0,3653	3.1043	1.5931	1	-0.8367	0.3182
		14.9442	1.1769	0.8442	1	0.7835	14.9178	1.1464	-0.8367	1	-0,7631
		8.9834	0.9029	0.3653	0.7835	1	9.0463	0.8800	0,3182	-0,7631	1

Table II.4: Input Process Parameters and Simulated Process Parameters for Run 30 & 31

				Run: 40	·····				Run: 41		
		All	Positive C	orrelation	Coefficien	its	Two Neg	ative and On	e Positive Co	prrelation Coe	efficients
្ទ		μ	σ		ρ		μ	σ		ρ	
nete nete	Shift Size for	3	1.6	1	0.95	0,9	3	1.6	1	-0.95	0.9
lng aran	Simulation	15	1.2	0.95	1	0.875	15	1.2	-0.95	1	-0.875
Ľ.		9	0.9	0,9	0.875	1	9	0.9	0.9	-0.875	1
		$\overline{\overline{X}}_{i}$	<i>S</i> _{<i>x</i>}		R		$\overline{\overline{X}}_{l}$	S _ī		R	
	+/- 0.25σ	2.9333	1.6435	1	0.9509	0.9071	3.0547	1.6084	1	-0.9467	0,8963
		14.9432	1.2203	0.9509	1	0.8819	14.9669	1.2084	-0.9467	1	-0,8656
		8.9715	0.9082	0.9071	0.8819	1	9.0284	0.90643	0,8963	-0.8656	1
		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{t}$	S _x		R	
رم س	+/- 0.5σ	3.1752	1.6084	1	0,9536	0.8953	3.0458	1.5635	1	-0.9481	0.9026
esult		15,1350	1.2084	0.9536	1	0.8659	14.9744	1.1806	-0,9481	1	-0.8776
ц Ц Ц		9.1095	0.9064	0.8953	0.8659	1	9.0215	0.8823	0,9026	-0.8776	1
Ilatio		$\overline{\overline{X}}_{l}$	S-x		R		$\overline{\overline{X}}_{i}$	S _x		R	
Simu	+/- 1.0σ	2.9452	1.6127	1	0.9495	0.9073	3.0145	1.5769	1	-0.9473	0.8851
		14.9755	1.2073	0.9495	1	0.8770	14.9679	1,1912	-0.9473	1	-0.8635
		8.9926	0.9327	0.9073	0.8770	1	8.9883	0.8372	0.8851	-0.8635	1
		$\overline{\overline{X}}_{i}$	<i>S</i> - <u></u> <i>x</i>		R		$\overline{\overline{X}}_{i}$	S ₋		R	
	+/- 1.5σ	2.9966	1.6636	1	0.9543	0.8984	2.9528	1,5382	1	-0.9505	0.8974
		14.9978	1.2236	0.9543	1	0.8788	15.0538	1.1715	-0,9505	1	-0.8798
		9.0209	0.9175	0.8984	0.8788	1	8.9926	0,8680	0.8974	-0.8798	1

Table II.5: Input Process Parameters and Simulated Process Parameters for Run 40 & 41

				Run: 50					Run: 51		
		All	Positive C	orrelation	Coefficier	nts	Two Neg	gative and On	e Positive Co	prrelation Coe	efficients
S		μ	σ		ρ		μ	σ		ρ	
out nete	Shift Size for	3	0.06	1	0.7	0,9	3	0.06	1	-0.7	0.9
lng aran	Simulation	15	0.12	0.7	1	0.6	15	0.12	-0.7	1	-0,6
۵.		9	0.09	0.9	0.6	1	9	0.09	0.9	-0.6	1
		$\overline{\overline{X}}_{i}$	<i>S</i> - <u></u> <i>x</i>		R		$\overline{\overline{X}}_{i}$	S _x		R	
	+/- 0.25σ	3.0010	0.0591	1	0.7133	0.8911	3.0003	0.0599	1	-0.7021	0.8909
		15.0003	0.0125	0.7133	1	0.6048	14.9997	0.0124	-0.7021	1	-0.6101
		8.9990	0.0892	0.8911	0.6048	1	9.0014	0.08880	0.8909	-0.6101	1
		$\overline{\overline{X}}_{i}$	$S_{\overline{x}}$		R		$\overline{\overline{X}}_{i}$	S _x		R	
s.	+/- 0.5σ	2.9949	0.0599	1	0.7301	0.9011	2.9983	0.0595	1	-0.7089	0.8936
esult		14.9988	0.0124	0.7301	1	0.6267	15.0004	0.0124	-0.7089	1	-0.5924
л В		8.9957	0.0888	0.9011	0.6267	1	8.9959	0.0855	0.8936	-0.5924	1
latio		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{i}$	S _x		R	
Simu	+/-10σ	2.9969	0.0629	1	0.6912	0.9077	2.9980	0.0582	1	-0.6907	0.8966
		14.9991	0.0124	0.6912	1	0.6117	14.9995	0.0122	-0.6907	1	-0.5846
		8.9936	0.0918	0.9077	0.6117	1	8.9943	0.0877	0.8966	-0,5846	1
		$\overline{\overline{X}}_{i}$	S _x	_	R		$\overline{\overline{X}}_{i}$	S _x		R	
	+/- 1.5g	3,0008	0.0631	1	0.7457	0.9087	2,9972	0.0592	1	-0.6777	0.9011
	,	15.0008	0.0129	0.7457	1	0.6294	15.0002	0.0117	-0.6777	11	-0.5700
		8.9987	0.0967	0.9087	0.6294	1	8.9947	0.0887	0.9011	-0.5700	1

Table II.6: Input Process Parameters and Simulated Process Parameters for Run 50 & :
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				Run: 60					Run: 61		
		All	Positive C	orrelation	Coefficier	nts	Two Neg	ative and On	e Positive Co	prrelation Coe	efficients
S		μ	σ		ρ		μ	σ		ρ	
out	Shift Size for	3	0.06	1	0.2	0.1	3	0.06	1	-0.2	0.1
lnl aran	Simulation	15	0.12	0,2	1	0.15	15	0.12	-0.2	1	-0,15
ä		9	0.09	0.1	0.15	1	9	0.09	0.1	-0.15	1
		$\overline{\overline{X}}_{l}$	\$,		R		$\overline{\overline{X}}_i$	S _x		R	
	+/- 0.25σ	2.9981	0.0608	1	0.1849	0.1229	2,9941	0.0616	1	-0.1877	0.0185
		14.9998	0.0119	0.1849	1	0.1382	15.0004	0.0118	-0,1877	1	-0.1226
		8.9958	0.0917	0.1229	0.1382	1	9.0010	0.09016	0.0185	-0.1226	1
		$\overline{\overline{X}}_{i}$	<i>S</i> - <u></u> <i>x</i>		R		$\overline{\overline{X}}_{i}$	S _x		R	
S S	+/- 0.5σ	3.0005	0.0616	1	0.2197	0.0933	3.0003	0.0564	1	-0.2542	0.1536
ssul		14.9996	0.0118	0.2197	1	0.2266	15.0000	0.0123	-0.2542	1	-0.1502
L R L		8.9993	0.0902	0.0933	0.2266	1	9.0053	0.0944	0,1536	-0.1502	1
latio		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{t}$	S _x		R	
Simu	+/- 1.0σ	3.0000	0.0586	1	0.1667	0.0560	3.0012	0.0611	1	-0.1580	0.0712
		14.9996	0.0120	0.1667	1	0.1575	14.9998	0.0119	-0.1580	1	-0.1421
		8.9956	0.0892	0.0560	0.1575	1	9.0063	0.0874	0,0712	-0.1421	1
		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{i}$	S-x		R	
}	+/- 1.5σ	2.9983	0.0560	1	0.1210	0.0911	3.0039	0.0577	1	-0.1042	0.0800
		15.0002	0.0112	0.1210	1	0.1633	14.9993	0.0120	-0.1042	1	-0.1368
		9.0067	0.0893	0.0911	0.1633	1	9.0058	0.0914	0.0800	-0.1368	1

Table II.7: Input Process Parameters and Simulated Process Parameters for Run 60 & 61

	[· · · · · · · · · · · · · · · · · · ·		Run: 70					Run: 71		
		All	Positive C	orrelation	Coefficien	its	Two Neg	ative and On	e Positive Co	orrelation Coe	officients
ъ		μ	σ		ρ		μ	σ		ρ	
nete	Shift Size for	0.5	1.6	1	0.7	0.9	0.5	1.6	1	-0.7	0,9
lng aran	Simulation	0.65	1.2	0.7	1	0.6	0,65	1.2	-0,7	1	-0.6
<u> </u>		0.25	0.9	0.9	0.6	1	0,25	0.9	0.9	-0.6	1
		$\overline{\overline{X}}_{I}$	<i>S</i> _{<i>x</i>}		R		$\overline{\overline{X}}_{i}$	$S_{\overline{x}}$		R	
	+/- 0 25σ	0.4112	1.5148	1	0.6714	0.8847	0.5659	1.6321	1	-0.6965	0.9004
		0.5881	1.2070	0.6714	1	0.5743	0.6976	1.2123	-0.6965	1	-0.6191
		0.2009	0.8677	0.8847	0.5743	1	0.2801	0.92480	0.9004	-0.6191	1
		$\overline{\overline{X}}_{i}$	<i>S</i> _{<i>x</i>}		R		$\overline{\overline{X}}_{i}$	S- x		R	
Ś	+/- 0.5σ	0.4446	1.6321	1	0.7354	0.9008	0.4933	1,6004	1	-0.7202	0.8991
esult		0.6843	1.2123	0.7354	1	0.6466	0.6533	1.1924	-0.7202	1	-0.6112
л R		0.2379	0.9248	0.9008	0.6466	1	0.2486	0.9146	0.8991	-0.6112	1
llatic		$\overline{\overline{X}}_{i}$	<i>S</i> ₋		R		$\overline{\overline{X}}_{t}$	<i>S</i> - <u></u> ,		R	
Simu	+/- 1 0σ	0.5135	1.6255	1	0.7306	0.9086	0.5559	1,5625	1	-0.6787	0.8911
		0.6199	1.2279	0.7306	1	0.6302	0.6811	1.1734	-0.6787	1	-0.5843
		0.2562	0.9180	0.9086	0.6302	1	0.2752	0.8704	0.8911	-0.5843	1
		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{t}$	S _x		R	
	+/- 1.5σ	0.5413	1.5768	1	0.7113	0.9023	0.5413	1.5768	1	-0.6658	0.9055
		0.6528	1.2370	0.7113	1	0.5912	0.6094	1.1652	-0.6658	1	-0.5935
		0.2741	0.9070	0.9023	0.5912	1	0.2724	0.9089	0.9055	-0.5935	1

Table II.8: Input Process Parameters and Simulated Process Parameters for Run 70 & 71

	[Run: 80					Run: 81		
		All	Positive C	orrelation	Coefficier	its	Two Neg	ative and On	e Positive Co	orrelation Coe	efficients
ស		μ	σ		ρ		μ	σ		ρ	
out nete	Shift Size for	0.5	1.6	1	0.2	0.1	0,5	1.6	1	-0.2	0.1
	Simulation	0.65	1.2	0.2	1	0.15	0.65	1.2	-0.2	1	-0.15
		0.25	0,9	0.1	0.15	1	0.25	0,9	0.1	-0,15	1
		$\overline{\overline{X}}_{i}$	<i>S</i> - <u></u> ,		R		$\overline{\overline{X}}_{i}$	S _x		R	
	+/- 0 25σ	0.5842	1.5983	1	0.1483	0.2163	0.5601	1.6163	1	-0.2022	0.1531
		0.7021	1.1586	0.1483	1	0.1932	0.6024	1,2223	-0.2022	1	-0.2178
		0.2217	0.9033	0.2163	0.1932	1	0.2526	0.86516	0,1531	-0.2178	1
		$\overline{\overline{X}}_{i}$	S _x		R		$\overline{\overline{X}}_{i}$	<i>S</i> _{<i>x</i>}		R	
l vi	+/- 0.5σ	0.4908	1.6163	1	0.1961	0.0855	0.3076	1.5583	1	-0.1413	0.1062
esult	,	0.6148	1.2223	0.1961	1	0.1264	0.6348	1,1519	-0.1413	1	-0.1665
Ъ. К.		0.2673	0.8652	0.0855	0.1264	1	0.2764	0.9137	0.1062	-0.1665	1
Ilatio		$\overline{\overline{X}},$	<i>S</i> - <u></u> <i>x</i>		R		$\overline{\overline{X}}_{i}$	S _ī		R	
Sim	+/- 1.0σ	0.5935	1.5688	1	0.1971	0,2063	0.4109	1.6096	1	-0.2020	0.0690
		0.6890	1.1922	0.1971	1	0.2346	0.7073	1.2373	-0.2020	1	-0.0882
		0.2405	0.9353	0.2063	0.2346	1	0.2486	0.8795	0.0690	-0.0882	1
		$\overline{\overline{X}}_{i}$	S _ī		R		$\overline{\overline{X}}_{i}$	S _x		R	
	+/- 1.5σ	0.4159	1.6040	1	0.2075	0.1116	0.5033	1.6301	1	-0.1609	0,1140
		0.5821	1.1958	0.2075	1	0.1976	0.7009	1.2480	-0,1609	1	-0.1072
		0.2993	0.8814	0.1116	0.1976	1	0.2749	0.9403	0.1140	-0.1072	1

Table II.9: Input Process Parameters and Simulated Process Parameters for Run 80 & 81

	[· · · · · · · · · · · · · · · · · · ·		Run: 90					Run: 91		
		All	Positive C	orrelation	Coefficien	its	Two Neg	ative and On	e Positive Co	prrelation Coe	efficients
ទា		μ	σ		ρ		μ	σ		ρ	
nete	Shift Size for	0.5	0.06	1	0,7	0.9	0,5	0.06	1	-0.7	0,9
Inj	Simulation	0.65	0.12	0.7	1	0.6	0,65	0.12	-0.7	1	-0.6
<u> </u>		0.25	0.09	0.9	0.6	1	0.25	0.09	0.9	-0.6	1
		$\overline{\overline{X}}_{i}$	S-x		R		$\overline{\overline{X}}_{i}$	S _x		R	
	+/- 0.25σ	0.5030	0.0594	1	0.6734	0,9036	0.4985	0.0602	11	-0.6664	0.8881
	,	0.6508	0.0119	0.6734	1	0.5885	0.6496	0.0123	-0.6664	1	-0.5616
		0.2553	0.0896	0.9036	0.5885	1	0.2478	0.09036	0.8881	-0.5616	1
		$\overline{\overline{X}}_{i}$	S _{-x}		R		$\overline{\overline{X}}_{i}$	<i>S</i> - <u></u>		R	
S.	+/- 0.5 0	0.5049	0.0602	1	0.7321	0.9006	0.5025	0.0569	1	-0.7119	0.8894
esult		0.6506	0.0123	0.7321	1	0.6321	0.6498	0.0120	-0.7119	1	-0.5975
L L L		0.2580	0.0904	0.9006	0.6321	1	0.2558	0.0858	0.8894	-0.5975	1
latio		$\overline{\overline{X}}_{i}$	$S_{\overline{x}}$		R		$\overline{\overline{X}}_{i}$	S _x		R	
Simu	+/- 1.0σ	0.4997	0.0597	1	0.7127	0.9013	0.4955	0.0595	1	-0.6915	0.8968
		0.6501	0.0123	0.7127	1	0.6445	0.6505	0.0124	-0.6915	1	-0.5958
		0.2494	0.0915	0.9013	0.6445	1	0.2434	0.0871	0.8968	-0,5958	1
		$\overline{\overline{X}}_{l}$	S _x		R		$\overline{\overline{X}}_{i}$	S _x		R	
}	+/- 1.5σ	0.5015	0.0629	1	0.7126	0,9066	0.4943	0.0620	1	-0.7138	0.8965
		0.6503	0.0117	0.7126	1	0.6351	0.6511	0.0121	-0.7138	1	-0.6230
l		0.2490	0.0953	0.9066	0.6351	1	0.2440	0.0909	0.8965	-0.6230	1

Table II.10: Input Process Parameters and Simulated Process Parameters for Run 90 & 91

	[Run: 100					Run: 101		
		All	Positive C	orrelation	Coefficier	nts	Two Neg	ative and On	e Positive Co	prrelation Coe	efficients
S		μ	σ		ρ		μ	σ		ρ	
out nete	Shift Size for	0.5	0,06	1	0.2	0.1	0.5	0.06	1	-0.2	0.1
	Simulation	0,65	0.12	0.2	1	0,15	0.65	0.12	-0,2	1	-0.15
Ŭ.		0.25	0.09	0.1	0.15	1	0.25	0.09	0.1	-0.15	1
		$\overline{\overline{X}}_{l}$	\$ <u>-</u>		R		$\overline{\overline{X}}_{i}$	<i>S</i> _{<i>x</i>}		R	
	+/- 0.25g	0.4991	0.0586	1	0.2114	0.0582	0.4987	0.0587	1	-0.0959	0.0945
		0.6497	0.0115	0.2114	1	0.1532	0.6492	0.0122	-0.0959	1	-0.1385
		0.2488	0.0905	0.0582	0.1532	1	0.2509	0.09303	0.0945	-0.1385	1
		$\overline{\overline{X}}_{l}$	S ₋		R		$\overline{\overline{X}}_{i}$	S _x		R	
ທ	+/- 0.5σ	0.4980	0.0587	1	0.1610	0.1021	0.4987	0.0605	1	-0.2106	0.1598
lluse		0.6501	0.0122	0.1610	1	0.2036	0.6501	0.0119	-0.2106	1	-0.1291
n Re		0.2569	0.0930	0.1021	0.2036	1	0.2521	0.0879	0.1598	-0.1291	1
latio		$\overline{\overline{X}}_{t}$	S-x		R		$\overline{\overline{X}}_{I}$	S-x		R	
Sim	+/-1.0σ	0.4980	0.0641	1	0.2190	0.0895	0.5024	0.0631	1	-0.1693	0.0956
		0.6503	0.0123	0.2190	1	0.1804	0.6492	0.0127	-0.1693	1	-0.1383
		0.2553	0.0830	0.0895	0.1804	1	0.2518	0.0916	0.0956	-0.1383	1
		$\overline{\overline{X}}_{l}$	\$ <u>-</u>		R		$\overline{\overline{X}}_{i}$	S-		R	
	+/- 1.5σ	0,5007	0.0588	1	0.1644	0.1606	0.4997	0.0583	1	-0,1515	0.1149
ĺ		0.6502	0.0119	0.1644	1	0.2077	0.6493	0.0122	-0.1515	1	-0.2021
		0.2524	0.0890	0.1606	0.2077	1	0.2480	0.0876	0.1149	-0.2021	1

Table II.11: Input Process Parameters and Simulated Process Parameters for Run 100 & 101

Appendix III. Sample Major Element Control Limits Information and Sample Major Element Control Charts

Simulation	Shift	All Positive Correlation Coefficients						Simulation	Shift Two Negative and One Positive Correlation Coefficients						cients
Run	Size	UCL _{M1}	LCL _{M1}	UCL _{M2}	LCL _{M2}	UCL _{M3}	LCL _{MS}	Run	Size	UCL _{M1}	LCLMI	UCL _{M2}	LCL _{M2}	UCL _{MS}	LCL _{MS}
00	+/- 0.25 a	6,6649	-6,6649	1,7158	-1.7158	5.3010	-5,3010	01	+/- 0.25o	6.5871	-6,5871	2.0456	-2.0456	4,8288	-4.8288
	+/- 0,5σ	5.4349	-5,4349	1,7856	-1.7856	4.2131	-4.2131		+/- 0,5σ	6.3076	-6,3076	1,6868	-1.6868	5,0598	-5.0598
	+/- 1.0σ	6.2777	-6.2777	1.7745	-1.7745	5,1398	-5,1398		+/- 1.0σ	6,3465	-6,3465	1.7318	-1.7318	4,9743	-4.9743
	+/- 1,50	5.5597	-5,5597	1,7842	-1.7842	4.4459	-4.4459		+/- 1.5σ	5.3137	-5.3137	1.7699	-1.7699	4.2825	-4.2825
10	+/- 0,250	0.9374	-0,9374	0,9258	-0,9258	0.9196	-0.9196	11	+/- 0.25σ	0.9123	-0.9123	0.9382	-0,9382	0,9077	-0.9077
	+/- 0.50	0.9586	-0,9586	0.9754	-0,9754	0,8984	-0.8984		+/- 0,5σ	0.9135	-0.9135	0,9200	-0.9200	0,9209	-0,9209
	+/- 1.00	0.9223	-0.9223	0,9749	-0,9749	0,9339	-0.9339		+/- 1.0o	0.9224	-0.9224	0.9446	-0.9446	0,9475	-0.9475
	17-1.50	0.9351	-0.9351	0.9332	-0,9332	0.8914	-0.8914		+/- 1.5σ	0.9443	<u>-0.9443</u>	0,9494	-0.9494	0.9361	-0.9361
20	+/- 0.250	2.6406	-2,6406	1.0159	-1.0159	2.7050	-2.7050	21	+/- 0.25σ	2.1670	-2.1670	0,9859	-0,9859	2.2718	-2.2718
	+/- 0.50	2.4524	-2.4524	1.0919	-1.0919	2.6187	-2.6187		+/- 0,5σ	2.2524	-2.2524	1.0140	-1.0140	2.4165	-2.4165
	+/- 1.00	2.5097	-2,5097	1.0331	-1.0331	2.6097	-2.6097		+/- 1.0a	2.4464	-2.4464	0.9973	-0.9973	2.5411	-2.5411
	1+/- 1.50	2.5392	-2,5392	1.0037	-1.0037	2,6670	-2,6670		+/- 1.5a	2.6130	-2.6130	1,0860	-1.0860	2.7714	-2.7714
30	+/- 0.250	15.0063	-15,0063	33,1915	-33.1915	11.3681	-11.3681	31	+/- 0.25σ	14.5044	-14.5044	33,8263	-33,8263	11.0952	-11.0952
	+/- 0.50	13,9060	-15,9060	38.2234	-38,2234	11.2127	-11.2127		+/- 0,5a	13,4393	-13.4393	30.8108	-30.8108	10.3667	-10.3667
	+/- 1.00	14 6108	-13,9101	33,0737	-33,8/3/	11.5167	-11.518/		+/- 1.00	15.3152	-15.3152	36,6023	-36.6023	12.5755	-12.5755
	1.1 0.25-1	14.0100	-14.0100	32,1092	-32,7892	10.8746	-10.8740		1+1-1.50	16.2398	-16,2398	34,9396	-34,9396	11.6585	-11.6585
40	+/ 0.250	11.0105	-11.0100	9.4224	-9,4224	5,0905	-5.0905	41	+/- 0.25g	10.9922	-10,9922	8.6223	-8.6223	4,5492	-4.5492
	+/ 1.0-	12.3/04	-12.3/64	9,8202	-9.8202	4.4801	-4.4801		+/- 0,5σ	11.0933	-11.0933	8,9440	-8.9440	4,8844	-4.8844
	+1-1.00	11.0025	-11,0025	9,0860	-9,0880	5,0564	-5,0564		+/- 1.0σ	10.3773	-10,3773	8,8367	-8.8367	4,1903	-4,1903
[110 0 05-1	<u> </u>	-11.5539	10,1547	-10.1547	4,6988	-4.6988		+/- 1.5σ	11.0153	-11.0153	9,4918	-9.4918	4.7091	-4.7091
50	+1-0.200	5,5799	-5,5/99	1.812/	-1.8127	4.3216	-4.3216	51	+/- 0.25g	5,3061	-5.3061	1.7432	-1.7432	4.2859	-4.2859
	+/- 1.00	6.0153	-0,1049 6 0163	1.5050	-1.9090	4,7410	-4,7410		+/- 0.50	5,8065	-5.8065	1.8032	-1.8032	4.4505	-4,4505
	+/- 1.50	7.0966	-0,0155	2 0482	-1.0934	5.0199	-5,0199		+/- 1.00	5./316	-5,/316	1.7068	-1.7068	4,5530	-4,5530
╠	4 0.25-1	0.0224	-1,0300	2.0402	-2.0402	0.0000	-5.2175	/	1.00	5.9521	-5,9521	1,0560	-1.6580	4,/0/0	-4./6/6
	4/-0.50	0.9224	-0.9224	0,9202	-0.9262	0,9082	-0.9082	61	+/- 0.250	0.9142	-0.9142	0.9278	-0.9278	0,8955	-0.8955
60	46 1 0-	0.9207	-0,9207	0,9704	-0,9704	0.9317	-0.9317		+/- 0.50	0.9569	-0,9569	0,9558	-0.9558	0.9157	-0,9157
	+/- 1.00	0.9000	-0,5060	0,9202	-0.9282	0.9053	-0.9053		+/- 1.00	0,9068	-0,9068	0.9208	-0.9208	0,9024	-0,9024
	+/- 0.25-	4 0712	4 0712	1 6111	-0.9100	4.0727	-0.9110		1.00	0,8957	-0.8957	0,9069	-0.9069	0,9028	-0.9028
70	+/- 0.250	5 0488	-4,9712	1.0111	-1.0111	4.0/3/	-4.0737	71	+/- 0.250	5,5869	-5.5869	1.7139	-1.7139	4,6647	-4.6647
	+/- 1.0-	6 6 2 9 6	-5,5400	1 9187	-1.9207	4.0332	-4.0932		+/ 1.0-	5.0/83	-8.0/83	1.8593	-1.8593	4.6696	-4.6696
	+/- 1.50	6 4293	-6.4293	1 8367	-1.8367	4 8820	-0.1207		+1-1.00	5,24/2	-3.2412	1.0413	-1.6413	4.29/5	-4.2975
	+/+ 0 25-	0.0360	0.3601	1.0007	- 1,0007	9.0023	-1.0029	<u> </u>	1.00	0.0045	-3,/045	0000.1	-1.5656	4.9031	-4,9031
80	+/= 0.200	0.9309	-0.9309	0.9277	-0.9277	0,9518	-0,9518	81	+/- 0,250	0.9317	-0.9317	0.9552	-0.9552	0,9381	-0.9381
	+/- 1 0-	0.9203	-0.9209	0.9290	-0,9290	0,0990	-0,8998		+/- 0.50	0,9065	-0,9065	0.9218	-0.9218	0.9137	-0.9137
	+/- 1.5π	0.9267	-0.9443	0.9507	-0.9507	0.9004	-0,9004		+/- 1.00	0,9220	-0.9220	0.9248	-0.9248	0.8914	-0.8914
90	+/- 0 25g	5 7676	5 7676	1 6200	1 6200	4 9221	4 9224	91	1.1 0.05	0,9143	-0.9143	0.9129	-0.9129	0,9010	-0.9010
	+/- 0.200	6.0935	-5,7076	1.0200	1.0200	4,0231	-4.0231		+/- 0.250	5,1/99	-5.1799	1.5989	-1.5989	4.2065	-4.2065
	+/- 1.0-	5 5864	-5 5864	1 7027	-1.9100	4.7032	4,7092		+/- 0.50	5,5693	-5,5693	1.8105	-1.8105	4.2720	-4.2720
	+/- 1.5g	6.0097	-6 0097	1.7945	-1.7527	4 9576	-4.7015		+1.150	5,0008	-3.0008	1.7000	-1./000	4.5312	-4.5312
	+/- 0 25c	0.9239	-0 9230	0 94201	-1.7 0420	0.0010	-0.0030		4 0.25-	0.0242	0.9000	0.0050	-1.0034	4,5087	1800.8-
100	+/- 0.50	0.9101		0.0725	-0.5425	0.0000	-0,5030	101	1. 0.200	0.0302	-0,6962	0.9056	-0.9056	0.9054	-0.9054
	+/- 1.0a	0.9289	0.9289	0.9525	-0,5050	0.5245	-0.5249		+/- 0.50	0,9405	-0.9405	0,9320	-0.9320	0,9140	-0.9140
	+/- 1.5σ	0.9223	-0.9223	0.9390	-0,0020	0.0141	-0.9141		+1-1.00	0,9130	-0.9130	0.9223	-0,9223	0.9041	-0.9041
	L. 100	0.0220	-0,544.0	0,5050	-0.5050	0,53/9	•0,93/9		1.00 I.O	0,9096	-0,9096	0,9358	-0.9358	0.9265	-0,9265

Table III.1: Sample Major Element Control Limits Information for 22 Simulation Runs



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10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27

Chart III-11.1: $\rho_{12} = -0.2$; $\rho_{13} = 0.1$; $\rho_{23} = -0.15$ (+/- 0.25 σ)

M'11

3

•2

1 2 3 4 -5 6 8 9


















165













172





174









177

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Appendix IV. Analysis of Simulation Experiment for the Study of the Effects of Sample Size and Number of Samples

Rep = 25		M ₁₁			M ₂₂			M ₃₃		
n	k	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range
6	25	5.38%	2.81%	11.62%	4.92%	1.90%	6.38%	5.31%	3.26%	13.52%
6	35	3.34%	2.74%	11.65%	4.49%	1.52%	5.93%	2.44%	1.19%	4.87%
6	50	1.88%	1.07%	3.47%	2.25%	1.49%	6.02%	1.71%	2.27%	9.12%
6	75	1.49%	1.60%	7.47%	2.02%	0.95%	4.58%	2.26%	1.87%	9.79%
6	100	1.19%	0.62%	2.31%	1.51%	1.28%	6.76%	2.02%	1.01%	3.56%
6	250	1.13%	0.86%	2.91%	1.20%	0.68%	2.59%	1.06%	0.68%	3.24%
6	500	1.12%	1.37%	5.63%	0.81%	0.40%	1.60%	1.20%	1.24%	5.23%
6	750	0.70%	0.82%	3.05%	0.36%	0.37%	1.51%	1.01%	0.42%	1.65%
6	1000	0.55%	0.39%	1.79%	0.66%	0.53%	1.90%	0.93%	0.95%	3.72%
8	25	2.65%	2.30%	9.98%	2.69%	2.66%	9.89%	2.74%	2.40%	10.63%
8	35	2.52%	1.64%	5.97%	1.39%	1.03%	4.70%	3.08%	3.54%	18.74%
8	50	2.02%	2.41%	12.19%	1.51%	1.65%	6.73%	2.22%	1.62%	8.24%
8	75	1.45%	0.87%	2.73%	1.27%	0.88%	4.44%	1.57%	1.18%	5.72%
8	100	1.35%	0.90%	4.84%	1.35%	1.13%	3.82%	1.80%	0.94%	5.33%
8	250	1.20%	1.12%	3.81%	1.08%	1.38%	5.28%	1.01%	1.17%	3.83%
8	500	0.97%	0.66%	3.11%	0.52%	0.56%	1.92%	1.05%	0.93%	3.20%
8	750	0.77%	1.16%	4.43%	0.47%	0.35%	1.82%	0.84%	1.06%	4.39%
8	1000	0.59%	0.60%	1.88%	0.23%	0.23%	1.03%	0.48%	0.47%	2.44%
10	25	2.71%	3.78%	13.58%	2.71%	3.12%	13.52%	3.15%	2.06%	11.03%
10	35	1.71%	1.03%	4.61%	2.76%	1.09%	5.61%	2.68%	1.92%	7.85%
10	50	1.58%	1.08%	5.65%	1.47%	1.02%	5.16%	2.02%	2.36%	12.02%
10	75	1.47%	0.96%	4.31%	1.53%	1.66%	5.38%	1.72%	0.73%	2.57%
10	100	1.30%	1.45%	7.06%	1.31%	1.28%	5.88%	1.31%	0.91%	4.00%
10	250	1.35%	2.59%	13.24%	1.29%	0.97%	4.83%	0.93%	0.96%	3.86%
10	500	0.44%	0.37%	1.19%	0.86%	0.54%	2.27%	1.11%	0.79%	3.22%
10	750	0.65%	0.81%	3.11%	0.47%	0.62%	2.98%	0.58%	0.68%	2.37%
10	1000	0.27%	0.35%	1.77%	0.21%	0.21%	0.83%	0.34%	0.28%	1.12%
15	25	2.38%	2.22%	9.40%	2.42%	2.27%	9.24%	2.12%	1.79%	6.59%
15	35	2.50%	1.54%	6.40%	1.56%	2.10%	7.93%	1.70%	1.33%	5.10%
15	50	1.32%	0.86%	3.54%	1.21%	0.88%	4.38%	1.31%	1.29%	6.14%
15	75	0.86%	0.69%	2.49%	1.10%	0.41%	1.77%	1.19%	0.50%	1.94%
15	100	0.79%	0.48%	2.08%	0.55%	0.64%	3.22%	1.03%	0.78%	3.45%
15	250	0.49%	0.34%	1.25%	0.38%	0.37%	1.47%	0.79%	0.76%	2.83%
15	500	0.60%	1.00%	3.86%	0.40%	0.36%	1.64%	0.54%	0.81%	2.78%
15	750	0.33%	0.59%	2.88%	0.34%	0.24%	0.75%	0.45%	0.80%	3.96%
15	1000	0.33%	0.41%	2.16%	0.41%	0.56%	2.38%	0.55%	0.84%	3.88%

Table IV. 1: Bias_{rep}% Information for Run 110

 $\mu_1 = 3, \sigma_1 = 1.6; \mu_2 = 15, \sigma_2 = 1.2; \mu_3 = 9, \sigma_3 = 0.9; \rho_{12} = 0.7, \rho_{13} = 0.9, \rho_{23} = 0.6$
Rep	= 25		M ₁₁			M ₂₂			M ₃₃	
n	k	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range
6	25	1.34%	0.80%	3.92%	2.95%	1.24%	4.82%	1.57%	1.35%	5.07%
6	35	1.45%	0.89%	4.88%	1.00%	0.92%	4.77%	0.89%	0.67%	2.28%
6	50	0.77%	0.60%	2.11%	0.94%	0.71%	2.03%	0.43%	0.40%	1.66%
6	75	0.36%	0.18%	0.69%	0.53%	0.38%	1.35%	1.01%	0.23%	0.96%
6	100	0.34%	0.24%	0.89%	0.19%	0.16%	0.62%	0.24%	0.27%	1.21%
6	250	0.38%	0.18%	0.73%	0.32%	0.20%	0.66%	0.34%	0.28%	1.26%
6	500	0.15%	0.14%	0.47%	0.32%	0.23%	1.01%	0.26%	0.20%	0.74%
6	750	0.24%	0.37%	1.88%	0.37%	0.21%	0.81%	0.10%	0.11%	0.48%
6	1000	0.08%	0.11%	0.44%	0.14%	0.08%	0.34%	0.06%	0.04%	0.17%
8	25	1.19%	0.76%	3.87%	1.37%	1.69%	7.97%	1.12%	0.70%	2.22%
8	35	1.09%	1.32%	4.56%	1.18%	1.62%	5.26%	0.45%	0.20%	0.76%
8	50	0.59%	0.43%	1.42%	1.21%	0.76%	2.73%	0.34%	0.41%	1.73%
8	75	0.44%	0.50%	2.60%	0.49%	0.39%	1.87%	0.64%	0.39%	1.83%
8	100	0.25%	0.34%	1.35%	0.21%	0.23%	0.92%	0.20%	0.22%	0.89%
8	250	0.22%	0.14%	0.48%	0.26%	0.23%	0.82%	0.42%	0.20%	0.96%
8	500	0.22%	0.35%	1.29%	0.14%	0.17%	0.63%	0.24%	0.18%	0.76%
8	750	0.11%	0.06%	0.27%	0.12%	0.20%	0.91%	0.24%	0.27%	1.15%
8	1000	0.08%	0.07%	0.31%	0.08%	0.07%	0.33%	0.04%	0.03%	0.10%
10	25	0.54%	0.47%	1.66%	1.06%	0.54%	2.15%	1.97%	0.77%	2.84%
10	35	0.30%	0.54%	2.02%	0.77%	0.42%	2.31%	0.51%	0.34%	1.57%
10	50	0.36%	0.40%	1.70%	0.44%	0.48%	1.96%	0.35%	0.42%	2.12%
10	75	0.42%	0.35%	1.81%	0.33%	0.44%	1.87%	0.35%	0.45%	1.40%
10	100	0.39%	0.26%	1.04%	0.24%	0.13%	0.51%	0.10%	0.09%	0.28%
10	250	0.45%	0.43%	1.39%	0.28%	0.32%	1.13%	0.22%	0.11%	0.52%
10	500	0.27%	0.14%	0.63%	0.20%	0.12%	0.56%	0.28%	0.27%	1.34%
10	750	0.12%	0.13%	0.51%	0.20%	0.10%	0.45%	0.07%	0.05%	0.25%
10	1000	0.08%	0.16%	0.67%	0.17%	0.11%	0.34%	0.12%	0.06%	0.25%
15	25	0.85%	0.20%	0.99%	0.36%	0.31%	1.15%	0.34%	0.37%	1.66%
15	35	0.37%	0.31%	1.37%	0.93%	0.50%	1.65%	0.31%	0.15%	0.52%
15	50	0.38%	0.33%	1.74%	0.43%	0.41%	1.48%	0.39%	0.50%	1.61%
15	75	0.52%	0.20%	0.91%	0.32%	0.22%	0.76%	0.20%	0.14%	0.63%
15	100	0.17%	0.18%	0.61%	0.30%	0.20%	0.72%	0.22%	0.23%	1.09%
15	250	0.14%	0.13%	0.51%	0.21%	0.16%	0.68%	0.14%	0.15%	0.60%
15	500	0.10%	0.08%	0.23%	0.20%	0.10%	0.52%	0.17%	0.10%	0.45%
15	750	0.12%	0.17%	0.73%	0.09%	0.06%	0.28%	0.08%	0.06%	0.28%
15	1000	0.06%	0.05%	0.20%	0.10%	0.10%	0.45%	0.06%	0.11%	0.51%

Table IV. 2: Bias_{rep}% Information for Run 120

 $\mu_1 = 3, \sigma_1 = 1.6; \mu_2 = 15, \sigma_2 = 1.2; \mu_3 = 9, \sigma_3 = 0.9; \rho_{12} = 0.2, \rho_{13} = 0.1, \rho_{23} = 0.15$

Rep	= 25		M ₁₁			M ₂₂			M ₃₃	
n	k	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range
6	25	4.55%	3.07%	12.77%	3.97%	1.54%	5.75%	4.91%	3.02%	12.28%
6	35	1.66%	2.56%	10.08%	1.54%	1.04%	3.09%	2.66%	1.15%	5.01%
6	50	1.16%	1.27%	5.37%	1.55%	1.12%	5.82%	1.86%	0.88%	2.96%
6	75	1.47%	1.11%	3.95%	0.84%	0.61%	2.09%	1.64%	1.86%	6.75%
6	100	1.83%	0.92%	3.09%	0.23%	0.27%	0.97%	1.72%	1.38%	5.47%
6	250	1.05%	0.60%	2.47%	0.57%	0.32%	1.20%	1.13%	0.63%	2.47%
6	500	1.05%	1.23%	5.00%	0.21%	0.11%	0.37%	1.11%	1.11%	4.54%
6	750	0.82%	0.70%	2.85%	0.46%	0.29%	0.96%	0.89%	0.88%	3.40%
6	1000	0.78%	0.46%	2.10%	0.45%	0.32%	1.43%	0.79%	0.33%	1.51%
8	25	2.33%	1.73%	7.52%	1.75%	2.20%	10.14%	2.91%	3.17%	16.56%
8	35	2.50%	2.70%	14.11%	1.65%	2.15%	6.96%	1.96%	0.96%	5.53%
8	50	1.78%	0.95%	5.10%	1.69%	1.04%	3.79%	2.15%	1.73%	7.94%
8	75	1.54%	1.79%	8.11%	0.68%	0.48%	2.07%	1.46%	1.00%	4.59%
8	100	1.41%	0.83%	2.81%	0.26%	0.33%	1.31%	1.16%	1.27%	5.43%
8	250	0.99%	0.99%	3.25%	0.38%	0.34%	1.24%	0.64%	0.74%	2.70%
8	500	0.56%	0.36%	1.40%	0.19%	0.31%	1.38%	0.38%	0.38%	1.84%
8	750	0.71%	1.04%	4.03%	0.21%	0.30%	1.13%	0.73%	0.93%	3.76%
8	1000	0.81%	0.78%	2.53%	0.12%	0.09%	0.39%	1.03%	. 0.98%	3.49%
10	25	2.75%	1.70%	8.61%	1.64%	0.93%	3.88%	3.74%	1.62%	6.74%
10	35	2.42%	2.02%	8.15%	1.07%	0.58%	3.04%	2.28%	1.97%	8.01%
10	50	2.00%	1.82%	9.13%	0.70%	0.85%	3.44%	1.56%	1.91%	9.36%
10	75	1.38%	0.74%	3.07%	0.51%	0.64%	2.60%	1.43%	0.92%	4.15%
10	100	1.43%	0.61%	2.90%	0.36%	0.20%	0.82%	0.90%	0.93%	3.54%
10	250	1.07%	1.16%	5.20%	0.44%	0.52%	1.81%	1.55%	0.65%	2.22%
10	500	0.69%	0.61%	2.15%	0.29%	0.17%	0.74%	0.97%	0.83%	3.52%
10	750	0.59%	0.68%	2.46%	0.30%	0.17%	0.69%	0.51%	0.70%	2.32%
10	1000	0.26%	0.28%	1.47%	0.24%	0.15%	0.48%	0.34%	0.28%	1.15%
15	25	2.04%	1.64%	5.90%	1.37%	0.80%	2.64%	1.50%	1.13%	4.49%
15	35	1.27%	0.92%	4.68%	0.53%	0.43%	1.61%	1.57%	1.46%	5.15%
15	50	1.58%	1.58%	6.82%	0.66%	0.61%	2.28%	1.47%	1.36%	6.37%
15	75	0.69%	0.50%	2.18%	0.45%	0.32%	1.09%	0.93%	0.58%	2.33%
15	100	0.92%	0.56%	2.64%	0.41%	0.29%	1.04%	0.95%	0.72%	3.06%
15	250	0.67%	0.62%	2.40%	0.27%	0.22%	0.91%	0.67%	0.69%	2.59%
15	500	0.54%	0.83%	2.92%	0.31%	0.15%	0.76%	0.51%	0.79%	2.59%
15	750	0.39%	0.74%	3.56%	0.12%	0.09%	0.39%	0.42%	0.82%	3.97%
15	1000	0.38%	0.58%	2.90%	0.16%	0.14%	0.65%	0.51%	0.75%	3.59%

Table IV. 3: Bias_{rep}% Information for Run 130

 $\mu_1 = 3, \sigma_1 = 1.6; \mu_2 = 15, \sigma_2 = 1.2; \mu_3 = 9, \sigma_3 = 0.9; \rho_{12} = 0.3, \rho_{13} = 0.8, \rho_{23} = 0.35$

Rep	= 25		M ₁₁			M ₂₂			M ₃₃	
n	k	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range
6	25	7.65%	2.24%	8.91%	4.85%	2.59%	13.63%	2.20%	3.58%	16.44%
6	35	3.93%	2.37%	10.13%	6.59%	2.33%	9.95%	7.00%	2.72%	14.26%
6	50	3.08%	2.02%	6.87%	2.33%	1.67%	5.60%	2.15%	1.19%	5.11%
6	75	2.54%	2.71%	14.00%	1.75%	1.27%	4.39%	1.42%	0.95%	3.57%
6	100	1.20%	1.00%	4.95%	1.42%	0.97%	3.28%	2.61%	1.42%	6.05%
6	250	1.21%	0.67%	2.56%	1.56%	0.95%	3.63%	1.52%	0.87%	3.85%
6	500	1.54%	0.90%	4.88%	1.82%	0.75%	3.49%	1.16%	0.78%	4.15%
6	750	1.29%	0.67%	3.01%	1.43%	0.80%	2.75%	1.22%	0.67%	2.25%
6	1000	0.88%	0.99%	3.25%	0.69%	0.45%	1.99%	0.68%	0.49%	1.86%
8	25	4.31%	1.86%	6.58%	3.10%	2.91%	13.56%	4.41%	4.66%	14.61%
8	35	2.04%	2.98%	13.80%	1.74%	2.64%	10.67%	3.66%	1.24%	5.43%
8	50	1.51%	0.96%	2.95%	3.23%	1.60%	6.83%	2.81%	2.08%	10.37%
8	75	1.27%	1.93%	10.14%	1.76%	1.86%	9.14%	1.53%	2.54%	9.84%
8	100	1.09%	0.98%	4.61%	1.49%	1.11%	4.89%	1.62%	1.07%	5.46%
8	250	1.66%	0.79%	3.66%	2.64%	1.03%	4.40%	2.18%	0.99%	3.36%
8	500	0.85%	0.62%	3.37%	0.82%	0.72%	2.89%	0.72%	0.70%	2.58%
8	750	0.82%	0.97%	3.84%	0.70%	0.70%	2.52%	0.65%	0.40%	1.31%
8	1000	0.61%	0.33%	1.22%	0.57%	0.47%	2.06%	0.49%	0.59%	3.07%
10	25	4.61%	2.72%	11.31%	3.19%	3.42%	16.12%	3.52%	2.55%	10.53%
10	35	2.94%	4.05%	20.32%	4.07%	3.68%	15.76%	2.42%	2.86%	12.73%
10	50	2.18%	1.62%	5.93%	1.74%	0.91%	3.48%	1.88%	2.53%	7.13%
10	75	1.36%	1.85%	9.03%	1.41%	1.13%	4.24%	1.28%	2.79%	14.13%
10	100	1.69%	0.91%	3.00%	1.39%	2.83%	14.53%	1.54%	0.71%	2.14%
10	250	0.93%	0.70%	2.89%	0.64%	0.75%	3.19%	0.60%	0.82%	4.06%
10	500	0.69%	0.52%	2.66%	0.80%	0.44%	2.13%	0.83%	0.57%	3.26%
10	750	0.59%	0.64%	2.09%	0.65%	0.68%	2.33%	0.95%	0.96%	4.91%
10	1000	0.56%	0.73%	3.25%	0.58%	0.77%	2.71%	0.36%	0.51%	2.14%
15	25	2.82%	1.76%	5.54%	2.34%	1.43%	4.55%	2.82%	1.40%	4.64%
15	35	1.58%	1.55%	4.83%	1.74%	1.70%	7.80%	1.27%	1.71%	7.73%
15	50	1.52%	0.74%	3.11%	1.29%	1.02%	3.58%	1.16%	1.71%	8.41%
15	75	1.10%	1.86%	8.19%	1.27%	1.11%	4.36%	1.61%	1.45%	5.80%
15	100	1.00%	1.05%	3.16%	1.13%	1.24%	4.23%	1.56%	1.11%	4.33%
15	250	0.76%	0.77%	2.62%	0.82%	1.42%	5.90%	1.16%	1.54%	6.02%
15	500	0.62%	0.68%	3.06%	0.64%	0.71%	2.74%	0.71%	1.25%	5.89%
15	750	0.76%	0.71%	3.46%	0.50%	0.95%	4.68%	0.52%	0.65%	2.95%
15	1000	0.31%	0.45%	2.35%	0.53%	0.57%	2.97%	0.35%	0.50%	2.15%

Table IV. 4: Bias_{rep}% Information for Run 140

 $\mu_1 = 3, \sigma_1 = 1.6; \mu_2 = 15, \sigma_2 = 1.2; \mu_3 = 9, \sigma_3 = 0.9; \rho_{12} = 0.85, \rho_{13} = 0.4, \rho_{23} = 0.8$

Rep	= 25		M ₁₁			M ₂₂			M ₃₃	
n	k	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range	Mean	Std. Dev.	Range
6	25	7.33%	2.74%	14.25%	9.06%	2.76%	12.12%	5.47%	3.05%	12.22%
6	35	4.11%	4.38%	16.55%	3.02%	1.56%	5.00%	2.59%	1.22%	4.68%
6	50	3.05%	1.29%	6.12%	2.32%	2.43%	10.56%	1.92%	0.95%	3.09%
6	75	3.89%	1.65%	5.99%	3.12%	0.90%	4.39%	1.68%	2.03%	7.87%
6	100	2.48%	0.79%	2.96%	2.14%	2.26%	6.71%	1.83%	1.61%	8.04%
6	250	1.15%	0.74%	2.58%	1.35%	0.76%	2.90%	1.21%	0.68%	2.96%
6	500	0.52%	0.66%	2.38%	0.59%	0.57%	2.55%	1.23%	1.20%	4.97%
6	750	0.68%	0.95%	3.94%	0.67%	0.74%	2.26%	0.79%	0.88%	3.41%
6	1000	0.48%	0.36%	1.48%	0.51%	0.44%	1.63%	0.86%	0.40%	1.80%
8	25	4.53%	3.62%	10.80%	3.52%	2.76%	12.00%	2.96%	3.40%	17.68%
8	35	1.35%	1.31%	4.36%	1.24%	1.00%	3.58%	2.45%	1.91%	8.61%
8	50	1.46%	1.04%	3.80%	2.52%	2.01%	6.87%	1.54%	1.16%	5.57%
8	75	2.31%	1.19%	4.88%	2.48%	0.70%	3.07%	1.69%	1.27%	5.34%
8	100	0.85%	0.99%	4.49%	0.94%	1.04%	3.83%	1.84%	0.92%	5.24%
8	250	0.93%	0.59%	3.18%	1.15%	1.28%	4.43%	0.82%	1.02%	4.19%
8	500	1.49%	1.34%	5.51%	0.97%	1.10%	4.28%	1.04%	0.98%	3.42%
8	750	0.50%	0.71%	2.66%	0.33%	0.31%	1.15%	0.75%	0.85%	3.02%
8	1000	0.52%	0.50%	2.36%	0.79%	1.20%	5.56%	0.48%	0.39%	2.00%
10	25	2.08%	2.33%	11.88%	2.36%	2.78%	9.66%	3.21%	2.08%	11.00%
10	35	3.50%	2.55%	11.75%	2.90%	1.94%	8.91%	2.78%	2.17%	8.91%
10	50	1.79%	2.11%	7.57%	4.11%	3.56%	11.86%	1.62%	1.93%	9.51%
10	75	1.59%	0.92%	3.19%	1.76%	1.44%	5.38%	1.43%	0.96%	3.86%
10	100	1.78%	2.02%	10.48%	1.56%	1.30%	6.84%	1.69%	0.73%	2.61%
10	250	1.37%	1.78%	6.43%	1.37%	1.43%	4.81%	1.01%	0.83%	3.41%
10	500	0.60%	0.56%	2.59%	0.46%	0.36%	1.29%	0.92%	0.94%	3.58%
10	750	0.47%	0.97%	4.30%	0.67%	0.83%	4.18%	0.55%	0.75%	2.55%
10	1000	0.37%	0.27%	0.92%	0.30%	0.37%	1.38%	0.37%	0.30%	1.12%
15	25	3.58%	2.10%	9.38%	2.52%	1.17%	4.32%	1.72%	1.28%	4.82%
15	35	1.87%	1.83%	9.04%	2.37%	3.03%	11.82%	1.84%	1.53%	5.50%
15	50	1.27%	0.86%	2.86%	1.83%	1.70%	6.04%	1.43%	1.35%	6.42%
15	75	0.67%	0.68%	3.56%	0.78%	1.00%	5.05%	1.04%	0.56%	2.03%
15	100	0.88%	0.41%	1.68%	0.94%	0.74%	3.12%	0.93%	0.74%	3.27%
15	250	1.14%	0.74%	3.13%	0.65%	0.64%	2.65%	0.77%	0.78%	2.87%
15	500	0.51%	1.13%	5.06%	0.75%	0.84%	4.22%	0.53%	0.85%	2.81%
15	750	0.31%	0.34%	1.45%	0.43%	0.45%	1.88%	0.44%	0.83%	4.06%
15	1000	0.40%	0.44%	1.64%	0.44%	0.35%	1.32%	0.54%	0.80%	3.81%

Table IV. 5: Bias_{rep}% Information for Run 150

 $\mu_1 = 3, \sigma_1 = 1.6; \mu_2 = 15, \sigma_2 = 1.2; \mu_3 = 9, \sigma_3 = 0.9; \rho_{12} = 0.95, \rho_{13} = 0.9, \rho_{23} = 0.875$

Appendix V. Simulation Study of Bootstrap Percentile Control Limits for Major Elements

V.1 Simulation Study Design

To study the Bootstrap Percentile Control limits, the following simulation study is designed to evaluate how the total number of observations ($n \times k$) and the size of resample will effect on the estimates of the major element control limits. The study include the following steps.

 Choose the process with the correlation structure, standard deviations, and means are listed below.

$$\mathbf{R}_{00} = \begin{bmatrix} 1 & 0.7 & 0.9 \\ 0.7 & 1 & 0.6 \\ 0.9 & 0.6 & 1 \end{bmatrix}, \mathbf{S}_{R_{00}} = \begin{bmatrix} 1.6 \\ 1.2 \\ 0.9 \end{bmatrix}, \mu_{R_{00}} = \begin{bmatrix} 3 \\ 15 \\ 9 \end{bmatrix}$$

- 2. Use the process parameters chosen above to simulate the in-control sample data according to the design of sample size, number of sample size, and bootstrap resampling size at different levels, which are listed in Table V.1.
- 3. Replicate each pool of the total observations from the in-control process sample data A times that is also listed in the Table V.1.
- 4. Use the replicated data pool to resample B times of size n, and calculated the sample major elements for B samples.
- 5. Compute the control limits by percentile method and estimated by the chi-square distribution of sample major elements.

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6. Calculated Bias% of the percentile control limits from the sample major elements control limits calculated from chi-square distribution.

	n	K	В	A
	Sample Size	number of	Resamples	No of
No	_	samples		Replicates
1	6	25	1000	40
2	6	25	1500	60
3	6	25	2000	80
4	6	25	2500	100
5	6	50	1000	20
6	6	50	1500	30
7	6	50	2000	40
8	6	50	2500	50
9	8	25	1000	40
10	8	25	1500	60
11	8	25	2000	80
12	8	25	2500	100
13	8	50	1000	20
14	8	50	1500	30
15	8	50	2000	40
16	8	50	2500	50

Table V.1 Sampling Plan for the Simulated Study

V.2 SAS Program for Bootstrap Percentile Control Limits of Major Elements

The original SAS program for Bootstrap Resampling is written in SAS/MACRO language and can be obtained from the user support documents supplied by SAS Institute Inc. The original program is modified to accommodate the purposes of computing the sample major elements and percentile control limits for the major elements. The coding of the program is relatively long; therefore, it is not listed in this appendix. However, interested reader can obtain the original program from the web site address listed below, or contact the author for the modified program.

http://www.sas.com/techsup/dowload/stat/jackboot.sas

V.3 Study Results

Chi-Square Control Limits for Sample Major Elements							
n	k	M11_UCL	M22_UCL	M33_UCL		······································	
6	25	5.0174	1.5761	4.1401			
8	25	4.4436	1.4190	3.4032			
6	50	5.7124	1.5120	4.6807	ĺ		
8	50	4.1447	1.3910	3.2012	1		
	B	lootstrap Pe	rcentile Co	ntrol Limits	for Major E	lemnts	
Resam	ple (B)=	=1000			[Bias%	
n	k	M 11_UCL	M 22_UCL	M _{33_UCL}	(M _{11_UCL})	(M _{22_UCL})	(M _{33_UCL})
6	25	5.7239	1.7931	4.5556	14.08%	13.77%	10.04%
8	25	4.9077	1.2435	3.8257	10.44%	12.37%	12.41%
6	50	6.1043	1.6250	4.9337	6.86%	7.47%	5.40%
8	50	4.3015	1.4502	3.3167	3.78%	4.26%	3.61%
Resam	ple (B)=	=1500				Bias%	
n	k	M 11_UCL	M 22_UCL	M _{33_UCL}	(M_{11_UCL})	(M _{22_UCL})	(M _{33_UCL})
6	25	5.3798	1.6564	4.3626	7.22%	5.10%	5.37%
8	25	4.7422	1.4986	3.6189	6.72%	5.61%	6.34%
6	50	6.0015	1.5751	4.8928	5.06%	4.18%	4.53%
8	50	3.9587	1.3559	3.2763	4.49%	2.53%	2.35%
Resam	ple (B)=	=2000				Bias%	
n	k	M 11_UCL	M 22_UCL	M _{33_UCL}	(M _{11_UCL})	(M _{22_UCL})	(M _{33_UCL})
6	25	5.1578	1.6528	4.2415	2.80%	4.87%	2.45%
8	25	4.5897	1.4652	3.4744	3.29%	3.26%	2.09%
6	50	5.8258	1.5352	4.7888	1.98%	1.53%	2.31%
8	50	4.0985	1.4115	3.1545	1.11%	1.47%	1.46%
Resam	ple (B)=	2500				Bias%	
n	k	M 11_UCL	M 22_UCL	M _{33_UCL}	(M _{11_UCL})	(M _{22_UCL})	(M _{33_UCL})
6	_25	5.1175	1.5996	4.2425	1.99%	1.49%	2.47%
8	25	4.4988	1.3959	3.5238	1.24%	1.63%	3.54%
6	50	5.8354	1.4846	4.6087	2.15%	1.81%	1.54%
8	50	4.1678	1.3815	3.1987	0.56%	0.68%	0.08%

VITA

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