

Profile Monitoring - Control Chart Schemes for Monitoring Linear and Low  
Order Polynomial Profiles

by

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A Dissertation Presented in Partial Fulfillment  
of the Requirements for the Degree  
Doctor of Philosophy

ARIZONA STATE UNIVERSITY

December 2010

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Order Polynomial Profiles

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## ABSTRACT

The emergence of new technologies as well as a fresh look at analyzing existing processes have given rise to a new type of response characteristic, known as a profile. Profiles are useful when a quality variable is functionally dependent on one or more explanatory, or independent, variables. So, instead of observing a single measurement on each unit or product a set of values is obtained over a range which, when plotted, takes the shape of a curve. Traditional multivariate monitoring schemes are inadequate for monitoring profiles due to high dimensionality and poor use of the information stored in functional form leading to very large variance-covariance matrices. Profile monitoring has become an important area of study in statistical process control and is being actively addressed by researchers across the globe. This research explores the understanding of the area in three parts.

A comparative analysis is conducted of two linear profile-monitoring techniques based on probability of false alarm rate and average run length (ARL) under shifts in the model parameters. The two techniques studied are control chart based on classical calibration statistic and a control chart based on the parameters of a linear model. The research demonstrates that a profile characterized by a parametric model is more efficient monitoring scheme than one based on monitoring only the individual features of the profile.

A likelihood ratio based changepoint control chart is proposed for detecting a sustained step shift in low order polynomial profiles. The test statistic

is plotted on a Shewhart like chart with control limits derived from asymptotic distribution theory. The statistic is factored to reflect the variation due to the parameters in to aid in interpreting an out of control signal.

The research also looks at the robust parameter design study of profiles, also referred to as signal response systems. Such experiments are often necessary for understanding and reducing the common cause variation in systems. A split-plot approach is proposed to analyze the profiles. It is demonstrated that an explicit modeling of variance components using generalized linear mixed models approach has more precise point estimates and tighter confidence intervals.

## DEDICATION

To Dad, Mom, Stueti and Shashi

## ACKNOWLEDGEMENTS

First of all, I thank Dr. Montgomery and Dr. Woodall for introducing me to the field of profile monitoring. I am deeply grateful to Dr. Montgomery for his guidance, support and immense patience. He is an inspiration. I am thankful to Dr. Borrer for being a great mentor throughout.

I appreciate the timely and invaluable guidance and help provided by my committee members, Dr. Fowler, Dr. Kulahci and Dr. Prewitt.

A very special thank you to all the colleagues who have helped along the way especially Busaba, Dana, Fang, Jing, Nat, Aziz, and Darshit. Also would like to acknowledge the support of colleagues at Risk Management Solutions.

I want to acknowledge the unconditional love and support of my amazing parents, parents-in-law, Stueti, Shashi, Anu, and wonderful friends Shampa, Payal, and Rati.

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## 1. Introduction

Every process is affected by random fluctuations. These random fluctuations can be due to chance causes or assignable causes. An assignable cause is a result of an external change in the process and can be corrected by taking appropriate actions. A chance cause is due to the inherent variability in the process and it is difficult to eliminate or sometimes control. The primary aim of statistical process control is to identify the assignable cause variability in the process and to signal to the operating personnel to take appropriate actions. One tool that is used as a quick visual detection aid is a control chart. The research in the field of statistical process monitoring and control was initiated by the emergence of control charts in 1924, when Dr. W. A. Shewhart proposed the concept of a visual monitoring scheme with control limits to detect changes in the process mean over time, Shewhart (1925, 1931). This formed the basis of the Shewhart control chart for monitoring process mean and variance. Since then, significant contributions have been made in the field and new charting schemes with improved performances have been proposed.

### 1.1. Univariate Control Chart

In process monitoring the type of quality characteristics of interest can be broadly grouped into two categories – univariate and multivariate. A typical control chart has two basic components, the time evolution of the statistics being tracked and the control limit(s), upper or lower or both, signaling process behavior beyond the control limits of an expected probability of occurrence less than equal to 0.005. If the process is in-control, almost all the values of the characteristic fall within the control limits. The most basic univariate control chart

is the Shewhart chart. For a univariate characteristic  $w$ , if the mean and standard deviation of  $w$  be  $\mu_w$  and  $\sigma_w$ , the control limits are defined as, see Montgomery (2005):

$$\begin{aligned} LCL &= \mu_w - L\sigma_w \\ CL &= \mu_w \\ UCL &= \mu_w + L\sigma_w \end{aligned} \quad (1.1)$$

where  $L$  is the distance of the control limits from the center line. Univariate control chart to monitor the process standard deviation can be expressed as:

$$\begin{aligned} LCL &= C_l \sigma_w \\ CL &= C_c \sigma_w \\ UCL &= C_u \sigma_w \end{aligned} \quad (1.2)$$

where  $C_l$ ,  $C_c$ , and  $C_u$  are appropriate constants for the lower, upper and center limits. Other charts commonly used for monitoring a univariate response are the cumulative sum (Cusum) where the control chart statistic is the cumulative sum of the deviations of the sample average from the in-control process mean,  $C_i = \sum_{j=1}^i (\bar{x}_j - \mu_0)$ . Another control chart which weighs the past observations is the exponentially weighted moving average (EWMA),  $z_j = \lambda x_i + (1 - \lambda)z_{i-1}$ . Here  $\lambda$  is a constant and typically the starting value is set at the process mean, i.e.  $z_0 = \mu_0$ . These charts weigh past observations, unlike the Shewhart chart, and are shown to be better in detecting shifts of smaller magnitude. There are additional univariate charts designed for special situations and the reader is referred to Montgomery (2005) for more details.

Process monitoring using control charts is a two stage process - Phase I and Phase II, Woodall (2000). The goal in Phase I is to evaluate the statistical stability of the process and to estimate the in-control values of the process parameters after the out of control points are dealt with. In Phase II, process is monitored with the objective to quickly detect out of control shifts in the process from the in-control behavior established in the Phase I. Different types of statistical methods are appropriate for the two phases with each type requiring different measures of statistical performance. In Phase I it is important to assess the probability of deciding whether the process is stable or not. It is gauged by the probability of obtaining an out of control signal.

In Phase II, the emphasis is on detecting process changes as quickly as possible. This is usually measured by parameters of the run length distribution. The run length is the number of samples taken before a sample falls outside the control limits and is distributed according to a geometric distribution with parameter  $p$ , where  $p$  is the probability of the sample statistic falling outside the control limits. Hence the average run length (ARL) for the in-control situation for the Shewhart control charts can be defined as

$$ARL = \frac{1}{\alpha} \quad (1.3)$$

For the out of control situation, ARL is the inverse of probability of detecting the shift in the first subsequent sample, which is  $\frac{1}{(1-\beta)}$ . ARL is used as a metric to evaluate the performance of a control chart simulated under varies types of shifts such as sustained shift, step shift or a run-up or run-down.

When designing a control chart there are two types of errors one can make

- fail to detect an out of control behavior or signal an out of control situation when it did not occur, also known as a false alarm.

The objective of any control chart is to minimize the time to detect an out of control situation while controlling for the false alarm rate.

### **1.2. Multivariate Control Charts**

When the overall quality of a product or process is characterized by several correlated quality characteristics measured at a particular sample point in the process, it is more efficient to monitor the joint distribution of the metrics. The univariate Shewhart-type, Cusum and EWMA charts have been extended to the multivariate case, Hotelling's  $T^2$  chart, multivariate EWMA (MEWMA) chart and multivariate Cusum (MCUSUM) charts respectively. The Hotelling's  $T^2$  statistic is based on multivariate normal distribution and the control chart statistic can be viewed as the generalized distance between the observed vector from the mean vector weighted by the covariance matrix,  $(\bar{\mathbf{x}} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu})$ . Please refer to Montgomery (2005) for details on these charts.

### **1.3. Profiles**

Consider a case when the quality characteristic of interest is a curve. So each sample consists of ordered values of the variable of interest measured over a range of another temporal or spatial variable. This is also been referred to as functional data [Ramsay and Silverman (1997)], waveform or signature. Profiles are different from a multivariate quality characteristic in that the observed

responses are ordered and the relationship between the quality variable over the range of explanatory variable is of interest.

Profiles are of interest in various situations from food production, manufacturing, testing or calibration, process industries. One of the initial applications of profile monitoring was in calibration to ascertain performance of the measurement method and to verify that it remained unchanged over time. It has also been used to determine optimum calibration frequency and to avoid errors due to over-calibration. Rosenblatt and Spiegelman (1981) discuss these issues in calibration and suggest the use of control charts to determine the need for recalibration. Various control charts have been proposed to monitor measurement gauges and calibration curves thus obtained, see Croarkin and Varner (1982), Mestek et al. (1994), Stover and Brill (1998), Kang and Albin (2000), and Chang and Gan (2007).

Profiles occur in many other areas, such as performance testing where the response is a performance curve over a range of an independent variable such as frequency or speed, Bisgaard and Steinberg (1997). Nair et al. (2002) present an example from injection molding where the response of interest is the compression strength of foam measured over different amounts of compression level. They also gave an example of designing a robust alternator, where the aim is to obtain a desired current profile over a range of speed.

Jin and Shi (2001) refer to profiles as waveform signals and cite examples of force and torque signals collected from online sensors. Boeing (1998, pp. 89-



92) proposed a location control chart for the case when numerous measurements of the same variable are made on several locations. The control limits are constructed based on the responses at that location, ignoring the multivariate structure of the data. Sahni et al. (2005) presents an example of a profile response from a mayonnaise production process in the food industry. Some of the examples of the profiles are shown in (Figures 1 and 2). Further examples of profiles and profile monitoring methods are given by Woodall et al. (2004) and Woodall (2007) who reviewed papers related to this topic, identified some weaknesses in existing methods, and identified research directions.

Profile monitoring ideas have been extended to detecting clusters of disease incidence. Woodall (2006) provide an overview of the approaches used in public health surveillance. Zhou and Lawson (2007) demonstrate application of the MEWMA to a spatial map of disease incidence.

There are processes when one observes a series of observations which generate curves over time. The key feature that separates profiles is that the curves over time or space are obtained sequentially and it has been assumed that the two profiles sampled are assumed to be independent. Jiang et al. (2007) discuss a case study when they observe a concurrent time series of telephone usage for multiple customers. Woodall (2007) argue that such processes with time series curves do not fall under the definition of profiles and hence will not be discussed further. For more examples of what does not constitute as a profile under the definition considered here please refer to Woodall (2007).

#### **1.4. Importance of the work**

In profile monitoring the parameters of the interest are often the relationship between the dependent and independent variables and the nature of the variance between and with the curves. The multivariate techniques often are inadequate for monitoring since the existing methods fail to capture the relationship between the response and explanatory variable and autocorrelation between the observations. This might lead to scheme with little interpretability of the control chart statistic. Further in most of the situations, the sampling points per profile are usually more than ten points. This would make multivariate scheme cumbersome to design. Hence research is needed to identify schemes that would be efficient to monitor the distance or features between the profiles. Till date many monitoring schemes have been proposed that smooth the profile using a parametric model and then designs a control chart on the parameters of the model. The work has been grouped by the nature of the model fit to the profile, which could be linear, polynomial, nonlinear or a waveform.

#### **1.5. Problem Statement and the Scope of the Proposed Research**

The objective of profile monitoring like any other process monitoring situation, is to detect the out of control behavior as quickly as possible while maintaining the occurrence of false alarms to a minimum. The out of control event for a stable process is defined such that a probability of occurrence of less than three sigma. Control schemes based on existing multivariate methods fail to account for the correlation between the sequentially sampled measurements

within a profile. Further the schemes which monitor only local features of the profiles have a high probability of missing a shift occurring in another location.

In the recent past, many monitoring schemes have been proposed and some have been compared, but there is need for more research in the area as discussed by Woodall, Spitzner, Montgomery, and Gupta (2004). The article is the result of the initial work on the topic of profile monitoring and forms the basis for the literature review. Since the time the study was conducted, there has been quite a lot of interest in the area across the globe. So in the next chapter, there is an up to date literature review of the work in the field.

In chapter 3, a comparative study of two linear profile monitoring techniques is presented. The comparison criterion is the average run length performance under shifts of different magnitude in the intercept, slope and the error variance. The two techniques studied are the Croarkin and Varner (1982) control chart (henceforth referred to as the NIST Method) and a modified version of the combined control chart of Kim et al. (2003) (henceforth referred to as KMW). It is found that the KMW scheme of simultaneous monitoring the intercept, slope and error standard deviation either with Shewhart control charts or EWMA control charts detects shifts more quickly than the NIST scheme. In addition, the KMW methods are found to be much easier to interpret unlike the classical estimator based technique, the NIST method in which the estimator is plagued with infinite variance and undefined expectation. This work has been

published in the *International Journal of Production Research*, Gupta et al. (2005).

In Chapter 4, results of changepoint method to monitor low order polynomial profiles is presented. A likelihood ratio test is used to detect a sustained step shift in the process. The test statistic is plotted on a Shewhart like chart with control limits derived from asymptotic distribution theory. Further, the test statistic is factored to reflect the variation due to the parameters to aid in interpreting an out of control signal. This work was presented at the 2006 Joint Research Conference, Gupta et al. (2006).

In Chapter 5 we briefly discuss experimental robust experimental design and analysis of profile experiments. Profile generating systems in the robust parameter design literature are often referred to as signal-response system. We demonstrate that explicit modeling of variance components using a generalized linear mixed model leads to more precise point estimates of important model coefficients with shorter confidence intervals. This work has been published in the *Quality and Reliability Engineering International*, Gupta et al. (2010).

Chapter 6 ends with a summary of the major findings from this research and some recommendations for future research.

## 2. Profile Monitoring – Literature Review

Profiles as quality characteristics have existed in various fields since the start of the industrial revolution, but tools and methodology to monitor those have matured only in the recent few years. This has been brought about by advances in sensing technology for capturing and storing multidimensional data and faster computing technologies that has enabled complex transformations and manipulations of the large datasets quickly and economically.

Before we review the literature, we discuss various issues that are critical for designing a profile monitoring control chart; namely model selection, control chart statistic and phase I and phase II applications of control charts.

### 2.1. Model Selection

Most of the early work in the area of profile monitoring has focused on techniques for parametric single factor fixed effect models, see Woodall et al. (2004) and references therein. Staudhammer et al. (2007) discuss the issue of autocorrelation within the profile resulting from closely sampled observations and propose ARIMA models to represent the profiles. Jensen, Birch and Woodall (2007) and Jensen and Birch (2008) propose fitting a mixed effects models to account for the randomness component of the parameters and also include the autocorrelated variance structure. Gupta et al. (2006), Kazemzadeh et al. (2008) study situations where the profile can be modeled using a low order polynomial model. Williams, Woodall and Birch (2003) model the dose response profiles using a four parametric logistic model. Jensen, Hui, and Ghare (1984), Mahmoud

(2007) and Zou, Wang, and Tsung (2007) consider multiple regression models. Colosimo, Pacella and Semeraro (2007) have studied geometric profiles and modeled them using a spatial autoregressive error model with Fourier-based regressors. Quite a few researchers have worked on smoothing the profile using a nonparametric model, see Kernel Smooth regression of Winistorfer et al. (1996), two dimensional splines of Gardner et al. (2007), spline of Boeing (1998, pp. 140-144). Additionally, Ding et al. (2006), Colosimo and Pacella (2007) and Moguerza et al. (2007) have proposed reducing the dimensionality of the data by independent component analysis models, functional principal components analysis and support vector machines respectively. Jin and Shi (2001) use wavelets to model stamping force profiles. Other work on using wavelets include Reis and Saraiva (2006), Zhou Sun and Shi (2006), Jeong Lu and Wang (2006), Chicken and Pignatiello (2009).

Among the parametric models, more work has been published for the linear models as compared to the nonlinear models. It can be seen that a wide variety of the models have been used to model the profile. We recommend using the simplest adequate model. When using more elaborate models, one has to be careful about the control chart statistic that would be efficient in detecting and diagnosing the out-of-control situation.

## **2.2. Control Chart Statistic**

As we discuss in chapter 1, it is very important to define a statistic which captures the functional form into values that can be tracked easily. Any profile

can be represented by an adequate model, a statistic which is a function of the parameters would be sufficient in tracking changes in the model. For parametric models, the parameters of the model namely the coefficients and the error variance are sufficient statistics to describe the model. In fact, out-of-control signal explained in terms of the parameters is quite efficient in diagnosing the shift. For the cases where the coefficients of the model can be made independent, especially for the linear and the polynomial models, individual control charts can be constructed for all the parameters or only for the parameters of interest, Kim Mahmoud and Woodall (2003). In case of the linear model, the intercept and the slope parameter can be made independent. Various authors have proposed monitoring the coefficients individually using a Shewhart or an EWMA chart or the vector of coefficients using a  $T^2$  statistic or a MEWMA chart. The coefficients of the polynomial model can be made independent by using orthogonal polynomials. This also helps in reducing the multicollinearity issue which might lead to an ill-conditioned matrix and hence inaccurate estimates of the parameters. Several authors have also proposed metrics based on residuals. For example, Croarkin and Varner (1982), Kang and Albin (2000), likelihood statistic by Mahmoud et al. (2006). For nonlinear models, the coefficients of the model are dependent and cannot be monitored using individual charts, so a multivariate statistic like the MEWMA or a  $T^2$  has to be proposed. There are multiple ways to construct the  $T^2$  statistics, Williams et al. (2007b) study various methods in detail

and demonstrate that the  $T^2$  statistic based on successive difference of the parameters is very efficient in detecting shifts.

For the nonparametric profiles, Gardner et al. (1997) have suggested using a distance based metric. But as Ding et al. (2006) point out that one has to be cautious in using the simple descriptive statistics as control chart statistics since these types of statistics would miss other local feature and would lead to a scheme which has high false alarm rate.

### **2.3. Phase I and Phase II**

Process monitoring using control charts is a two stage process - Phase I and Phase II. The goal in Phase I is to evaluate the statistical stability of the process, and after dealing with any assignable causes, to estimate the in-control values of the process parameters. In Phase II, one is concerned with monitoring the on-line data to quickly detect shifts in the process from the in-control behavior established in the Phase I. Different types of statistical methods are appropriate for the two phases with each type requiring different measures of statistical performance. In Phase I, it is important to assess the probability of deciding whether the process is stable or not. It is gauged by the probability of obtaining an out of control signal.

In Phase II, the emphasis is on detecting process changes as quickly as possible. This is usually measured by parameters of the run length distribution. The run length is the number of samples taken before a sample falls outside the control limits and is distributed according to a geometric distribution with



parameter  $p$ , where  $p$  is the probability of the sample statistic falling outside the control limits. Hence the average run length (ARL) for the in-control situation can be defined as

$$ARL = \frac{1}{\alpha}$$

For the out of control situation, the ARL is the inverse of probability of detecting the shift in the first subsequent sample, which is  $\frac{1}{(1-\beta)}$ . ARL is used as a metric to evaluate the performance of a control chart simulated under various types of sustained shifts, step shift or a run-up or run-down.

Another objective of Phase I is to characterize the common cause variation among profiles. It is hard to detect changes in profiles when they are plotted on top of each other. Jones and Rice (1992) proposed a principal component approach to identify the first few modes of variation. In the case of profiles, viewing the first few eigenfunctions that indicate modes along which the profiles vary a lot, simplifies the visual representation of the profiles and also provides a perspective on subspace of the explanatory variable that has the highest variability. Colosimo and Pacella (2007) illustrate the PCA approach to study the variation among roundness profile. Woodall et al. (2004) illustrate the approach on particle density board profiles. Ding et al. (2006) treat PCA as a dimension reduction algorithm and highlight that PCA might not be optimal approach in clustering the in-control data separate from out-of-control profiles. Instead they propose independent component analysis (ICA) and define an interestingness metric that is maximized when the data is in-control. Gonzalez and Sanchez

(2008) propose monitoring the first few principal components. We caution against using such schemes unless it is supplemented by control charts on the rest of the principal components. Since any shift in the least significant principal components would make the process behave out-of-control but would be missed by scheme monitoring only the first few principal components.

#### **2.4. Linear Profile Monitoring**

Much of the literature in linear profile monitoring deals with Phase II application, assuming that the underlying in-control model parameters are known. Stover and Brill (1998) used the Hotelling  $T^2$  chart and a univariate chart based on the first principal component of the vectors of the estimated regression parameters to determine the response stability of a calibration instrument and the optimum calibration frequency. Kang and Albin (2000) suggested the use of a Hotelling  $T^2$  chart or a combination of an exponentially weighted moving average (EWMA) and the R chart based on residuals for monitoring Phase II linear profiles. They recommended the use of similar methods for Phase I. Kim et al. (2003) proposed transforming the  $x$ -values to achieve an average coded value of zero and then monitoring the intercept, slope and process standard deviation using three separate EWMA charts (called the EWMA3 method). They conducted performance studies and showed their method to be superior to the multivariate  $T^2$  and EWMA – R charts of Kang and Albin (2000).

For Phase I analysis Kim et al. (2003) suggested replacing the Phase II EWMA charts with Shewhart charts. Mahmoud and Woodall (2004) proposed the

use of a global F statistic based on an indicator variable technique to compare  $k$  regression lines in conjunction with a control chart to monitor the error variance term. They compared various Phase I methods with their procedure based on the probability of a signal under various shifts in the process parameters, and showed that their method often performed better than the use of the  $T^2$  control chart of Stover and Brill (1998), the  $T^2$  control chart of Kang and Albin (2000) and the three Shewhart control charts of Kim et al. (2003).

Croarkin and Varner (1982) have proposed monitoring the deviations of the three observations (one at each of the end points of the measurement range and one near the centre) from the standard for checking the calibration relationship. The quantities plotted on the control chart are obtained by correcting the measured or the  $y$ -values and then subtracting the standard or the  $x$ -values from it and it is of the form:

$$z_{ij} = \frac{y_{ij} - \beta_0}{\beta_1} - x_i ; i = 1, 2, \dots, n \quad (2.1)$$

Croarkin and Varner (1982) suggested plotting the deviations over the sample number. That means that the three deviations would line up vertically, and would be indicated by U, M or L for upper, middle and lower respectively. The method is pretty competitive as compared to the method of Kim et al. (2003) but performs poorly when there are more sampling points per profile as shown in Gupta, Montgomery and Woodall (2006). Further the statistic is also plagued with infinite variance, thus reducing the confidence in the method. See Kurtchkoff (1967, 1969), Williams (1969) and Berkson (1969). Chang and Gan (2007)

illustrate the application of profile monitoring to track the relationship between two measurement gauges. This relationship between two measurement gauges is also known as measure of linearity and is often expressed by the slope coefficient of the linear model obtained from regression one from the other. The model form assumed by the authors is  $y_i = g + bx_i + c$ , where  $c \sim N(0, bs_x^2 + s_y^2)$ . The authors then derive the distribution of beta which is a measure of linearity. Shewhart chart for the measure of linearity is proposed based on asymptotic distribution of standardized beta (standardized via dividing by the precision ratio  $s_y^2/s_x^2$ ). The authors propose building  $q$  charts for  $q$  pairs of measurements, but have not elaborated about the correlation between the pairs.

Kang and Albin (2000) suggested monitoring the residuals using a EWMA and R chart. They define the residuals as  $e_{ij} = y_{ij} - \beta_0 - \beta_1 x_i$  and suggest plotting the average of the residuals for each profile  $\bar{e}_j = \frac{1}{n} \sum_{i=1}^n e_{ij}$ , as a chart statistic for EWMA and R Chart. Kim et al. (2003) showed that these methods are pretty competitive to the individual coefficient monitoring scheme for a simple linear profile.

Approaches based on nonparametric control charting methods have been proposed. Wang and Tsung (2005) argue for monitoring  $q$ - $q$  plot of the samples collected from processes where sampling time is very small, especially when sensors are deployed for collecting data. The process or the quality characteristic of interest need not be a profile, but transforming the data into quantiles per

sampling time, lends this problem into the domain of profile monitoring. The authors believe that the shift in the process leads to change in the in-control distribution. Due to obvious ordering of the measurements within a  $q$ - $q$  profile, authors use generalized least squares to estimate the parameters. Authors propose monitoring each parameter using an EWMA chart and demonstrate the superiority of the proposed method with a performance study. The idea of monitoring  $q$ - $q$  curves is extension of the method proposed by Grimshaw and Alt (1997) to a profile monitoring case. The idea of transforming the univariate data to a  $q$ - $q$  plot to set up a profile monitoring case is novel. In spite of its attractive features, this method is limited by quick detection of the root cause of the out-of-control situation.

Several authors have also suggested representing the profile as a mixed effect model, where the variation between the profiles is captured by random effects coefficient. Staudhammer et al. (2007) illustrate the application in a wood product manufacturing facility. They found that high level of autocorrelation had no effect on the efficiency of the control chart. Jensen et al. (2007) also discuss  $T^2$  chart to monitor the fixed effects and random effects coefficients. However presence of autocorrelation helps more than hurts the profile monitoring case and Jensen et al. (2007) demonstrate that for a balanced case, least square approach is quite sufficient. However under the following conditions mixed models are better suited to characterize the profiles, namely sample size between profiles is

different, there is missing data, the autocorrelation within the profile is small or if the sampling points per profile are quite small.

### **2.5. Change point Analysis**

Mahmoud et al. (2007) have proposed looking at profile monitoring as a changepoint detection problem and propose a likelihood ratio statistic (*lrt*) to detect the location and magnitude of the shift in linear profiles. Further the authors propose to split the *lrt* into three variance components, one each for the error variance, intercept, and the slope to get an idea about individual contributions of the intercept, slope and the error variance. Their split is similar to the one by Gulliksen and Wilks (1950). Zhou et al. (2007) look at self starting mechanism for change point based control charts for linear profiles. They extend the Hawkins et al. (2005) method of monitoring the likelihood ratio of the unknown parameters to profiles scenario. The authors propose once the subset of the sample has been shown to be in-control, the samples are excluded from the likelihood ratio test statistic and suggest using EWMA to offset the potential delay caused by small number of samples. The authors demonstrate the average run length performance of the proposed chart and do comparative analysis with the EWMA<sub>3</sub> chart of Kim et al. (2004).

Zhang, Li and Wang (2009) use an exponential weighting scheme for all the parameters that are eventually used for constructing the likelihood statistic. The authors compare their proposed ELR (exponentially smoothed likelihood ratio) control chart to the KMW chart of Kim et al. (2003) and MEWMA

approach of Zou et al. (2007). The simulations conducted shows comparative behavior of the all the three charts and the proposed chart performs modestly better than the other charts for detecting shifts in error variance.

Zou, Tsung and Wang (2007) proposed MEWMA chart for monitoring general linear profiles. They define their MEWMA statistic of parameters to include the error variance. The MEWMA statistic is defined as

$$W_j = \lambda Z_j + (1 - \lambda)W_{j-1}; \text{ where } Z_j \text{ is } (Z'_j(\beta), Z_j(\sigma))'. Z_j(\beta) = \left( \frac{\hat{\beta}_j - \beta}{\sigma} \right)$$

$$Z_j(\sigma) = \phi^{-1}\{F((n-p)\hat{\sigma}_j^2/\sigma^2; n-p)\}$$

Kazemzadeh, Noorossana, and Amiri (2008) extended the Mahmoud et al. (2007) approach to polynomial profile and the authors suggested centering the  $x$ -values to reduce the multicollinearity problem. The authors demonstrate the superiority of the changepoint approach as compared to the Williams et al. (2007)  $T^2$  statistic and Mahmoud and Woodall (2004)  $F$ -approach. We believe the multicollinearity among regression variables will result in an ill conditioning of the  $X$  matrix and will lead to unstable coefficients. In chapter 4 we discuss potential solution for avoiding the multicollinearity problem.

## 2.6. Non Linear Profile Monitoring

Non linear profiles occur as commonly as the linear profiles. Walker and Wright (2002) use additive models to compare particle density boards. This is a non parametric technique. Sahani et al. (2005) monitor the principal components of the NIR spectra data obtained from mayonnaise production. Williams et al.

(2003, 2007b) suggests using  $T^2$  chart to monitor parameters of the non linear function simultaneously. The authors proposed estimating the variance-covariance matrix using successive difference vector and demonstrate that the resultant chart is effective in detecting step and ramp shifts in the process. It is well known that  $T^2$  control chart is good at detecting changes in the process but it is extremely cumbersome to pin point the changes in the subset of the parameters as the number of parameters increase.

Ding et al. (2006) study the process with high dimensional dataset and propose reducing the dimensions using Independent Component Analysis and a Phase I control chart based change point approach. Colosimo and Pacella (2007) study circular profiles modeled using Fourier basis functions and develop a test statistics based on functional PCA. Moguerza et al. (2007) propose a phase I approach based on regression support vector machines to identify the extreme observations. Vaghefi et al. (2009) study two different approaches to monitor a nonlinear profile. One based on the parameters of the nonlinear regression and the other is based on a deviation metric from a standard profile.

Jin and Shi (2001) model the response of a tonnage stamping process using wavelets and monitor wavelet coefficients of the torque signals to detect changes in the stamping process. Reis and Saraiva (2006), Zhou, Sun and Shi (2006), Jeong, Lu and Wang (2006), and Chicken et al. (2009) also study approaches based on wavelets. This is a sophisticated method to monitor the data, but I would think that tracing the actual cause of the shift would be difficult.



## 2.7. Multivariate Profile Monitoring

So far it has been seen that control chart techniques based on monitoring the parameters of the regression line the profile takes shape is very efficient for the univariate straight profile. Among the first to take this approach for multiple regression case were Jensen, Hui and Ghare (1984). They propose control charts for monitoring change in form of the model, change in model parameters, a control chart for isolating the coefficients that have changed and variance control chart based on  $F$  distribution.

Multivariate profiles are common in chemometrics and monitoring schemes based on latent variable methods, like partial least squares and principal components are used. Krouti and MacGregor (1996) suggest one such approach. There is a difference between the profiles studied by Krouti and MacGregor (1996) and ours. We study the case when the response is a function, whereas in their case the predictor is a function and response is a univariate value or a multivariate vector. For example, temperature profile in the boiler and response could be the molecular weight of the end product. Bharati and MacGregor (1998) proposed methods for the analysis of image data, where the images can be considered to be profiles. Gardner et al. (1997) consider two-dimensional wafer surfaces as profiles and proposed distance based metrics to monitor the presence of a systematic shift. No performance comparison was conducted. Zhou and Lawson (2007) monitor disease maps over time using spatial model.

## 2.8. Conclusion

Since Woodall et al. (2004), there has been considerable interest in profile monitoring and it is evident in the growing number of publications in the field. Few general themes emerge among the research so far, namely, 1) there is consensus among the researchers to reduce the dimensionality of the data, either by using a latent variable or reducing the profile to parameters of the smooth function, 2) most of the work has focused on shifts in the mean profile, and, 3) there has been almost equal emphasis on the Phase I and Phase II applications of profile monitoring. There are a few topics that would need more consideration. Very little work has been done in this area involving profiles with multiple covariates and multivariate profile surfaces. In non linear analysis, it is expected that the number of parameters will increase and it becomes essential to have a technique that will provide quick way to trace the root cause of the problem. There has been considerable work done in using Principal Component Analysis. Profile monitoring is a widely applicable and an active area of research.

### 3. Performance evaluation of two methods for online monitoring of linear calibration profiles

#### 3.1. Introduction

The focus of this paper is to perform a Phase II comparative study between the Croarkin and Varner (1982) control chart (henceforth referred to as the NIST Method) and the combined control chart of Kim et al. (2003) (henceforth referred to as KMW). We compare the two methods on the basis of ARL performance under sustained shifts of different magnitudes in the intercept, slope and the error variance.

#### 3.2. Description of the Methods

The in-control model for the  $i^{\text{th}}$  observation within the  $j^{\text{th}}$  random sample is assumed to be of a simple linear form  $y_{ij} = \beta_0 + \beta_1 x_i + \varepsilon_{ij}$ ,  $i = 1, 2, \dots, n$ , where the  $\varepsilon_{ij}$ 's are independent, identically distributed (i.i.d.) normal random variables with mean zero and known variance  $\sigma^2$ . The regression coefficients, the intercept ( $\beta_0$ ) and the slope ( $\beta_1$ ), are assumed to be known.

Croarkin and Varner (1982) suggest using monitoring techniques for calibration curves similar to those for individual measurements. The method is described in the NIST/SEMATECH e-Handbook of Statistical Methods (see references for the website). The control chart statistic is obtained by first 'correcting' the measured values ( $y$ -values) and then subtracting the standard  $x$ -value from it. The quantities plotted on the control chart at the time of the  $j^{\text{th}}$  sample are

$$z_{ij}^{**} = \frac{y_{ij} - \beta_0}{\beta_1} - x_i \quad ; i = 1, 2, \dots, n. \quad (3.1)$$

The control limits are established as

$$\text{Upper Control Limit } l_1 = s_c Z_\zeta^* \quad (3.2a)$$

$$\text{Lower Control Limit } l_2 = -s_c Z_\zeta^*, \quad (3.2b)$$

where,

$$s_c = \frac{\sigma}{\beta_1} . \quad (3.3)$$

Here  $\sigma$  is the assumed known standard deviation and  $\beta_1$  is the assumed known in-control value of the slope. The value  $Z_\zeta^*$  corresponds to the upper  $\zeta$  percentage point of the standard normal distribution, where  $\zeta$  is defined as

$$\zeta = \frac{1}{2} \left\{ 1 - e^{\left( \frac{\ln(1-\alpha)}{n} \right)} \right\}, \quad (3.4)$$

where  $n$  is the number of standards evaluated at each time period and  $\alpha$  is chosen to provide the desired in-control ARL using the relationship  $ARL_0 = 1/\alpha$ . The control limits in equation 3.2 are constructed using the standard normal value, instead of the  $t$  distribution value [as proposed by Croarkin and Varner (1982)], as the in-control parameter values are assumed to be known. The NIST method recommends measuring three standards (one near each end point of the measurement range and one near the centre) for checking the calibration relationship.

Kim et al. (2003) propose fitting a straight line to the calibration data in each sample over time and using separate EWMA or Shewhart charts for monitoring each of the regression coefficients and the standard deviation. The independent variable is subtracted from its mean to obtain a transformed variable. This technique makes the estimated least squares regression coefficients independent and they can be monitored individually using separate control charts. In our study we replace the EWMA charts by X-bar charts to monitor the intercept and slope and by an  $S^2$  chart to monitor the error variance. This modification makes the KMW procedure more similar to the NIST procedure.

The control limits for monitoring the intercept are

$$\begin{aligned}
 \text{UCL} &= \beta_0 + Z_{\alpha/2} \sqrt{\frac{\sigma^2}{n}} \\
 \text{Centre Line} &= \beta_0 \\
 \text{LCL} &= \beta_0 - Z_{\alpha/2} \sqrt{\frac{\sigma^2}{n}}.
 \end{aligned} \tag{3.5}$$

The control limits for monitoring the slope are

$$\begin{aligned}
 \text{UCL} &= \beta_1 + Z_{\alpha/2} \sqrt{\frac{\sigma^2}{S_{xx}}} \\
 \text{Centre Line} &= \beta_1 \\
 \text{LCL} &= \beta_1 - Z_{\alpha/2} \sqrt{\frac{\sigma^2}{S_{xx}}},
 \end{aligned} \tag{3.6}$$

where  $S_{xx}$  is defined as  $\sum_{i=1}^n (x_i - \bar{x})^2$  (refer Montgomery et al. (2001 pp. 15

-17)). Finally, the control limits for monitoring the error variance are

$$\begin{aligned}
\text{UCL} &= \frac{\sigma^2}{n-2} \chi_{\alpha/2, n-2}^2 \\
\text{Centre Line} &= \sigma^2 \\
\text{LCL} &= \frac{\sigma^2}{n-2} \chi_{(1-\alpha/2), n-2}^2,
\end{aligned} \tag{3.7}$$

where  $\chi_{\alpha/2, (n-2)}^2$  and  $\chi_{(1-\alpha/2), (n-2)}^2$  are the upper and lower  $\alpha/2$  percentage points of the chi-square distribution with  $n-2$  degrees of freedom associated with the residuals (see Montgomery (2004, pp. 212-248)). The value of  $\alpha_{overall}$  is calculated using the equation  $\alpha_{overall} = 1 - (1 - \alpha)^3$  and the in-control ARL is computed by taking the reciprocal of  $\alpha_{overall}$

### 3.3. Comparisons

In our comparisons the underlying in-control linear model assumed for both the methods is  $y_{ij} = 3 + 2x_i + \varepsilon_{ij}$ , with  $\varepsilon_{ij}$  i.i.d normal random variables with zero mean and unit variance. The  $x$ -values for each sample are initially fixed at 2, 4, 6, and 8 (a four-level case). Different numbers of levels of the  $x$ -values are also investigated, (3 and 10), and are discussed subsequently. For both the charts the same  $x$ -values are used for each sample. The transformed model following the KMW scheme is  $y_{ij} = 13 + 2x_i + \varepsilon_{ij}$  with the  $x$ -values of -3, -1, 1 and 3.

Monte Carlo simulation is used to obtain the ARL performance for both the methods. All simulations are conducted by tuning the NIST and the KMW charts to achieve an overall in-control ARL of 200. The ARL value is estimated by averaging the run lengths obtained by running 10 000 simulated charts. For the KMW-Shewhart charts,  $\alpha$  is set at 0.00167 to achieve a combined in-control

ARL of the three charts to be approximately 200. The individual in-control ARL for each of the Shewhart charts is 598.8. The  $\alpha$ -value for the NIST control chart is set at  $1/200 = 0.005$ . We consider various shifts in the parameters for the comparison study which are listed in (Table 3.1.)

Table 3.1. Shifts considered for the two methods

Type of shift	Notation	Values of the shift
Shift in Intercept	$\beta_0$ to $\beta_0 + \lambda\sigma$	For $\lambda = 0.2, 0.4, 0.6, \dots, 2.0$
Shift in Slope	$\beta_1$ to $\beta_1 + \delta\sigma$	For $\delta = 0.025, 0.050, 0.075, \dots, 0.25$
Shift in Standard Deviation	$\sigma$ to $\gamma\sigma$	For $\gamma = 1.2, 1.4, 1.6, \dots, 3.0$

There are two ways to compute the ARL for the Shewhart chart – analytically and using simulation. It is fairly easy to compute ARLs for each of the Shewhart charts monitoring the intercept and slope parameters using the equations in Montgomery (2004, pp. 233-235). The ARL calculation for the control chart for variance and for the situations involving combined charts and shifts would be more complicated. Simulation proves to be a straightforward alternative. To maintain uniformity in our comparisons, we use simulation to find the ARLs for all the control charts.

In the first part of the study we compare the performance of the original EWMA<sub>3</sub> procedure of KMW and the Shewhart chart version of KMW under shifts in the intercept and the error variance under the model  $y_{ij} = 3 + 2x_i + \varepsilon_{ij}$ . There are two ways a shift can occur in the slope, either in the original model ( $y_{ij} = 3 + 2x_i + \varepsilon_{ij}$ ) or in the transformed model ( $y_{ij} = 13 + 2x_i + \varepsilon_{ij}$ ). These shifts are depicted in (Figure 3.1.)

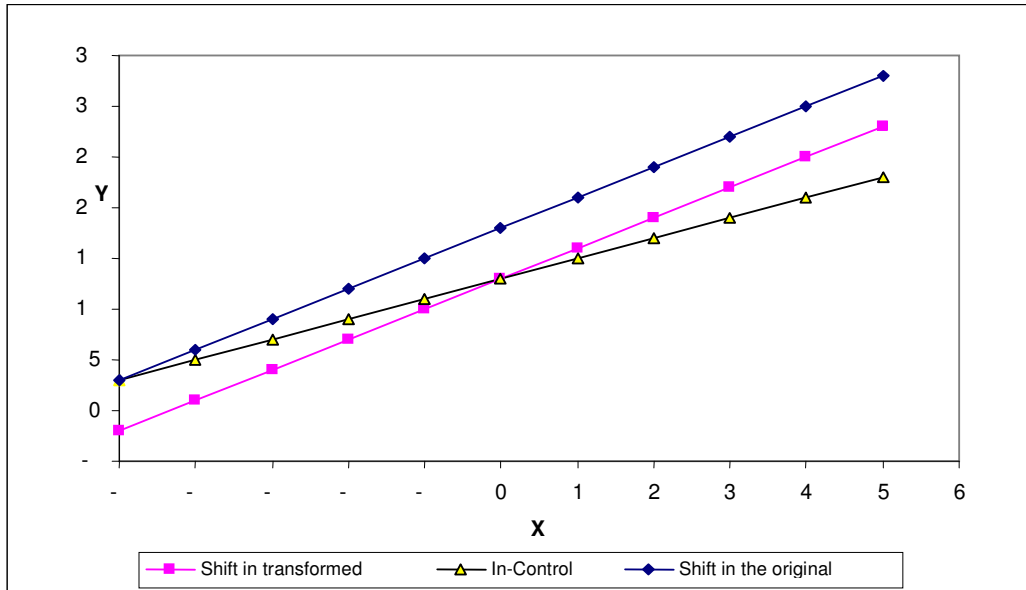


Figure 3.1. Comparison of the introduction of the shifts for unit shift in slope

From (Figure 3.1) it is apparent that the change in the shifted model from the baseline model is smaller when a unit shift in the slope was introduced in the coded model as compared to when the unit shift in slope was introduced in the original model. The combined ARL values for the three separate control charts for intercept, slope and standard deviation for the EWMA<sub>3</sub> and KMW-Shewhart methods are shown in (Tables 3.2, 3.3, and 3.4.)



Table 3.2. ARL comparison of KMW-Shewhart and KMW-EWMA charts under Intercept shifts

Shift in the intercept (Lambda)	EWMA <sub>3</sub> Chart (as reported by KMW)	Shewhart Charts
0	200	199.9
0.2	59.1	151.4
0.4	16.2	77.9
0.6	7.9	33.8
0.8	5.1	15.5
1	3.8	7.7
1.2	3.1	4.3
1.4	2.6	2.7
1.6	2.3	1.9
1.8	2.1	1.5
2	1.9	1.2

Table 3.3. ARL comparison of KMW-Shewhart and KMW-EWMA charts under Slope shifts

Shift in slope (Delta)	EWMA <sub>3</sub> (as reported by KMW – shift in the original model)	EWMA <sub>3</sub> (shift in the coded model)	Shewhart Charts (shift in the original model)	Shewhart Charts (shift in the coded model)
0	200	198.1	199.9	199.1
0.025	101.6	172.5	178.3	195.0
0.05	36.5	119.4	125.0	181.8
0.075	17	76.7	79.2	166.9
0.1	10.3	49.1	46.7	142.1
0.125	7.2	32.4	27.9	120.8
0.15	5.5	23	17.1	99.2
0.175	4.5	16.7	10.9	81.2
0.2	3.8	13.2	7.1	63.8
0.225	3.3	10.6	5.0	51.0
0.25	2.9	8.8	3.6	41.0

Table 3.4. ARL comparison of KMW-Shewhart and KMW-EWMA charts under Standard Deviation shifts

Shift in standard deviation (Gamma)	EWMA <sub>3</sub> (as reported by KMW )	Shewhart Charts
1	200	199.9
1.2	33.5	40.1
1.4	12.7	13.5
1.6	7.2	6.5
1.8	5.1	4.0
2	3.9	2.8
2.2	3.2	2.2
2.4	2.8	1.8
2.6	2.5	1.6
2.8	2.3	1.5
3	2.1	1.4

The larger ARL values for the case when the shift in the slope is introduced in the transformed model support our observations from (Figure 3.1.) We also considered the case where the shift is introduced in the original line. The EWMA charts did well at detecting small sustained shifts in the parameter coefficients. The performance of Shewhart charts is found to be very comparable to the performance of the EWMA charts for large shifts in the parameters. Both the charts have almost the same power of detection for shifts in the error standard deviation. These results are expected as it is well known that the EWMA chart is superior to a Shewhart chart in detecting small sustained shifts while for larger shifts the Shewhart chart is very effective. ARL values for the shift in the slope in the transformed model are larger than the ones in the original model. This part of the study demonstrates that to capture small sustained shifts EWMA charts are

better, whereas if the interest is in capturing spikes (or unsustained big disturbances), it is known that the Shewhart chart is the right choice. In situations where both kinds of shifts are of interest, Montgomery (2004) and others suggest a combined approach. For the second part of the study we choose Shewhart charts for KMW method to have a more direct comparison with Shewhart-type chart in the NIST method.

When we compare the KMW-Shewhart approach and the NIST method, we also vary the number of observations on the calibration curve that are being used, i.e.,  $n$ . Three, four, and ten levels are considered. The  $x$ -levels used in these cases are in (Table 3.5.)

Table 3.5.  $x$ -values considered

Number of levels	Notation	$x$ Levels
3	3a	2, 5, 8
	3b	1, 5, 10
4	4a	2, 4, 6, 8
10	10	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

The ARL values for various sustained shifts in intercept, slope and error standard deviation are shown in (Figures 3.2, 3.3, and 3.4) respectively. We consider only shifts in the original model. Unless otherwise mentioned for the three levels of  $x$ , case 3a is to be assumed. The number in the bracket in the discussion below refers to the number of  $x$ -values considered, so Shewhart (3a) refers to the KWM-Shewhart charting scheme for three values of  $x$ .

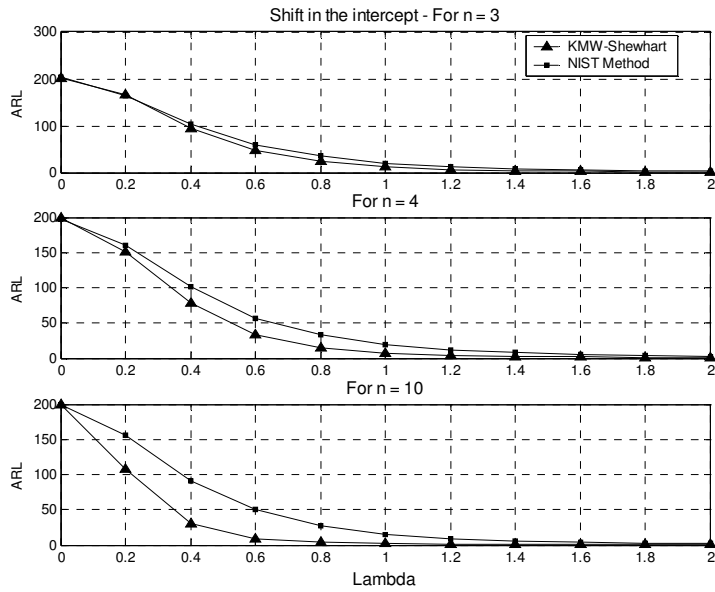


Figure 3.2. ARL comparison under Intercept shift from  $\beta_0$  to  $\beta_0 + \lambda\sigma$

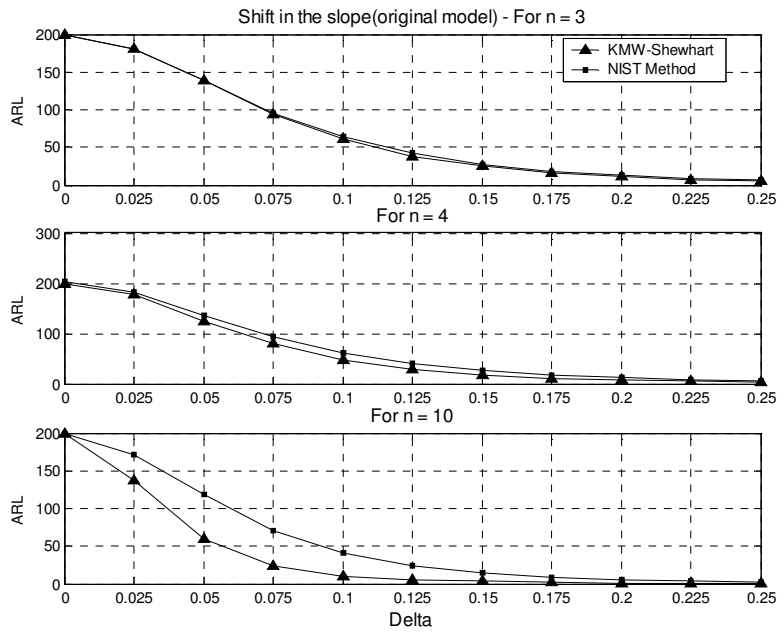


Figure 3.3. ARL comparison under slope shift from  $\beta_1$  to  $\beta_1 + \delta\sigma$

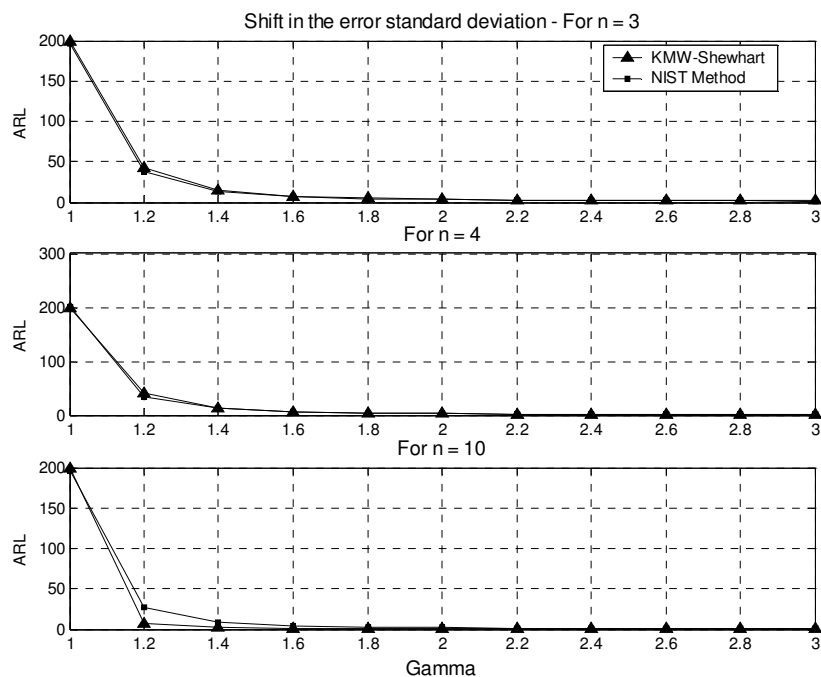


Figure 3.4. ARL comparison under Standard Deviation shift from  $\sigma$  to  $\gamma\sigma$

The plots of the ARLs under the intercept shift indicate that the KMW-Shewhart scheme performs better than the NIST scheme. The NIST scheme for monitoring 10 points, NIST (10), is approximately comparable to the KMW-Shewhart scheme for 3 points, Shewhart (3a), which indicates that we would need less time and fewer data points to reach the same conclusions by using the KMW-Shewhart scheme than we would by using the NIST Method. A similar pattern is seen for a shift in the slope. For a shift in the error standard deviation, both schemes have similar performance. These figures indicate that the Shewhart (10) scheme gives the overall best performance. Furthermore, the out-of-control ARL of the KMW-Shewhart scheme decreases much more quickly than the ARL for the NIST scheme as the number of the standard values increases.

Simultaneous sustained shifts in the intercept and slope are also considered. Kim et al. (2003) consider combined shifts in the coded regression coefficients for the intercept and the slope. We consider combined shifts in the original regression coefficients for the KMW-Shewhart method. The ARL values obtained are summarized in Appendix A where the first row in each cell contains the combined ARL values for the KMW-Shewhart method, the second row contains the combined ARL value for NIST method and the third row shows the percentage improvement in detecting sustained shifts by the KMW-Shewhart method as compared to the NIST method. The KMW-Shewhart method significantly outperforms the NIST method for all combinations of shifts in the slope and the intercept.

We also carried out several other studies to determine if the location of the values of the standards would improve the performance of the NIST method (not shown here). There is no significant improvement in the performance of the NIST method even if we increase the number of standards used.

### **3.4. An Example**

We use the example presented in the NIST/ SEMATECH e-Handbook of statistical methods (see references) to illustrate the two methods. The dataset consists of line widths of photomasks reference standards on 10 units (40 measurements) used for monitoring linear calibration profiles of an optical imaging system. The line widths are used to estimate the parameters of the linear

calibration profile,  $y_{ij} = 0.2817 + .9767x_i$  with a residual standard deviation of 0.06826 micrometers.

A monitoring scheme is established to monitor measurements on three units for upper, middle and lower end of the relevant measurement range from the estimated Phase I profile. The dataset is provided in (Table 3.7) and plotted in (Figure 3.5.) In the plot the in-control line is the established Phase I profile. On careful observation of the measurements for the fourth sample, the plotted values seem to be slightly offset from the in-control line. We employ both the KMW-Shewhart scheme and the NIST method to monitor the phase II line width data and the control charts are as shown in (Figures 3.6 and 3.7.)

Table 3.7. Line -width measurements for the example

DAY	POSITION	X	Y
1	L	0.76	1.12
1	M	3.29	3.49
1	U	8.89	9.11
2	L	0.76	0.99
2	M	3.29	3.53
2	U	8.89	8.89
3	L	0.76	1.05
3	M	3.29	3.46
3	U	8.89	9.02
4	L	0.76	0.76
4	M	3.29	3.75
4	U	8.89	9.3
5	L	0.76	0.96
5	M	3.29	3.53
5	U	8.89	9.05
6	L	0.76	1.03
6	M	3.29	3.52
6	U	8.89	9.02

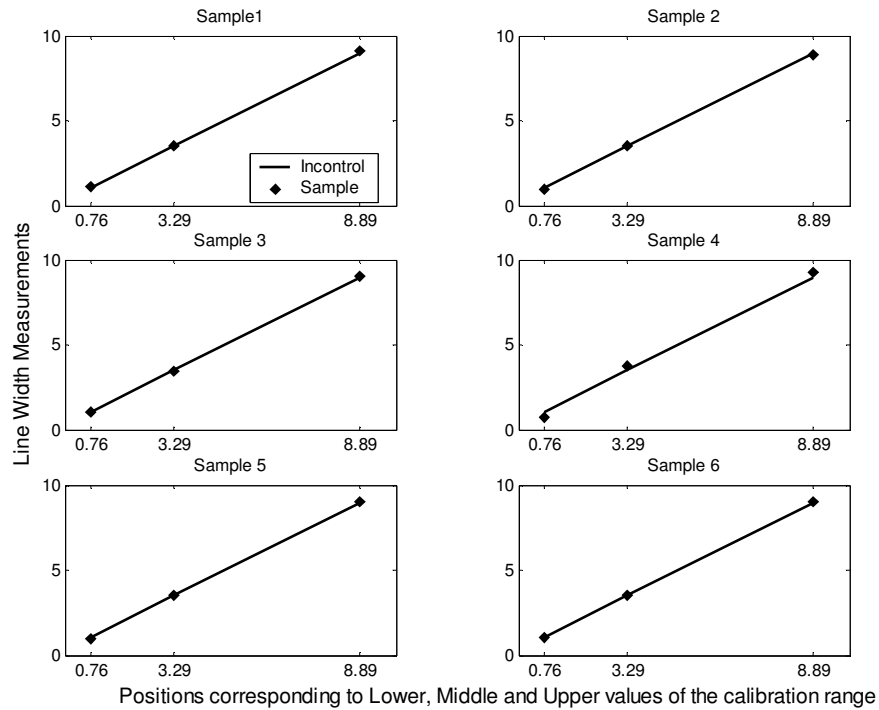


Figure 3.5. Plot of the line-width measurements



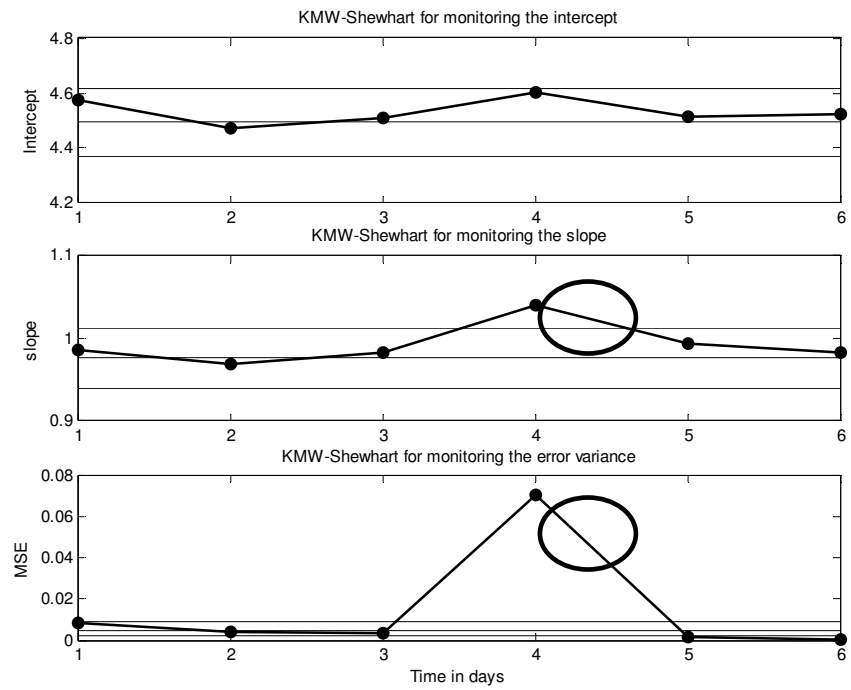


Figure 3.6. KMW-Shewhart charts for monitoring the parameters of the calibration line

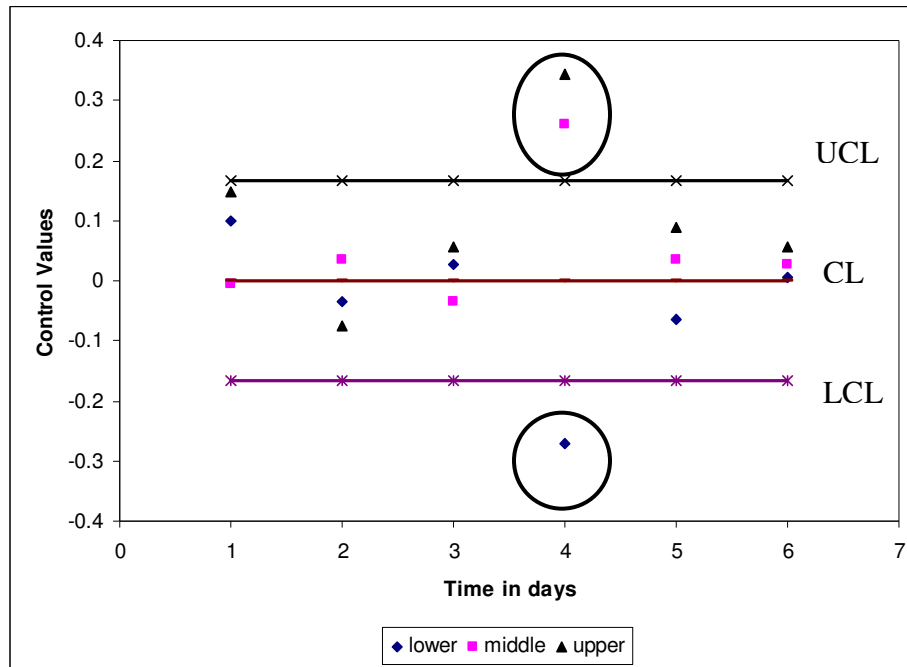


Figure 3.7. NIST chart for monitoring calibration line

In the KMW-Shewhart charts (see Figure 3.6), the three horizontal lines indicate upper control limit, centre line and lower control limits respectively, calculated using equations (3.5), (3.6) and (3.7). The numerical values of the upper control limit, centre line, and lower control limit for the intercept, slope and error variance charts are (4.62, 4.49, 4.37), (1.01, 0.98, 0.94) and (0.0087, 0.0046, 0.002), respectively. To achieve the overall in-control ARL of 200, the value of  $\alpha$  for KMW-Shewhart and NIST was adjusted to be 0.00167 and 0.005 respectively. The NIST chart is shown in (Figure 3.7.) Note that the measurements on the fourth day are out-of-control for both the NIST chart and the KMW-Shewhart charts. On the KMW-Shewhart, the error variance values on the fifth and sixth day are below the lower control limit with the values 0.0018 and 0.0000 respectively. Although this sample dataset is small, it is easily seen that

the KMW-Shewhart method provides more information and is easier to interpret than the NIST control chart.

### 3.5. Conclusions

Linear profiles occur often in calibration applications. A calibration curve is established based on the functional relationship between the measurement system values and the accepted values of the standard. Often large amounts of time and money are invested in recalibrating the system, even sometimes when the recalibration is not required. The aim has always been to optimize the calibration frequency and maintain a certain level of accuracy and precision. This could be achieved in part by monitoring the calibration curves over time. Among the two methods evaluated in this study, the KMW scheme of simultaneous monitoring the intercept, slope and error standard deviation either with Shewhart control charts or EWMA control charts detects sustained shifts more quickly than the NIST scheme. In addition the KMW methods are much easier to interpret.

The NIST method with an estimated in control calibration line is based on the classical method of calibration in which the calibration equation is

$$\hat{x} = \frac{y_o - \hat{\beta}_0}{\hat{\beta}_1} \quad (3.8)$$

where  $\hat{\beta}_0$  and  $\hat{\beta}_1$  are the estimates of the intercept and slope respectively,  $y_o$  is the measured variable, and  $\hat{x}$  is the estimated value of the variable of interest. The classical estimator is plagued with numerous weaknesses, Montgomery et al. (2001 pp. 503-508). Even though the estimator is minimum

variance unbiased and the estimator of the slope is assumed to be normally distributed and independent of  $y$  and  $\bar{y}$ , its reciprocal has infinite variance and it has undefined expectation. This leads to infinite mean square error and hence can result in poor performance of the method. Various researchers have discussed these points and some have proposed an alternative inverse method for calibration. Kurtchkoff (1967, 1969), Williams (1969) and Berkson (1969) have discussed in detail the weaknesses in the classical calibration method.

Considering the strengths of the KMW method compared to the NIST scheme, we suggest using the KMW scheme with either Shewhart charts or EWMA charts or a combination of both to monitor linear calibration curves.

## 4. The Use of Changepoint Statistics to Monitor Polynomial Profiles

### 4.1. Introduction

Non-linear profiles are as common as linear profiles, but techniques to monitor linear profiles have clearly outnumbered those for the non-linear situation. Non-linear profiles are common in engineering and sciences (Jin and Shi (2001), Walker and Wright (2001)). In the absence of prior mechanistic model form, most of the nonlinear profiles can be modeled adequately using a polynomial model or using piecewise polynomial models. In this article, we restrict our attention to the types of non linear profiles that can be adequately modeled using lower order polynomials. Few examples of polynomial profile include - acceleration and deceleration profile of an air bag in automotives, Marklund and Nilsson (2003). Sahni et al. (2005) discuss a scenario where monitoring the viscosity of mayonnaise over time is of interest.

In this study we investigate the changepoint approach for Phase I analysis of polynomial profiles and conclude the article with our comments on the Phase II aspect of profile monitoring using changepoint approach. The changepoint approach can be defined succinctly as follows. If  $y_1, y_2 \dots y_n$  are independent random vectors with probability distribution functions  $F_1, F_2 \dots F_n$ , respectively, the change point analysis can be defined as the problem of detecting the point in time when change(s) in the distribution of the observations occurred. The hypothesis being tested can be written as

$H_0: F_1 = F_2 = \dots = F_n$  versus  $H_a: F_1 = \dots = F_{m_1} \neq F_{m_1+1} = \dots = F_{m_q} \neq F_{m_q+1} = \dots = F_n$  ;

(4.1)

where  $m_1, m_2, \dots, m_q$  are the  $q$  unknown change point locations.

## 4.2. Development of the Changepoint Statistic

Various studies have been conducted to evaluate the changepoint approach, most of them assumed a linear sampling framework of the form  $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$ . In this study we focus on the techniques that have been proposed for a profile sample. A profile sample of  $k$  profiles is typically of the form  $\{(x_{i1}, y_{i1}), i = 1, 2, \dots, n_1\}, \{(x_{i2}, y_{i2}), i = 1, 2, \dots, n_2\}, \dots, \{(x_{ik}, y_{ik}), i = 1, 2, \dots, n_k\}$ , where each profile is assumed to have at least two observations [Mahmoud et al.(2004)].

The hypothesis being tested is whether the parameters of the model change from one profile to another, assuming the form of the model is the static and the parameters do not change within the profile. The changepoint model for a profile can be written as

$$y_{ij} = f(x_{ij}) + \varepsilon_{ij},$$

(4.2)

$$\text{and } \theta_{q-1} < j \leq \theta_q, q = 1, \dots, m, j = 1, \dots, k, i = 1, 2, \dots, n_j,$$

where  $\theta_q$  is the changepoint between the  $j$  profiles with  $i$  samples per profile and the  $\varepsilon_{ij} \sim N(0, \sigma_j^2)$ .

If we assume the distribution of the nuisance term to be  $N(0, \sigma_j^2)$ , then the likelihood ratio statistic (*lrt*) for a single changepoint or two segments ( $q = 2$ ) can be defined as (see Sullivan and Woodall (1996)):

$$lrt_{m_1} = N \log \hat{\sigma}^2 - N_1 \log \hat{\sigma}_1^2 - N_2 \log \hat{\sigma}_2^2, \quad \text{for } m_1 = 1, 2, \dots, m-1$$

(4.3)

where  $\hat{\sigma}^2$  is the maximum likelihood estimator (MLE) of the error variance of all the samples pooled together into a single sample of size  $N$ ,  $\hat{\sigma}_1^2$  is the MLE of the error variance of all the samples before the changepoint  $m_1$  of size  $N_1 (= \sum_{j=1}^{m_1} n_j)$

and  $\hat{\sigma}_2^2$  is the MLE of the error variance of all the samples after the changepoint  $m_1$  of size  $N_2 (= \sum_{j=m_1+1}^m n_j)$ . The likelihood ratio statistic in equation (3) can be used

to detect changes in both the mean and the error variance. Mahmoud et al. (2004) split the *lrt* for a linear profile into three variance components, one each for the error variance, intercept, and the slope to get an idea about individual contributions of the intercept, slope and the error variance. The splitting of the likelihood ratio into variance components is quite useful in diagnosing the cause of the shift and also detecting the potential cause of process deviance. It would be of interest to make sure that one of the components of variance is not dominating. Mahmoud et al. (2004) discuss inferring the status of the process by looking at the contribution of the variance components. Though it is a great diagnostic tool, care must be taken in not over adjusting the process based on the values. Gulliksen and

Wilks (1950) construct three step hierarchical hypothesis to tests the significance of the three variance components. We decomposed the likelihood ratio statistic for a second degree polynomial. Let's say that  $f(x_{ij})$  in equation (4.1) is represented by  $A_j + B_j x_{ij} + C_j x_{ij}^2$ , where the  $X$ -values are assumed to be fixed for each sample

and also assumed to be centered on zero. This implies that  $\sum_{i=1}^n x_i = \sum_{i=1}^n x_i^3 = 0$ .

Hence the maximum likelihood estimate, MLE of the total error variance can be written as

$$\sigma^2 = \hat{\sigma}^2 = \sum_{i=1}^N (Y_i - a - bx_i - cx_i^2)^2 / N$$

(4.4)

where  $N$  is the total number of samples ( $m*n$ ). For the samples before the split point  $m_1$  with a sample size of  $N_1$  and after the split point  $m_1$ , (sample size of  $N_2 = N - N_1$ ) the MLE of the error variance is defined as

$$\hat{\sigma}_1^2 = \sum_{i=1}^{N_1} (Y_i - a_1 - b_1 x_i - c_1 x_i^2)^2 / N_1,$$

$$\hat{\sigma}_2^2 = \sum_{i=N_1+1}^N (Y_i - a_2 - b_2 x_i - c_2 x_i^2)^2 / N_2$$

(4.5)

Hence the likelihood ratio statistic can be written as:

$$lrt_{m_1} = N \log[\hat{\sigma}^2 (\hat{\sigma}_1^2)^{-N_1/N} (\hat{\sigma}_2^2)^{-N_2/N}]$$

(4.6)



Further equation (4.4) can be expanded as the sum of the error variances defined in equation (5.5) and expressed as a function of the sum of squares

$$\begin{aligned}
\hat{\sigma}^2 &= \left[ \sum_{i=1}^{N_1} (Y_i - a_1 - b_1 x_i - c_1 x_i^2 - a - b x_i - c x_i^2 + a_1 + b_1 x_i + c_1 x_i^2)^2 \right. \\
&\quad \left. + \sum_{i=N_1+1}^N (Y_i - a_2 - b_2 x_i - c_2 x_i^2 - a - b x_i - c x_i^2 + a_2 + b_2 x_i + c_2 x_i^2)^2 \right] / N \\
&= [N_1 \hat{\sigma}_1^2 + N_1 \hat{\sigma}_1^2 + N_1 (a - a_1)^2 + N_2 (a - a_2)^2 + S_{x_1^2} (b - b_1)^2 + S_{x_2^2} (b - b_2)^2 \\
&\quad + S_{x_1^4} (c - c_1)^2 + S_{x_2^4} (c - c_2)^2 + 2(a - a_1)(c - c_1)S_{x_1^2} + 2(a - a_2)(c - c_2)S_{x_2^2}] / N
\end{aligned}
\tag{4.7}$$

where the sum of squares are defined as

$$S_{xy} = \sum x_i y_i; \quad S_{x^2} = \sum x_i^2; \quad S_{x^2 y} = \sum x_i^2 y_i; \quad S_{x^4} = \sum x_i^4$$

Now if  $d_a = \bar{Y}_2 - \bar{Y}_1$ ;  $d_b = b_2 - b_1$ ;  $d_c = c_2 - c_1$  and

$$\begin{aligned}
w_1 &= N_1 \hat{\sigma}_1^2 + N_1 \hat{\sigma}_1^2; \quad w_2 = \frac{S_{x_1^2} S_{x_2^2}}{S_{x^2}}; \quad w_3 = \frac{S_{x_1^4} S_{x_2^4}}{S_{x^4}}; \quad w_4 = \frac{N_1 N_2}{N}; \\
w_5 &= N_1 \left( c \frac{S_{x^2}}{N} - c_1 \frac{S_{x_1^2}}{N_1} \right)^2 + N_2 \left( c \frac{S_{x^2}}{N} - c_2 \frac{S_{x_2^2}}{N_2} \right)^2 - 2w_4 d_a \left( c_2 \frac{S_{x_2^2}}{N_2} - c_1 \frac{S_{x_1^2}}{N_1} \right) \\
&\quad + 2 \frac{(c_2 - c_1)}{S_{x^4}} \left( (a - a_1) S_{x_2^4} S_{x_1^2} - (a - a_2) S_{x_1^4} S_{x_2^2} \right)
\end{aligned}$$

Factoring and substituting the above expressions for the various terms in the equation (4.7), it can be written as

$$\begin{aligned}
\hat{\sigma}^2 &= [w_1 + w_2 d_b^2 + w_3 d_c^2 + w_4 d_a^2 + w_5] / N \\
&= \left( \frac{w_1}{N} \right) \left( 1 + \frac{w_2 d_b^2}{w_1} \right) \left( 1 + \frac{w_3 d_c^2}{w_1 + w_2 d_b^2} \right) \left( 1 + \frac{w_4 d_a^2 + w_5}{w_1 + w_2 d_b^2 + w_3 d_c^2} \right)
\end{aligned}
\tag{4.8}$$

Further

$$[w_1(\hat{\sigma}_1^2)^{-N_1/N}(\hat{\sigma}_2^2)^{-N_2/N}]/N = (N_1 r^{2N_2/N} + N_2 r^{-2N_1/N})/N; \text{ where } r = \hat{\sigma}_1/\hat{\sigma}_2$$

Hence likelihood ratio statistic can be written as

$$\begin{aligned} lrt_{m_1} &= N \log\{(N_1 r^{2N_2/N} + N_2 r^{-2N_1/N})/N\} + N \log\left(1 + \frac{w_2 d_b^2}{w_1}\right) \\ &\quad + N \log\left(1 + \frac{w_3 d_c^2}{w_1 + w_2 d_b^2}\right) + N \log\left(1 + \frac{w_4 d_a^2 + w_5}{w_1 + w_2 d_b^2 + w_3 d_c^2}\right) \\ &= Var_{\hat{\sigma}^2} + Var_B + Var_C + Var_A \end{aligned}$$

(4.9)

Simplifying the  $Var_A$  term further, let  $z_i = x_i^2$  and recall that the coefficient of the quadratic term can be expressed as

$$c = \frac{\sum x_i^2 y_i - \frac{\sum y_i \sum x_i^2}{n}}{\sum x_i^4 - \frac{(\sum x_i^2)^2}{n}} = \frac{\sum z_i y_i - \frac{\sum y_i \sum z_i}{n}}{\sum z_i^2 - \frac{(\sum z_i)^2}{n}} = \frac{\sum (z_i - \bar{z}) y_i}{\sum (z_i - \bar{z})^2}$$

(4.10)

and the intercept can be expressed as

$$a = \frac{\sum y_i - c \sum x_i^2}{n} = \frac{\sum y_i - c \sum z_i}{n} = \frac{\sum y_i - (\sum z_i) \frac{\sum (z_i - \bar{z}) y_i}{\sum (z_i - \bar{z})^2}}{n}$$

(4.11)

Now let

$$t_i = \frac{(\sum z_j)(z_i - \bar{z})}{\sum (z_j - \bar{z})^2}$$

Hence the equation (4.11) can be written as

$$a = \frac{1}{n} (\sum y_i - \sum t_i y_i) = \frac{1}{n} \sum y_i (1 - t_i)$$

(4.12)

So variance of the intercept can be written as

$$\begin{aligned} \text{Var}[a] &= \frac{1}{n^2} \sum (1 - t_i)^2 \sigma^2 = \frac{\sigma^2}{n^2} \sum (1 - t_i)^2 = \frac{\sigma^2}{n^2} \sum (1 - 2t_i + t_i^2) \\ &= \frac{\sigma^2}{n^2} \{n - 2\sum t_i + \sum t_i^2\} \end{aligned}$$

(4.13)

But we know that  $\sum t_i = 0$  hence equation can be simplified to

$$\begin{aligned} \text{Var}\{a\} &= \sigma^2 \left\{ \frac{1}{n} + \frac{(\sum z_i)^2 \sum (z_i - \bar{z})^2}{n^2 [\sum (z_i - \bar{z})^2]^2} \right\} = \sigma^2 \left\{ \frac{1}{n} + \frac{(\sum z_i)^2}{n^2 \sum (z_i - \bar{z})^2} \right\} \\ &= \sigma^2 \left\{ \frac{1}{n} + \frac{\bar{z}^2}{\sum z_i^2 - \frac{(\sum z_i)^2}{n}} \right\} \end{aligned}$$

(4.14)

Unlike the breakdown for the linear model, the components for the quadratic model are difficult to segregate and showed dependency. Hence it is difficult to clearly attribute an out-of-control shift to any one of the coefficients of the model.

To construct a control chart using the changepoint statistic, we simulated the value of the threshold for the  $lrt$  statistic using simulation for a given type I error. It is well known that the expected value of  $lrt_{m_1}$  is proportional to the value of  $m_1$ , implying that the  $E(lrt_{m_1})$  gets large if the change point is located close to either end of the profile sample. Hence it is necessary to standardize the  $lrt$  values. Similar to the method prescribed in Mahmoud et al. (2004) we simulate the normalization factor which makes the expected value same for all values of the location of the changepoint.

### 4.3. Methodology

For this study the model of interest is a second order polynomial in one variable,  $x$ , defined as:

$$f(x_{ij}) = A + Bx_i + Cx_i^2 \quad (4.15)$$

where  $A$ ,  $B$  and  $C$  are the known parameters, there are  $i = 1, \dots, n$  levels of  $x$  and  $j = 1, \dots, k$  profiles. We use orthogonal polynomials as the columns of the  $X$  matrix and compute the likelihood ratio statistic as defined by equation (4.3), for each segment. The first three orthogonal polynomials for equally spaced  $x$  levels for this study were computed using the following expressions (Montgomery, Peck and Vining (2007))

$$P_0(x_i) = 1$$

$$P_1(x_i) = \lambda_1 \left[ \frac{x_i - \bar{x}}{d} \right]$$

$$P_2(x_i) = \lambda_2 \left[ \left( \frac{x_i - \bar{x}}{d} \right)^2 - \left( \frac{n^2 - 1}{12} \right) \right]$$

(4.16)

where  $d = x_{i+1} - x_i$  and  $\lambda_l$  are constants. For the case where the  $x$  levels are not equally spaced, designs mentioned in Seber (1977) can be used to construct the orthogonal polynomials. The  $lrt$  values are then compared with the simulated threshold values to determine presence of a shift. This approach could be generalized to a polynomial model of any order.

For the performance comparison simulations we used 8, 4 and -5 respectively for the intercept, linear and quadratic coefficients. We also assumed 10 levels for each of the 20 profiles. The  $x$  values are assumed to be equally spaced and are generated using orthogonal polynomials. If  $m_l$  is the change point then the likelihood ratio statistic for the proposed model is defined in equation (4.3).

Table 4.1. Out of control shifts for simulation

Type of shift	Notation	Magnitude
Shift in Intercept	$\beta_0$ to $\beta_0 + \lambda\sigma$	$\lambda = 0(0.5)4$
Shift in Slope (Linear Term)	$\beta_1$ to $\beta_1 + \delta\sigma$	$\delta = 0(0.5)4$
Shift in slope (quadratic term)	$\beta_2$ to $\beta_2 + \theta\sigma$	$\theta = 0(0.5)4$
Shift in Standard Deviation	$\sigma$ to $\gamma\sigma$	$\gamma = 1(0.2)3$

The threshold values are simulated at different confidence levels such as 90%, 95% and 99%. The out of control situations were simulated by considering the following cases: individual shifts in the intercept, the coefficients of the linear and quadratic terms and the error variance. The various magnitudes of the shifts considered in the study are tabulated in (Table 4.1.) For each shift, the change points are simulated at 10, 15 and 19 which correspond to the middle, three-fourths and the end of the sample respectively. It is assumed that the shift in the order of the polynomial model would be reflected in the model residuals or the error variance.

#### **4.4. Performance Comparison**

The proposed change point control chart is compared with the individual control chart approach of Kim et al. (2003). For the predefined shifts in the parameters and the model error variance, it was observed that the change point technique was very quick in detecting changes in the error variance but relatively poor in detecting shifts in the intercept, linear and quadratic coefficients. The performance graphs for shifts in error variance and linear coefficients are shown in (Figures 4.1 and 4.2.) The graphs for shifts in the intercept and the quadratic terms look similar to the one for the linear term and not shown here.

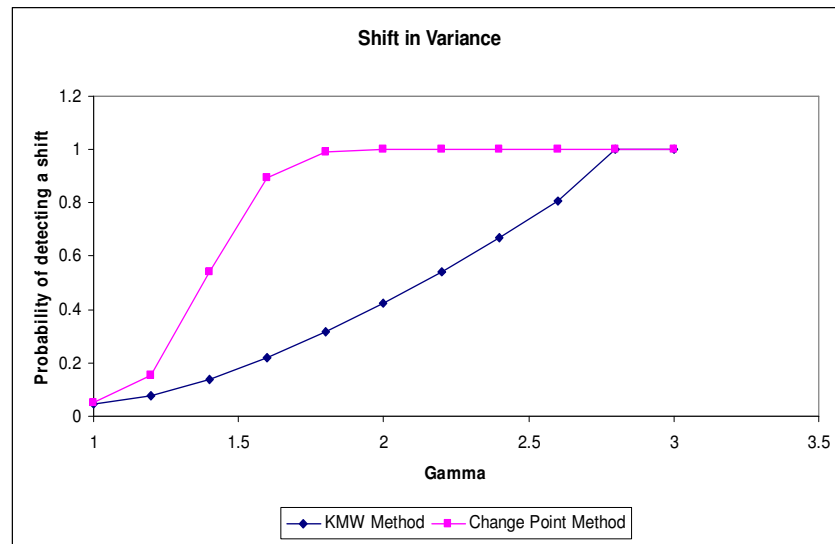


Figure 4.1. Probability of detecting shifts in the variance

To overcome the loss in efficiency in monitoring the coefficients we propose using a joint MEWMA chart along with changepoint likelihood ratio based chart. The MEWMA chart was designed using the tables presented in Prabhu and Runger (1997). The combined chart has a much better power of detecting the out of control shift for all the coefficients. The results are shown in (Figures 4.3-4.6.)

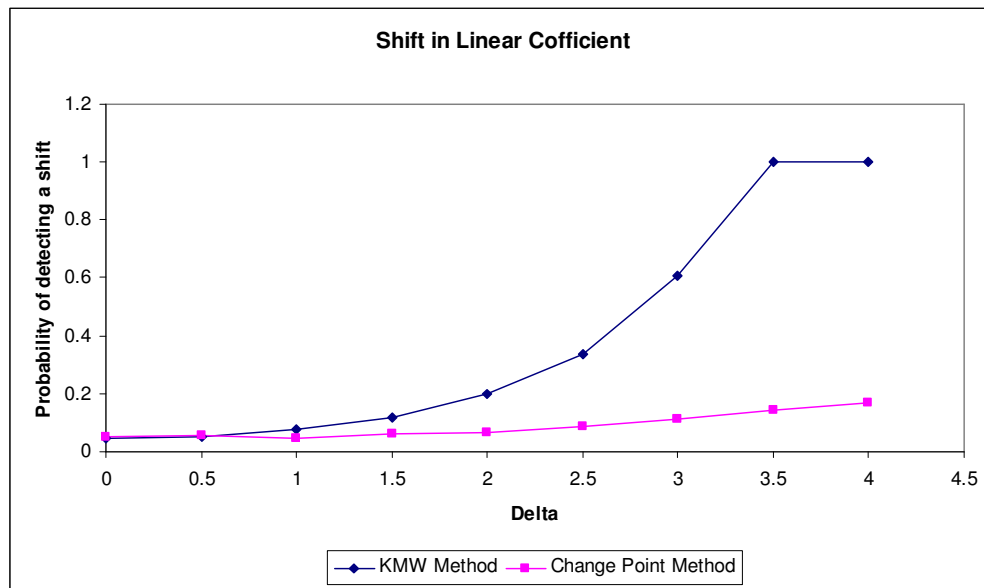


Figure 4.2. Probability of detecting shifts in the linear coefficients

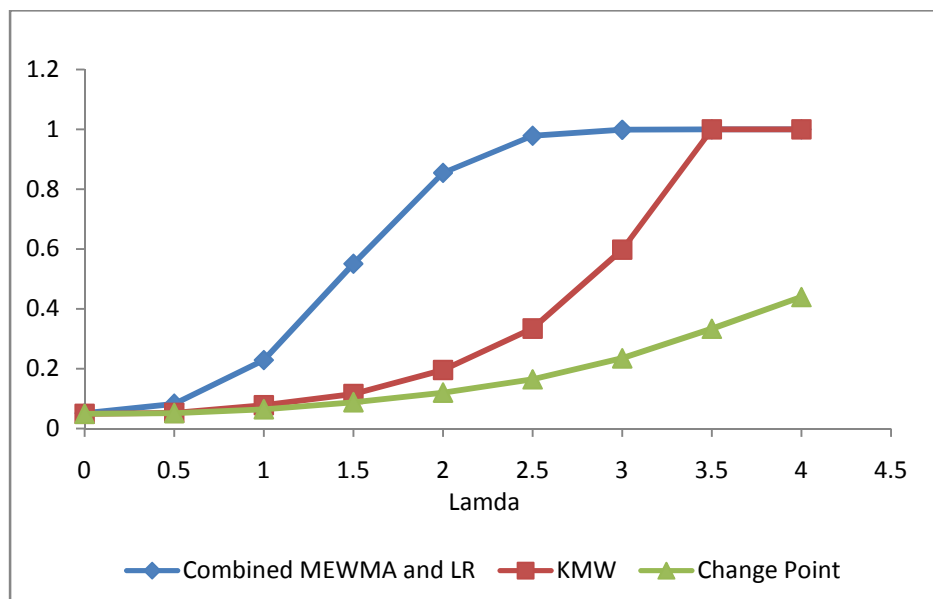


Figure 4.3 Probability of detecting shift in the intercept



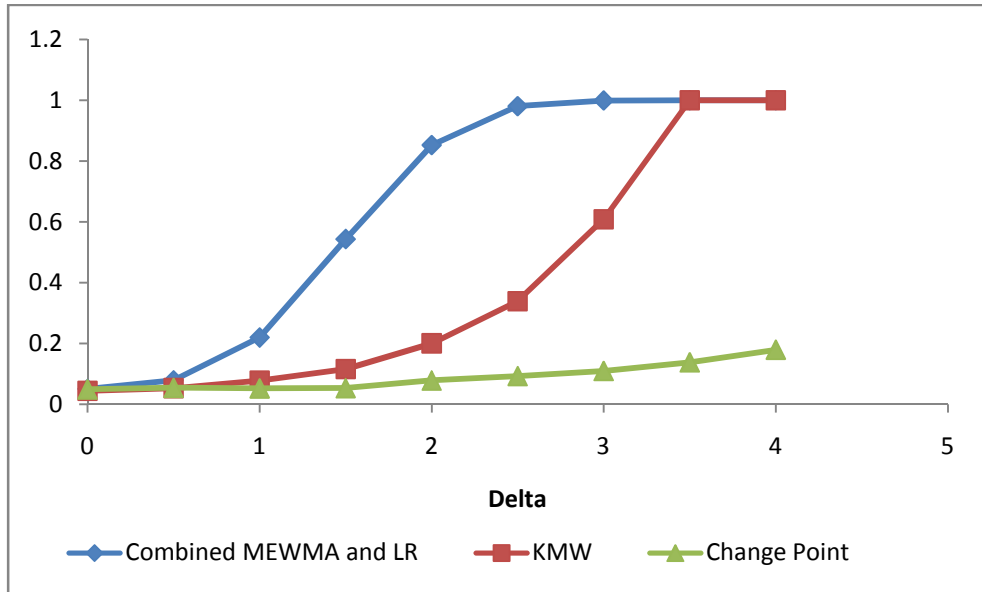


Figure 4.4. Probability of detecting a shift in the linear term

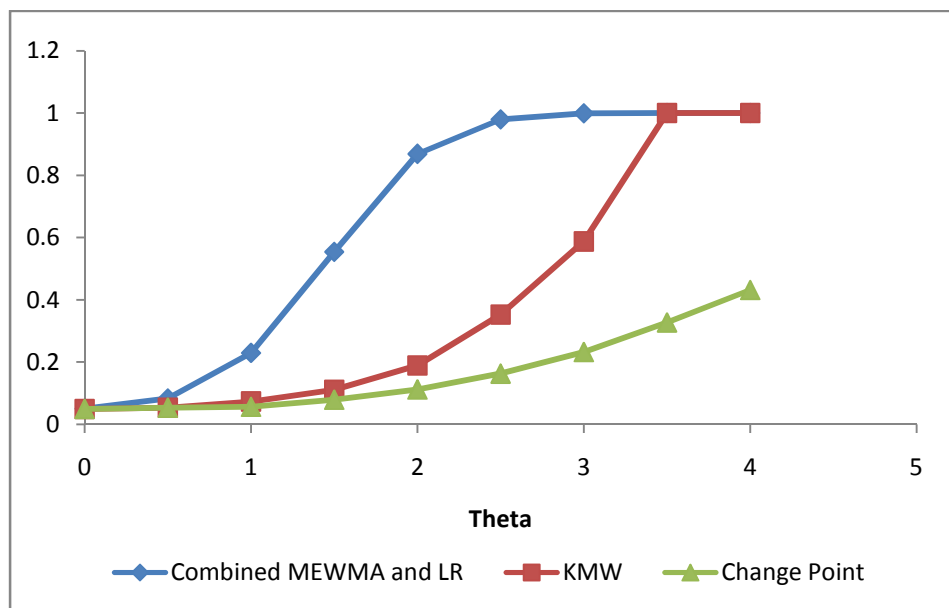


Figure 4.5. Probability of detecting a shift in the quadratic term

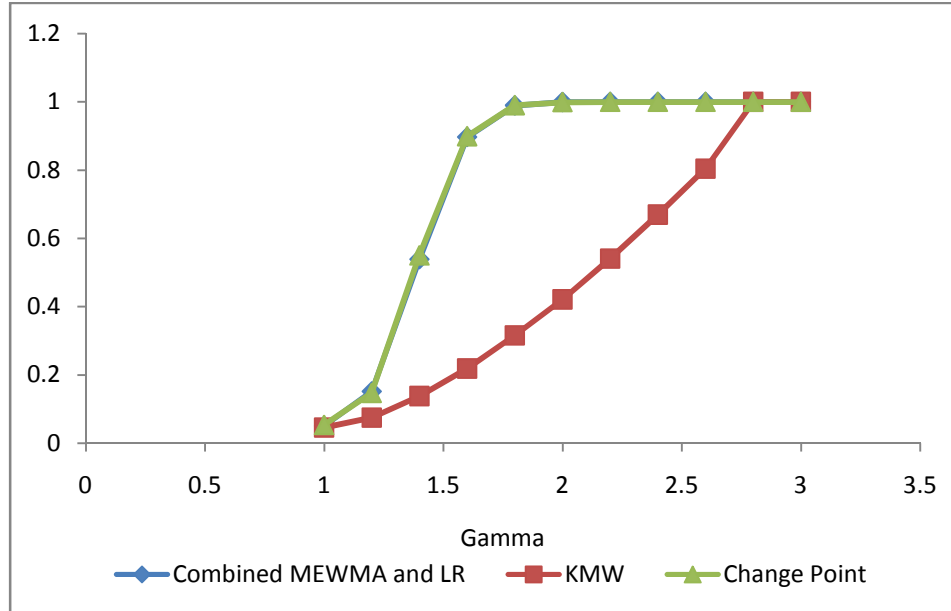


Figure 4.6 Probability of detecting a shift in the error variance

#### 4.5. Conclusion

This study extended the linear change point approach of Mahmoud et al. (2006) to a polynomial profile. Unlike the linear case, the polynomial case had dependencies among the parameters and it was difficult to segregate the contribution of the various parameters of the model as clear from the derived values in equation (4.9). The phase I performance of the changepoint approach was superior in detecting changes in the error variance but relatively poor for the intercept, linear and quadratic term. It is still a very useful technique since large fluctuations in the error variance can indicate process instability and it is imperative to control that to ensure that the other parameters are estimated accurately. Once the error variance is found to be stable, we propose the simultaneous use of the MEWMA chart for monitoring the coefficients of the model and the change point chart for monitoring the error variance.

We found the use of orthogonal polynomials to remove the ill conditioning of the hat matrix very useful and made the parameters of the models independent and easier to monitor. One could have possibly used the individual control charts but as the order of the polynomial model would increase, it would become cumbersome to track multiple control charts. An MEWMA approach in that situation would be much more efficient.

In the time since this study was conducted, Kazemzadeh, Noorossana, Amiri (2008) also extended the Mahmoud et al. (2006) approach to monitoring polynomial profile. The main differences between the proposed approach and the approach suggested by Kazemzadeh et al. (2008) are:

1. the authors conduct a performance comparison of the changepoint approach to the  $T^2$  control chart of Williams et al. (2007) and  $F$ -statistic control chart of Mahmoud and Woodall (2004). We compare the changepoint approach to the KMW method.
2. the authors suggested centering the  $x$ -values to reduce the multicollinearity problem and we propose using orthogonal polynomials. We believe the multicollinearity in polynomial regression is an important and a non trivial problem that results in the ill conditioning of the  $X$  matrix leading to unstable coefficients. Seber and Lee (2007) propose to tackle the problem by either normalizing the  $x$ -values or by using orthogonal polynomials. Bradley and Srivastava (1979) illustrate that centering the  $X$  matrix does not completely alleviate the problem of ill conditioning. The ill conditioning in the hat matrix

would lead to unstable and probably inaccurate parameter estimates. This would result in inaccurate or underestimated error coefficient and eventually lead to a poor estimation of likelihood ratio statistic. We suggest using orthogonal polynomials since there is one to one correspondence between the original variable and the orthogonal variable; it does not alter the directional interpretation of the out of control signal. Further, the use of orthogonal polynomials leads to nice properties of the model coefficients as well as it reduces the computation of the inverse of the hat matrix whenever the order of the polynomial model is increased.

## 5. Analysis of Signal-Response Systems Using Generalized Linear Mixed Models

### 5.1. Introduction

In signal-response systems, the quality characteristic or response of interest,  $y$ , is not a single characteristic, but a function over a range of output values. That is, the response takes on different values as a result of differences in some signal factor. We can model the response as

$$y = g(M) + \varepsilon$$

where  $g$  is the relationship between the signal,  $M$ , and the response,  $y$ . In addition,  $g$  can depend upon both controllable and uncontrollable (noise) factors. Generally, the signal-response systems are classified into three types based on the function of the system being studied: 1) multiple target systems; 2) measurement systems; and 3) control systems. We study the multiple target system where different levels of response are obtained by consciously adjusting the signal factor. We begin by describing a well-known signal-response example that will be fully analyzed in later sections.

### 5.2. Injection Molding Example

DeMates(1990) describes a factorial experiment conducted in an injection molding plant. It is a robust design study conducted to identify the control factors that increase the variability in the weight of the mold at two different compound noise levels. The response of interest is the weight of the mold measured over eight levels of the factor, high injection pressure. The performance characteristic

is a profile obtained by modeling the response over a range of the signal factor [Taguchi (1986)], see (Figure 5.1.) The hierarchical nature of the experiment adds to the complexity of the analysis in addition to the correlation between the part weights at different levels of pressure. The individual values of weight are correlated within a control and noise factor setting and can be assumed independent between different experimental runs.

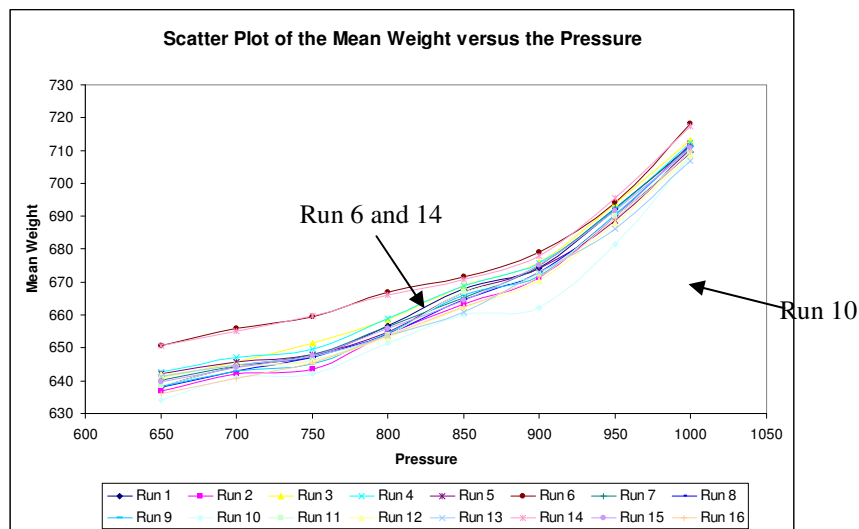


Figure 5.1. Plot of Injection Molding Responses

There are seven continuous control factors, each at two levels and four noise factors, also at two levels each. However, the four noise factors are combined to form one compound noise factor, at two levels. The continuous control factors and resulting compound noise factor and their ranges are displayed in (Table 5.1) and (Table 5.2), respectively.

Table 5.1. Control Factors for the Injection Molding Experiment

<b>Factor</b>	<b>Low Level (-1)</b>	<b>High Level (+1)</b>
A: Injection Speed	0.0	2.0
B: Clamp Time	49 s	44 s
C: High Injection Time	6.8 s	6.3 s
D: Low Injection Time	20 s	17 s
E: Clamp Pressure	1700 psi	1900 psi
F: Water Cooling	80° F	70° F
G: Low Injection Pressure	550 psi	650 psi

Table 5.2. Compound Noise Factor for the Injection Molding Experiment

<b>Factor</b>	<b><math>X_N = -1</math> (Low Level)</b>	<b><math>X_N = +1</math> (High Level)</b>
Melt Index	18	22
Percent Regrind	5%	0%
Operator	New	Experienced
Resin Moisture	High	Low

The signal factor in this application is high injection pressure since it is known that the amount of material injected could be affected by this factor. High injection pressure is varied over the range of 650 psi to 1000 psi. The experiments were conducted over two days, where the compound noise factor ( $X_N$ ) was set at its low level on the first day and high level on the second day. The control factors were varied according to a  $2^{7-4}$  fractional factorial design for each level of the compound noise factor (Table 5.2.) Four measurements were recorded for each run in the  $2^{7-4}$  design. To illustrate the type of measurements obtained, the resulting data for the first run on Day 1 are given in (Table B.2.)

Since the experiment was conducted so that for each level of the noise factor, a  $2^{7-4}$  with resolution III experiment was performed, the set up of the experiment is very similar to a split-plot experiment. In fact, the experiment can

be viewed as a split-split plot with the signals or curves within each experimental unit representing a sub-sub plot.

Analysis methods for signal-response systems have been addressed in the literature. Taguchi(1886, 1887) provided early examples of these systems, and new and better methods have been subsequently developed by Nair(1992), Miller and Wu(1996), Bisgaard and Steinberg(1997), and Nair et al.(2002), among others. The most commonly used method can be summarized in two steps, 1) estimation of the functional relationship between the response and the signal factor and 2) estimation of the relationship between the parameters of the functional models and the design parameters. Various researchers have also studied the robustness of the process with respect to predefined levels of noise variables. Since the studies involve systematically varying the noise factor in addition to the control factors, it results in large designs. Due to increase in execution costs compromises are often made on the randomization of the experimental runs. The relationship of the response with the control and noise factor is often modeled by methods based on ordinary least squares, which fails to accommodate for the various sources of variation introduced in restriction to randomization and also the departure of the response from the normal distribution. These two issues can be resolved by using the GLMM.

We propose and illustrate the use of generalized linear mixed models for analyzing an RPD for a signal response system and demonstrate the comparison with the ordinary least squares approach. The remainder of the paper is laid out as



follows. The next section is a brief survey of the current methods in the literature for analyzing a signal response system. We examine the experiment as if it were run as a split-plot design and present our arguments to support the claim in section 5.3. In section 5.4 we propose and explain the GLMM for analyzing the split plot structure of an RPD for a signal response system. Section 5.4 presents the illustration of the proposed method and results of the comparison of the proposed method to the traditional method based on ordinary least squares using the Injection Molding example presented previously. We then conclude the paper with discussion and future directions.

### **5.3. Analysis of Signal-Response Systems**

Miller and Wu (1996) propose two methodologies to analyze the results from the signal-response experiment described in DeMates (1990). The methods were performance measure modeling (PMM) and response function modeling (RFM). The PMM method involves reducing the functional response to a performance measure and analyzing the resulting measure as the response. Box (1988) demonstrates the weakness of this type of analysis by providing examples of different systems with different behavior that give rise to the same performance measure. RFM on the other hand involves modeling the relationship between the signal and response using the parameters of the model. This method makes intuitive sense to determine how the settings of the control and noise factors affect the parameters of the model. However, this approach must be used with caution when correlation between the parameters is present.

Other analysis techniques can be generalized as a two step procedure: 1) estimation of the functional relationship between the response and the signal factor followed by 2) modeling of the parameters or some function of the model parameters as a function of control and noise factors. Taguchi (1986, 1987) proposed analyzing a dynamic signal to noise ratio which has subsequently been criticized as being inefficient as it confounds the mean and the variance [Myers, Montgomery and Anderson-Cook(2009) , Miller and Wu(1996)].

Welch et al. (1990) suggest modeling the response using a combined array design and approximating the parameter estimates to form the intercept, slope, and error variance functions. These functions are then used as responses to optimize the process. This approach is referred to as the “response-model approach”. The loss model approach presented by McCaskey and Tsui (1997), and Tsui (1999) differs from the response-model approach since the intercept, slope and error variance for different levels of the control factors are estimated first and then these parameters are modeled as separate responses. The settings of the control factors that optimize the dynamic system are then identified.

Bisgaard and Steinberg (1997) describe a two-step procedure that involves fitting a polynomial to the signal response and treating the coefficients as multiple responses to study the effects of the experimental factors. Nair et al. (2002) suggest fitting a location-dispersion model to the response evaluated at each level of the signal factor. The location  $\mu$  and the log of the dispersion,  $\sigma^2$  are represented as a function of design ( $x_i$ ) and signal factors ( $s_k$ ):

$$\mu(x_i; s_k) = x_i' \beta(s_k) \quad \text{and} \quad \log \sigma^2(x_i; s_k) = x_i' \phi(s_k)$$

(5.2)

where  $\phi$  and  $\beta$  are the effect coefficients of design factors for mean and the variance as a function of the signal factor. Significant effects are then identified using a normal probability plot or as a function of the signal factor. Nair et al. (1986) further discuss the situation where the noise factor ( $z_j$ ) is explicitly controlled and varied, and can be incorporated in the model as

$$Y_{ijk} = \mu(\mathbf{x}_i; \mathbf{z}_j; s_k) + \sigma(s_k) \varepsilon_{ijk} \quad (5.3)$$

where the location model can be represented as

$$\mu(\mathbf{x}_i; \mathbf{z}_j; s_k) = \mathbf{x}_i' \boldsymbol{\beta}(s_k) + \mathbf{z}_j' \boldsymbol{\gamma}(s_k) + \mathbf{x}_i' \boldsymbol{\Lambda}(s_k) \mathbf{z}_j \quad (5.4)$$

where  $\boldsymbol{\gamma}$  and  $\boldsymbol{\Lambda}$  are the effects of the noise factor and the control by noise interactions, respectively, as a function of the signal factor. The dispersion effects can be estimated by the interaction between the control and noise factors. Nair et al. (2002) demonstrate their approach using three different functional response systems. There are a few studies conducted on using optimization techniques to identify the optimal settings for dynamic systems, including Chen (2003), Chang et al. (2007) and Tong et al. (2008). Chen (2003) structured the problem as a mathematical programming problem and proposed a sequential quadratic programming (SQP) approach to solve the nonlinear stochastic optimization problem. Chang et al. (2007) propose simulated annealing to find the optimal setting of a dynamic system, on the performance measures developed using a

back-propagation neural network. Tong et al. (2003) study the dynamic system with multiple quality characteristics and use the data envelopment analysis approach to develop relative efficiency measures of the location and dispersion effects and model the overall quality performance (OQP) as a function of design factors to assess the optimal factor level combination. Lesperance and Park (2003) use a joint generalized linear modeling approach to model the mean and the variance function, assuming the observations are independent within a response function. They also provide a comparison of the graphical approaches to their joint generalized linear modeling approach. Lunani et al. (1997) extend the Taguchi (1991a, 1991b) performance measure for dispersion and propose two graphical methods. They define dispersion in the response as a function of sensitivity measure  $\beta_i$  and a multiplicative error term  $\phi$ , such as

$$\sigma^2 = \beta^{\gamma} \phi^2 \quad (5.5)$$

The two proposed plots are the gamma-plot ( $\gamma$ -plot) and the sensitivity standard deviation plot (SS-plot).

Since the data is collected sequentially by adjusting the signal factor, it is important first to evaluate and then adjust for the correlation between the response levels. In the two-step approaches discussed so far, this correlation has been ignored which could lead to underestimation of the error variance.

Furthermore, these robust designs are usually carried out as split-plot systems similar to that described in the example presented earlier. In this article, we propose a general linear mixed model approach to analyze the response profiles

that will accommodate both the correlation structures and the split plot nature of the problem. We describe our approach using the injection molding example described in the previous section.

## 5.4. Split-Plot Designs and Generalized Linear Mixed Models

### 5.4.1. Split-Plot Designs and Mixed Models

An RPD with a signal-response system can be viewed as a split-split plot design. The compound noise factor is treated as a whole plot factor. The control factor treatments common to a particular level of the whole plot share the same whole plot error. The signal factor can be treated as a sub-sub plot factor which now shares the whole plot and sub-plot errors in addition to the random error associated with each of the levels. These errors are variance components and are explicitly represented by a mixed model.

Robinson et al. (2004) demonstrate that the analysis of results from a split-plot experiment can be carried out using generalized linear mixed models. They show that the general form of a model for a split-plot design can be written as a mixed model and given as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\varepsilon} \quad (5.6)$$

where  $\mathbf{X}$  is a matrix of fixed effects and  $\mathbf{Z}$  is a matrix of zeroes and ones. In a split-plot setting,  $\mathbf{X}$  represents the control factors and the signal factor while  $\mathbf{Z}$  would be used to model the various whole-plot levels. The vectors  $\boldsymbol{\gamma}$  and  $\boldsymbol{\varepsilon}$  consist of random effects where  $\boldsymbol{\gamma} \sim N(0, \sigma_{\gamma}^2)$  and  $\boldsymbol{\varepsilon} \sim N(0, \sigma_{\varepsilon}^2)$ . In addition,  $\boldsymbol{\gamma}$  and  $\boldsymbol{\varepsilon}$  are assumed to be independent. The error terms,  $\sigma_{\gamma}^2$  and  $\sigma_{\varepsilon}^2$ , are variance

components and represent the whole-plot error variance and sub-plot error variance, respectively. These components can be estimated using maximum likelihood. Modeling the response using Equation 5.5 naturally supports the assumption common to most split-plot experiments; that is, the responses within a whole plot (here represented by  $\mathbf{Z}$ ) are correlated. The analysis method used must take into account this correlation structure among the responses within a whole-plot level. We will discuss two approaches to incorporating this correlation structure for the injection-molding example presented earlier.

#### 5.4.2. Generalized Linear Mixed Models

One of the important assumptions underlying mixed models is that of normality of the random effects and the errors. There are situations where this assumption may be violated and the error may assume some distributional form other than normal. For an example, see the braking torque experiment discussed in Lesperance and Park (2003). In that example, the authors show that a gamma distribution, with a log link for the response, provides a better fit as compared to the case with the normality assumption.

For linear models, Nelder and Wedderburn (1972) propose generalized linear models (GLMs) that provide flexibility to model errors from any distribution in the exponential family, see McCullagh and Nelder (1989). Breslow and Clayton (1993) and later Wolfinger and O'Connell (1993) combine the principles of generalized linear models with the mixed model approach and proposed *generalized linear mixed models* (GLMM). In this approach, the

function of the response is regressed on fixed and random factors such as those given in Equation 5.5. The GLMM can be expressed as

$$E[Y | \boldsymbol{\gamma}] = g^{-1}(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}) \quad (5.7)$$

where  $g^{-1}(\cdot)$  is the inverse of a differentiable monotonic link function,  $g$ .

GLMMs provide flexibility in modeling the covariance or correlation structure between responses. Littell et al. (1996) provide details on implementing mixed models using SAS. Recall for split-plot experiments, responses are correlated within a whole-plot level and this correlation should be taken into account when conducting an analysis.

Two common models used to incorporate the covariance or correlation structure among responses in a GLMM are the batch-specific model (also referred to as the random-effects GLM) and the population-averaged model (also referred to as the covariance-pattern GLM). In the batch-specific approach, the whole-plots (which are treated as random effects) are modeled along with the regression coefficients for the control and signal factor simultaneously. By including the whole-plot effects in the model with the control and signal factors, we can adequately represent the correlation that exists among responses within a “batch” (i.e., whole plot). For the second approach, instead of treating the whole-plot as a random effect and modeling it simultaneously with the control and signal factors, a specific correlation structure among the responses within a whole-plot is assumed. That is, the user must define a specific correlation matrix prior to running the analysis. This is often referred to as the population-averaged

model or covariance-pattern GLM. Assuming a specific correlation structure instead of modeling the whole-plots themselves, is similar to averaging over all “batches” (i.e., whole-plots). For complete details on GLMMs and their applications to split-plot designs see Robinson et al. (2004). In the next section, we compare the population average model and the batch-specific model with the two-step modeling approach of Miller and Wu (1996).

### **5.5. Methodology**

The proposed methodology for analyzing a robust design of a signal response system can be summarized as follows:

1. Identify the whole-plot, sub-plot factors. Typically we have observed Taguchi experiments the compound noise factor is the whole-plot treatment, control factors are the sub-plot treatments and the signal factor is the sub-subplot treatment.
2. Identify the distribution of the mean response and the variance of the response to select the appropriate generalized linear mixed model
3. Use restricted maximum likelihood method to fit a GLMM. This can be achieved by using SAS Proc GLIMMIX. The same procedure can also be used to model the batch-specific model GLMM and population-average model GLMM by treating the whole-plot treatment as a random effect for the former modeling approach.
4. Asses the model fit using residual plots and goodness of fit statistic



The next section we illustrate the method by analyzing the Injection Molding experiment presented previously.

### **5.6. Analysis of the Injection Molding Example**

Miller and Wu (1996) analyze the experiment in DeMates (1990) by fitting a quadratic model involving the signal factor (high-injection pressure) for the mold weight for each combination of control and compound noise factors. The coefficients of these models are treated as random responses and modeled as a function of the control and compound noise factor levels. As mentioned previously, four observations are recorded for each level of the compound noise by control by signal factor. Since the exact details of the execution of the experiment are unclear, we assume the four observations are repeat observations and treat their mean and variance as responses. We fit generalized linear mixed models for the mean and the variance separately, treating the compound noise factor as the whole-plot treatment, the control factors as a sub-plot effect and the high injection pressure level as the sub-subplot effect.

#### **5.6.1. Analysis of the Mean Weight**

We used the SAS procedure GLIMMIX to build a GLMM for the mean weight. For the mean weight, we initially assume the normal distribution as the marginal distribution and restricted maximum likelihood (REML) method was used to estimate the parameters. (Figure 5.1) displays the mean weight as a function of the signal factor, high-injection pressure. It can be observed from (Figure 5.1), that a quadratic model in high-injection pressure would best

approximate the relationship between the mean weight and high-injection pressure. However, a polynomial model such as a quadratic model by nature induces linear dependency (collinearity) among the columns involving the signal factor, leading to unstable and hence unreliable model parameter estimates. To alleviate this problem, we use orthogonal polynomials to remove the collinearity. Orthogonal polynomials as the name indicates are polynomials generated such that the columns are linearly independent, see Montgomery et al. (2006). The values of the orthogonal polynomials used in this application are summarized in (Table 5.5.)

Next, we assume a gamma distribution for the responses. Though the parameter estimates were not much different from the results of Miller and Wu (1996), the diagnostic statistics indicated that underdispersion was present. As a result, we decided to work with a regression model. The model obtained for the mean weight is

$$\hat{y} = 667.54 - 1.134A - 1.771C + 1.397E - 0.998F + 1.778G + 4.783P_1 + 1.33P_2 + 0.168C \times P_1 - 2.177X_N \quad (5.7)$$

The residual graphs were satisfactory with the exception of a single outlier, which was not surprising as the plot of the responses displayed outlying curves (Figure 5.1). Since the resolution of the design for the control factors is III, the control factor interactions were confounded with main effects and it became difficult to ascertain which effects were significant. It is evident from the model that the compound noise factor ( $X_N$ ) can be manipulated to adjust the mean of the response, but the contribution of individual noise factors is not obvious. To

obtain larger values of the mean weight of the injection molds, factors *A* (injection speed), *C* (high injection time) and *F* (water cooling temperature) should be set at their low levels, and factors *E* (clamp pressure) and *G* (low injection pressure) at their high levels. The interaction of factor *C* (high injection time) with the linear signal-factor ( $P_1$ ) effect indicates that the level of the factors affect the shape of the response curve over the range of the high-injection pressure.

For the batch-specific model for the mean response, the noise factor was treated as a random effect. Point estimates, 95% confidence intervals, and the confidence interval length for all three methods are given in (Table 5.6.) The parameter estimates and the respective standard errors for the batch-specific model were similar to those found using the population average model. The difference between the two methods was in the confidence interval for the mean response (Table 5.6). The batch-specific model has shorter confidence intervals as compared to the population average. However, the precision of the confidence interval (measured by CI length) for either GLMM approach is significantly better than the OLS approach used by Miller and Wu (1996).

As noted in Robinson et al. (2004), for a split-plot design with signal response measurements, the random-effects or the batch specific model provides more precise estimates as compared to the population average model. This could be due to explicit modeling of the whole plot variance in the batch specific model. In the current example, the magnitude of the whole plot variance is not

large, hence the model estimates and their standard errors are similar for both cases.

### 5.6.2. Analysis of the Variance of the Mean Weight

Since the marginal distribution of the mean response was found to be normal, the variance is assumed to follow a chi-square distribution. A gamma distribution was employed for the variances while three different links were investigated. The three links were the identity, log and inverse. Since only the log link gave non-negative lower confidence intervals on the predicted variance, it was chosen as an appropriate link in the GLMM.

The diagnostic checks indicated a good fit to the data. Even though some of the factors were marginally significant at 10% significance, we decided to keep them as deleting them worsened the fit. The fitted model for the variance is

$$\begin{aligned} \text{Var}(\hat{y}) = & \exp(0.36 + 1.17A + 0.11B - 0.16C - 0.19G + 0.08P_1 \\ & + 0.02B \times P_1 + 0.23G \times P_1 + 0.04B \times P_2 + 0.03C \times P_2 \\ & + 0.05E \times P_2 - 0.03F \times P_2 + 0.07G \times P_2 - 0.7X_N) \end{aligned} \quad (5.8)$$

The residuals plots are again satisfactory. To minimize the variance, factor *A* (injection speed), should be set at its low level. Furthermore, we would set factor *G* (low injection pressure) at its high level keeping the remaining factors at levels determined when modeling the mean weight. The noise factor is significant and it is recommended that the compound noise factor be set so that melt index is at 22, 0% regrind, with an experienced operator and low resin

moisture. These results correspond to the ones obtained from the RFM analysis of Miller and W (1996).

### 5.7. Discussion

The conclusions from the joint GLMM approach correspond to the results recommended in Wu and Hamada (2000) in terms of what factor settings should be chosen for a robust design. In fact, the model for the intercept obtained by Miller and Wu (1996) approach given as

$$\beta_0 = 666.4 - 1.2A - 1.8C + 1.4E - 1.0F + 1.8G + 1.1X_N$$

(5.9)

is very similar to the mean GLMM (equation 5.7) with the inclusion of some additional terms. It is our recommendation that the GLMM approach should be preferred over an ordinary least squares approach implemented by Miller and Wu (1996). There are several reasons for this recommendation. First, a single equation is obtained for the mean response as opposed to an equation for each parameter of the model. For profiles with complicated shapes, the interpretation from a joint GLMM model is straightforward despite the increase in the number of parameters. More importantly, the GLMM approach results in more precise estimates. For example, consider the confidence intervals for the mean response displayed in (Figure 5.2.)

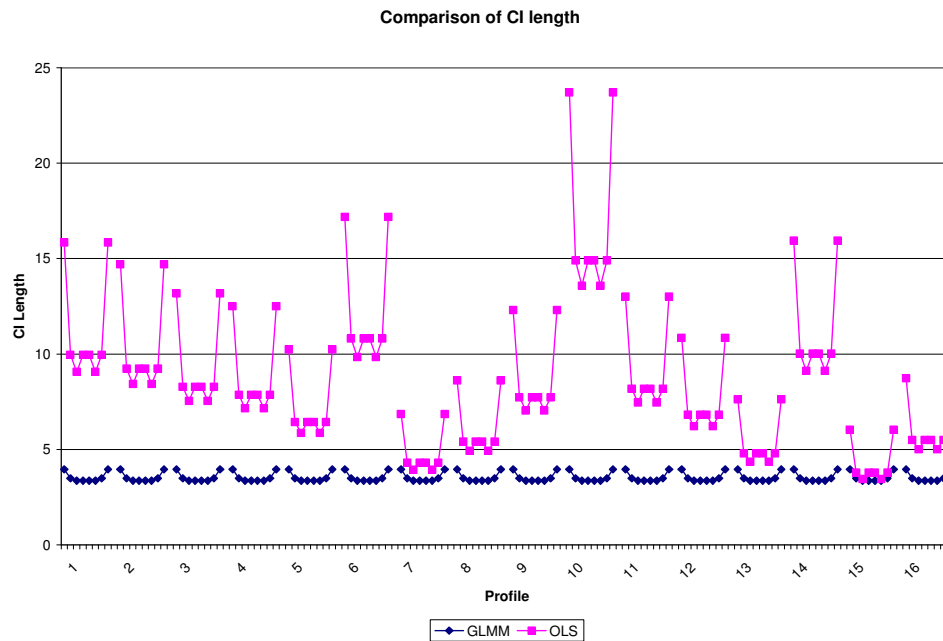


Figure 5.2. Confidence Interval Length with GLMM and OLS models

The confidence intervals for the mean response clearly show that the GLMM approach results in shorter confidence intervals which in turn indicate more precise estimation of the response. Point estimates, 95% confidence intervals, and the confidence interval length for all three methods are given in (Table 5.3.)

Table 5.3. Comparison of Population Average and Batch Specific Models

Y	$\hat{y}$	GLMM Batch Specific			$\hat{y}$	GLMM Population Average		
		95% Confidence Interval	CI Length	95% Confidence Interval		CI Length		
636.88	637.989	636.106	639.873	3.77	637.12	635.14	639.09	3.95
642.10	639.906	638.266	641.546	3.28	639.03	637.29	640.78	3.49
643.50	644.485	642.911	646.059	3.15	643.61	641.93	645.29	3.36
654.33	651.725	650.151	653.299	3.15	650.85	649.17	652.53	3.36
663.38	661.627	660.053	663.201	3.15	660.75	659.07	662.44	3.36
671.40	674.19	672.615	675.764	3.15	673.32	671.63	675.00	3.36
690.15	689.414	687.774	691.054	3.28	688.54	686.80	690.29	3.49
712.20	707.3	705.416	709.183	3.77	706.43	704.45	708.40	3.95
642.80	644.995	643.112	646.879	3.77	644.57	642.59	646.54	3.95
647.13	646.24	644.6	647.88	3.28	645.81	644.07	647.56	3.49
649.65	650.146	648.572	651.721	3.15	649.72	648.04	651.40	3.36
658.83	656.714	655.14	658.288	3.15	656.29	654.60	657.97	3.36
668.75	665.943	664.369	667.517	3.15	665.52	663.83	667.20	3.36
675.75	677.834	676.26	679.408	3.15	677.41	675.72	679.09	3.36
692.15	692.386	690.746	694.026	3.28	691.96	690.21	693.70	3.49
712.38	709.599	707.716	711.483	3.77	709.17	707.20	711.15	3.95
650.78	650.297	648.414	652.181	3.77	649.45	647.47	651.43	3.95
654.98	651.542	649.902	653.182	3.28	650.69	648.95	652.44	3.49
659.88	655.448	653.874	657.023	3.15	654.60	652.92	656.28	3.36
666.00	662.016	660.442	663.59	3.15	661.17	659.49	662.85	3.36
670.88	671.245	669.671	672.819	3.15	670.40	668.72	672.08	3.36
677.80	683.136	681.561	684.71	3.15	682.29	680.61	683.97	3.36
695.70	697.688	696.048	699.328	3.28	696.84	695.09	698.58	3.49
717.35	714.901	713.018	716.784	3.77	714.05	712.08	716.03	3.95

Table 5.4. Comparison of the CI for the two models

y	GLMM (Population Average)				$\hat{y}$	OLS		
	$\hat{y}$	95% Confidence Interval		CI Length		95% Confidence Interval	CI Length	
636.88	637.12	635.14	639.09	3.95	638.44	631.09	645.79	14.71
642.10	639.03	637.29	640.78	3.49	640.04	635.42	644.66	9.24
643.50	643.61	641.93	645.29	3.36	644.52	640.31	648.73	8.42
654.33	650.85	649.17	652.53	3.36	651.88	647.26	656.50	9.24
663.38	660.75	659.07	662.44	3.36	662.12	657.50	666.74	9.24
671.40	673.32	671.63	675.00	3.36	675.24	671.03	679.45	8.42
690.15	688.54	686.80	690.29	3.49	691.24	686.62	695.86	9.24
712.20	706.43	704.45	708.40	3.95	710.12	702.77	717.47	14.71
642.80	644.57	642.59	646.54	3.95	643.83	637.58	650.08	12.50
647.13	645.81	644.07	647.56	3.49	645.85	641.92	649.78	7.85
649.65	649.72	648.04	651.40	3.36	650.37	646.79	653.95	7.15
658.83	656.29	654.60	657.97	3.36	657.39	653.46	661.32	7.85
668.75	665.52	663.83	667.20	3.36	666.91	662.98	670.84	7.85
675.75	677.41	675.72	679.09	3.36	678.93	675.35	682.51	7.15
692.15	691.96	690.21	693.70	3.49	693.45	689.52	697.38	7.85
712.38	709.17	707.20	711.15	3.95	710.47	704.22	716.72	12.50
650.78	649.45	647.47	651.43	3.95	653.31	645.34	661.28	15.94
654.98	650.69	648.95	652.44	3.49	653.81	648.80	658.82	10.02
659.88	654.60	652.92	656.28	3.36	657.03	652.47	661.59	9.13
666.00	661.17	659.49	662.85	3.36	662.97	657.96	667.98	10.02
670.88	670.40	668.72	672.08	3.36	671.63	666.62	676.64	10.02
677.80	682.29	680.61	683.97	3.36	683.01	678.45	687.57	9.13
695.70	696.84	695.09	698.58	3.49	697.11	692.10	702.12	10.02
717.35	714.05	712.08	716.03	3.95	713.93	705.96	721.90	15.94

Again, the batch-specific and population-average models have similar results. However, the precision of the confidence interval (measured by CI length) for either GLMM approach is significantly better than the OLS approach used by Miller and Wu (1996).



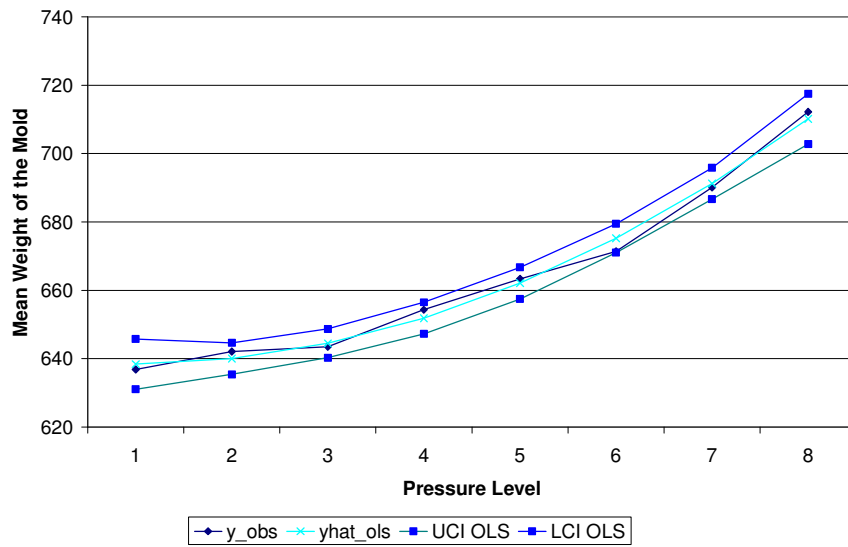


Figure 5.3. Confidence Interval from the OLS Model

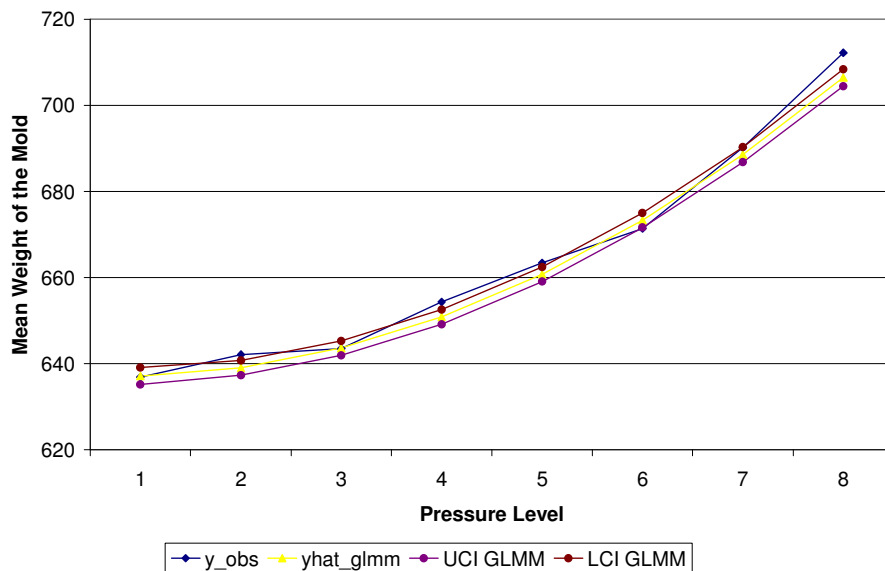


Figure 5.4. Confidence Interval from the GLMM

This is further demonstrated in (Figures 5.3 and 5.4) where the mean response, predicted response and the confidence intervals are displayed for OLS

and GLMM models. As a final note, the erratic nature of the interval length of OLS model indicates a presence of variation not accounted for by the model.

### **5.8. Conclusions**

The aim of this work was to illustrate the application of generalized linear mixed models for the analysis of robust parameter designs involving signal-response systems for use in the design stage of a product or process. The signal-response example considered clearly demonstrates that the ordinary least squares approach of the two-step modeling procedure does not correctly account for the error structure introduced by the split-split plot nature of these designs. The generalized linear mixed model provides explicit modeling of the covariance structure either as a population average model or as a batch-specific model and results in more precise estimates of the parameters. The choice between the population average and batch specific model is dependent upon the objective of the modeling being done. As noted in Robinson et al. (2004) the population average model is more applicable for situations where the batches are assumed to be similar in nature and the aim is to predict the response across batches. On the other hand, when there are differences between the batches and the interest is to either quantify the difference or account for the difference in the analysis, the batch-specific model is preferred. The latter approach provides more precise estimates as it avoids the loss of information due to the averaging of the effects. The result will be a product or process designed to be robust to uncontrollable factors and stresses.

## 6. Summary and Conclusions

The area of profile monitoring is relatively recent and an active area of research. There are a lot of questions that still need to be researched before a consensus is reached on the control charting schemes appropriate for most of the profile monitoring situations. This research has focused on answering three specific questions. In this chapter we summarize the findings from this piece of research and conclude with a discussion on some of the open problems for future research.

### 6.1. Contributions

In the study on Phase I analysis of linear profiles, we closely examined the specific application of profile monitoring in linear calibration situations and compared the efficiency of the method proposed by Croarkin and Varner (1982), referred here as NIST method, for monitoring profiles as compared to the KMW method proposed by Kim et al. (2003). The NIST control chart statistic is obtained from the deviation of the corrected measured value (by the parameters of the linear profile) from the standard value and has been shown to have very poor statistical properties. The control chart statistics for the KMW method, on the other hand, are the parameters of the linear model fit to the calibration profile and are minimum variance unbiased estimators. The average run length performance comparison demonstrated that the KMW method was more efficient in detecting shift in the individual parameters as well as the combined shifts in the intercept and slope. Further by monitoring the parameters of the model, it was visually

intuitive in diagnosing the state of the process as compared to monitoring individual points along the calibration line. This was an important result as the NIST method is incorporated in an ISO 5725-6 (1994) standard and is freely available in the NIST/SEMATECH e-Handbook of Statistical Methods. We also demonstrated that with as small as ten sampling points per profile, the performance of the NIST method, of monitoring the end and middle points, deteriorates. The results can be extended to a more general case implying that a method based on representing a linear profile by a parametric model and subsequently designing a control chart based on the parameters of the model is an efficient approach as compared to a chart based on deviation statistics. Another significant result illustrated by the study was the reduction in the effect of the magnitude of the shift in the slope when the model is transformed by centering the x-values. Based on our observation we recommended using KMW with EWMA charts instead of the Shewhart charts for monitoring the individual coefficients. The results from the study can be applied to optimize the calibration frequency without losing the accuracy and precision of the instrument. The methods proposed to study and develop would be widely applicable to calibration data, both in understanding the measurement process behavior and in preventing unnecessary calibrations. Frequent recalibration can be expensive and increase the variation of the measurement process.

The applicability of changepoint approach for monitoring polynomial profiles was studied. Profiles with nonlinear behavior over one independent

variable can be approximated with polynomial models over certain regions. The development of the changepoint statistic for a polynomial case was illustrated and a derivation of the breakdown of the variance components of the likelihood ratio statistic was presented. The derivation showed that the components of the variance breakdown were not as clearly distinguishable as in the linear case. As is the case with the polynomial profiles or with nonlinear profiles, the parameters of the profile are dependent. The run length performance comparison was conducted with the KMW control chart which has not been compared previously in the literature. The probability of detecting signal comparison of the changepoint approach with the KMW method indicated a superior performance for detecting shifts in error variance. Since stability of error variance is of primary importance before shifts in the other parameters can be ascertained. It clearly indicated that the changepoint was a more efficient approach in situations that coefficients of the model are not independent. The retarding of the approach in detecting shifts in the intercept and slope can be compensated by using the changepoint approach in conjunction with an MEWMA approach. Further with polynomial profiles, multicollinearity is a nontrivial issue. Centering of the independent variables [Kazemzadeh et al. (2008)] reduces the effect but a more robust method is needed if the technique has to extend to higher order polynomials, one such method is the orthogonal polynomials.

In chapter 5, the problem analyzing an experiment on the system that generates a profile, also known as signal-response system was presented. This

problem goes hand-in-hand with the monitoring problem and falls in the general space of problems aimed at understanding and reducing variability in the system to improve process performance. The signal-response system has been studied extensively using the Taguchi experimental design and conducted in a manner similar to a split plot experiment. Here the control factors were adjusted for a fixed level of the noise factors, and the response value is observed by sequentially changing the signal factor. Traditionally such systems have been analyzed using a two step OLS approach, where in the first step a parametric model is fit and in the second step the parameters of the model are treated as the responses. Very often, an OLS approach is used to fit the model in the first step, and multiple responses are optimized the control and noise factor settings. A generalized linear mixed model approach (GLMM) was proposed. This method has the flexibility to represent the error structure of a restricted randomization of the split plot experiment and also has the ability to model non-normal responses. A mean-variance modeling approach of an RPD was followed. Subsequently the GLMM approach was compared with the Miller and Wu approach (1996) and was demonstrated to provide a much better fit to the data as compared to the two step approach of Miller and Wu (1996). This was illustrated by the tighter confidence interval of the predicted response. Further the OLS approach of Miller and Wu (1996) does a poor job of explaining the variability in the model as demonstrated by the erratic pattern in the confidence intervals.

Finally in chapter 2, an updated literature review was provided since the comprehensive reviews of Woodall et al. (2004) and Woodall (2007).

## **6.2. Future Research Ideas**

In the past, the cost of sampling effort has driven the selection of optimal sample sizes and sampling frequency such that the within-sample variation is minimized so that the between-sample variation can be maximized to detect changes in the process. Increasing use of automatic sensing and measurement technologies has reduced the cost of sampling. For phase II approaches, it has become pretty standard to establish real time monitoring systems. One question that has not been addressed with enough stress is the question of appropriate phase I sample size to determine the parameters of the model. Jensen et al. (2006) investigate the effect of parameter estimation on control charts in general and argue that for phase II charts based on estimated quantities to behave as expected a larger sample size has to be used for phase I estimation. The authors suggest more research in this area and for profile monitoring in specific.

Any statistical monitoring scheme is depended on a successful distinction between the common-cause variation between and within profiles from the special cause variation between profiles. There have been steps made in the direction to incorporate a more flexible variance-covariance structure by using mixed models; see Jensen and Birch (2009) and Jensen et al. (2007). There has been no deliberate work done so far to show how robust the profile monitoring schemes are to the model assumption. Residuals charts or variance charts could

be used for tracking changes in lack of fit of the fitted models over time.

Residuals charts such as Kang and Albin (2000) average the residuals and much of the lack of fit information is smoothed out. Bulk of the research in profile monitoring has been focused on monitoring the mean profile. More work is needed in understanding the variance profile and using robust design studies can help in characterizing the function.

The literature indicates the ubiquitous presence of nonlinear profiles in varied industries. Profiles ranging from dose response curves which can be represented by well understood empirical nonlinear models to more complicated profiles quantified by a large class of functions. Some of the examples of such profiles include - stamping tonnage signals [Jin and Shi (1999)], force profile of rams inserting valve seats in automotive engine cylinder head [Mesesova et al. (2006)] and cross-sectional roundness profiles [Colosimo and Pacella (2007)] among others. Many authors resort to using nonparametric approaches to represent the profiles. Using smoothing techniques such as smoothing spline [Gardner et al. (1997)], much of the information is dependent on the choice of the smoothing parameter which has to be optimized so that it does not smooth out the local features that might distinguish the out-of-control profiles. Parametric or semi-parametric approaches like the spatial autoregressive model proposed by Colosimo et al. (2008) and wavelets of Jin and Shi (2001), Jeong et al. (2006), Chicken, Pignatiello and Simpson (2009), Chiang and Yadama (2010). Also, Jin and Shi (2001) and Jeong et al. (2006) proposed methods to



select subset of the wavelet coefficients to monitor. As cautioned by Woodall et al. (2004), in addition to the control chart based on the most significant wavelet coefficients, there should be an additional control chart established to monitor the remaining coefficients to reduce the risk of not detecting any shifts. Chicken, Pignatiello and Simpson (2009) discuss these issues in detail and highlight additional issues and proposed a changepoint based chart to monitoring the wavelet coefficients deviations from the established in-control profile. They run simulations for various types of shifts and demonstrate that likelihood statistic performs much better than the rest of the wavelet based methods. Their method is based on Phase II approach. Zarandi and Alaeddini (2010) show comparison between model free approaches versus model based approach, in particular they focus on comparing methods based on Fuzzy Inference Systems. More work needs to do be done in comparing the efficiency gained in using wavelets based approach especially for phase I as compared to the parametric or semiparametric model based approaches.

### **6.3. Conclusion**

The results of this work for linear and polynomial profile monitoring will serve as an input to the research on developing an optimal monitoring scheme, which will have a significant impact on the use of process monitoring and control charting methods by quality engineers. The approach to analyze profile experiments will help in understanding the behavior of common cause variation due to nuisance factors. The profile monitoring is the one of the

most active area of research in statistical process control and its scope is not restricted to engineering applications but has been extended to health care and public health surveillance of disease clusters, Woodall (2006).

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APPENDIX A

ADDITIONAL RESULTS FOR COMPARISON BETWEEN KMW AND NIST

Table A.1. KMW Shewhart Scheme – ARLs for combined shifts in Intercept and Slope

KMW-Shewhart NIST %Improvement over NIST Method		Delta (Shift in slope)										
		0	0.025	0.05	0.075	0.1	0.125	0.15	0.175	0.2	0.225	0.25
Lambda (shift in the intercept)	0	198.7*	175.4	125.0	79.2	47.4	27.7	17.2	10.7	7.2	5.0	3.6
		199.5†	181.3	138.7	95.6	61.9	40.4	26.7	17.8	12.2	8.4	6.2
		0.4‡	3.3	9.9	17.2	23.4	31.4	35.6	39.9	41.0	40.5	41.9
	0.05	195.8	161.8	105.8	64.8	38.9	23.7	14.5	9.1	6.2	4.4	3.2
		200.1	167.6	121.8	83.1	55.3	36.2	23.8	16.1	11.1	7.8	5.7
		2.1	3.5	13.1	22.0	29.7	34.5	39.1	43.5	44.1	43.6	43.9
	0.1	186.4	139.5	90.1	55.2	32.3	19.5	12.2	7.9	5.4	3.9	2.9
		188.3	151.6	106.5	71.9	47.5	30.9	20.8	14.3	9.9	7.1	5.2
		1.0	8.0	15.4	23.2	32	36.9	41.3	44.8	45.5	45.1	44.2
	0.15	170.3	119.4	75.3	45.4	26.5	15.9	10.3	6.8	4.7	3.5	2.6
		177.7	135.2	96.3	63.1	42.4	27.5	18.6	12.7	9.0	6.5	4.7
		4.2	11.7	21.8	28.1	37.5	42.2	44.6	46.5	47.8	46.2	44.7
0.2	153.1	101.3	61.7	36.9	22.1	13.4	8.6	5.8	4.2	3.1	2.4	
	164.2	120.7	85.2	55.6	36.1	24.4	16.5	11.7	8.0	5.8	4.4	
	6.8	16.1	27.6	33.6	38.8	45.1	47.9	50.4	47.5	46.6	45.5	
0.25	131.3	84.2	50.6	30.4	18.1	11.5	7.4	5.1	3.7	2.8	2.2	
	149.3	106.3	72.0	48.1	31.9	21.6	14.6	10.3	7.4	5.4	4.1	
	12.1	20.8	29.7	36.8	43.3	46.8	49.3	50.5	50.0	48.1	46.3	
0.3	112.1	69.4	40.6	24.3	14.9	9.5	6.4	4.5	3.3	2.5	2.0	
	132.5	92.5	63.6	42.3	28.2	18.9	13.0	9.4	6.6	4.8	3.8	
	15.4	25.0	36.2	42.6	47.2	49.7	50.8	52.1	50.0	47.9	47.4	
0.35	93.7	57.4	33.7	20.3	12.6	8.2	5.5	4.0	2.9	2.3	1.9	
	115.5	79.3	55.3	37.3	25.1	16.7	11.7	8.4	6.0	4.5	3.5	
	18.9	27.6	39.1	45.6	49.8	50.9	53.0	52.4	51.7	48.9	45.7	
0.4	78.3	47.2	27.6	16.8	10.6	6.9	4.8	3.5	2.7	2.1	1.7	
	100.6	71.0	47.7	32.2	22.3	14.9	10.5	7.6	5.5	4.2	3.3	
	22.2	33.5	42.1	47.8	52.5	53.7	54.3	53.9	50.9	50.0	48.5	
0.45	63	37.8	22.5	14	8.9	6.0	4.3	3.2	2.4	1.9	1.6	
	87.7	60.1	41.7	28.1	19.2	13.3	9.4	6.9	5.0	3.8	3.0	
	28.2	37.1	46.0	50.2	53.6	54.9	54.3	53.6	52.0	50.0	46.7	



		52.6	30.9	18.7	11.6	7.6	5.2	3.7	2.8	2.2	1.8	1.5
	0.5	76.9	52.7	36.2	24.8	17.2	11.9	8.5	6.3	4.6	3.6	2.8
		31.6	41.4	48.3	53.2	55.8	56.3	56.5	55.6	52.2	50.0	46.4

\* ARL KMW-Shewhart method  
† ARL NIST method  
‡ Percentage improvement over  
NIST method

APPENDIX B

ADDITIONAL TABLES FOR THE SIGNAL RESPONSE SYSTEM STUDY

Table B.1. Design Matrix for the Control Factors

Row	Control Factors						
	A	B	C	D	E	F	G
1	1	1	1	1	1	1	1
2	1	1	1	-1	-1	-1	-1
3	1	-1	-1	1	1	-1	-1
4	1	-1	-1	-1	-1	1	1
5	-1	1	-1	1	-1	1	-1
6	-1	1	-1	-1	1	-1	1
7	-1	-1	1	1	-1	-1	1
8	-1	-1	1	-1	1	1	-1

Table B.2. First Run for Day 1 of the Experiment

Row	Signal Factor Level								$X_N$
	650	700	750	800	850	900	950	1000	
1	639.7	642.3	645.5	653.9	666.6	672.1	692.2	711.6	-1
	640.5	641.7	644.8	655.1	665.8	670.8	690.6	710.8	
	636.2	643.6	646.1	654.7	667.1	673.3	689.7	711.1	
	637.2	644.0	644.3	654.2	665.4	671.1	689.8	710.5	

Table B.3. Design Matrix for the Control Factors

Signal Factor	Orthogonal Polynomial	
	P1	P2
650	-7	7
700	-5	1
750	-3	-3
800	-1	-5
850	1	-5
900	3	-3
950	5	1
1000	7	7

Table B.4. Model Specification

	Dimensions
G-side Cov. Parameters	1
R-side Cov. Parameters	2
Columns in X	11
Columns in Z per Subject	16
Subjects (Blocks in V)	16
Max Obs per Subject	8

APPENDIX C

SAS CODE FOR FITTING GLMM MODEL

```

% GLMM for Mean
%LET DDF = BETWITHIN;
proc glimmix data = mean_orth;
class id xn run tclss;
model mean_wt = a c e f g p1 p2 c*p1 xn/ dist =normal
solution
ddfm = &DDF;
random _residual_ /subject = id type = cs;
output out = glmout pred = yhat resid = residual UCL =
upperCI
LCL= LowerCI;
run;
data glmout1;set glmout;
gCIlengthid = upperCI - lowerCI;
run;

% GLMM for Variance
proc glimmix data = mean_orth ;
class id xn run tclss ;
model var_wt = a b c g p1 b*p1 g*p1 b*p2 c*p2 e*p2 f*p2
g*p2
xn/dist = gamma link = log ddfm = satterth solution;
random _residual_/subject = id type = simple;
output out = glmout pred = yhat resid = residual UCL =
upperCI
LCL= LowerCI;
run;
data glmout;set glmout;
gCIlengthid = upperCI - lowerCI;
run ;

```