Implementation of A Real-time Multivariate Data Analysis Methodology in Injection Molding and High Frequency Welding Process

By

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ABSTRACT

In this research two methodologies for data collection using a multivariate data analysis technique are proposed. The Continuous Methodology and Combination Methodology for data collection are used and evaluated in two distinct processes, injection molding and welding by radio frequency. These processes, which are of a multivariate nature, contain variables that have an effect on the quality of a product. The Continuous Modeling Methodology proposed the use of process data at three levels to create sub-matrices, which provided the most information of all the available batch characteristics. The Combination Methodology utilized gradual changes to critical variables of the process or product defect. A signal monitoring system is utilized for the validation of the methodologies proposed for each process. For the evaluation of the methods proposed, type I and type II errors are used along with process scrap rates. It has been shown that with the continuous and combination methodology, the type I error or the scrap rate are decreased. The variables that are significant for the identification of product defect have been identified.

RESUMEN

En esta investigación, dos metodologías son propuestas para la adquisición de data que es usada con una técnica de análisis de múltiples variables. La metodología Continua y la Combinada, usadas para la adquisición de data, son evaluadas en dos procesos diferentes, moldeo por inyección y soldadura usando radio frecuencia. Estos procesos son de por naturaleza constituidos por múltiples variables que pueden tener un efecto en la calidad de un producto. La metodología Continua propone usar data del proceso en tres niveles de operación para la creación de matrices que proveen la mayor cantidad de información de la característica de los lotes. La metodología Combinada utiliza cambios graduales a variables críticos para el defecto del proceso o el producto. Un sistema de monitoreo de señales es utilizado para la validación de las metodologías propuestas para cada proceso. Para la evaluación de cada metodología propuesta, el error tipo I, tipo II y la razón de desperdicios son calculado. Se ha demostrado que usando la metodología continua y combinada se disminuye el error tipo I o la razón de desperdicios. Las variables que son significantes para la detección de defectos son identificados en ambos procesos.

DEDICATION

To my family who throughout the years has understood that some things in life take a bit more of time for different individuals. Success does not arrive immediately, but with patience and perseverance some goals may be achieved.

ACKNOWLEDGEMENTS

I want to thank the following people for giving me the opportunity to reach some of my goals: Felix Ortiz, who always said to give an inexperienced person the opportunity to shine, gave me the opportunity to work with his automation group. Carlos Rios and Franklin Sifre had the confidence in my work to run the show. Ramon Rivera whose expertise rivaled all engineers and Roberto Lopez whose trust and wisdom guided me through rough times.

Finally and not least, to David Serrano who since 1998 has been a friend and my counselor in various projects and classes and with much patience has endured the voyage.

TABLE OF CONTENT

TABLE LIST

FIGURE LIST

NOMENCLATURE

I	Identity matrix
N	Sample
PC	Principal Component
R^2	Goodness of fit
S	Covariance matrix
T^2	Hotelling's multivariate analog to uni-variate statistic t^2
U	Vector of Principal Components
w_n	Loading
x_n	Observed variable
$\overline{X}$	Mean
X	Random Vector

Greek Symbols

α	Confidence Level
β	Column Vector
ε	Variance
ϕ	Function
λ	Lagrange Multiplier
θ	Angle measurement

Chapter 1 Introduction

1.1 Background

The detection and identification of part defects and its causes in medical devices is an important task for the personnel involved in the manufacturing process. Defects in medical devices can affect the different phases of product life. A defect in a medical device used for fluid transport may obstruct the flow of fluid through the device, create loose particles within the fluid and may prevent the proper assembly to other devices. Defects can also be responsible for the wear and possible breakage of the various mechanical components in an assembly machine; therefore, increasing the manufacturing costs due to an increase of scrap, labor time and machine downtime. If a defective medical device is used it may provoke possible complications in the patient's treatment, recovery and even worse, death. These can open an array of legal dilemmas that may affect the credibility of the medical device manufacturer and may lead to the possible loss of quality certifications, which allow the manufacturer to continue the production of its devices.

Currently, there are various methods of identifying defective parts. Vision systems can be used to detect part defects, such as a short or flash or missing components, which in high-speed machine output may range from 500 to 900 parts per hour. Manual inspection of parts is also used for low output processes such as in the production of bags for intravenous fluids. In special cases where a vision system and manual inspection is not feasible other methods have to be implemented to detect and segregate the good and bad parts. Some production machines have programmed features, which allow the process specialist to identify the ranges of operation for each parameter of interest, for example pressure or temperature. If the parameter goes above or below the set range a digital output can be sent to a conveyor or any part segregation equipment, which can mechanically accept and discard parts. Although these features are helpful they do not contribute to the understanding of the process. The process specialist cannot see if there are any relationships between the parameters being monitored and the defects that are produced by these parameters going out of the established range.

1.2 Research Objectives

In many cases of study, a problem is encountered which may be due to variables that may or may not contribute to the occurrence and magnitude of the problem. We are faced with the dilemma of having a process with multiple variables that need to be monitored at all times. The variables may have an effect on the quality of the product. The amount of data is also so abundant that manual calculations or analysis of the data would be time consuming and render little or no improvements in the long term.

The principal objectives of this research are:

a. Provide an effective methodology to monitor a process in real time.
b. Establish a means of determining which variables are to be monitored.
c. Validate the methodology proposed by implementing in a process and obtaining measurable results.

Chapter 2 Overview of Multivariate Techniques

2.1 Multivariate Data Analysis

Multivariate data analysis (MVDA) is simply defined as any statistical technique used to analyze data that arises from more than one variable. MVDA can be used in any field of study were large amounts of data are collected and analyzed. It has been used in the areas of biology, medicine, engineering, business and psychology to name a few. Chapter 2 sections 2.2 will provide an overview of the classification of multivariate techniques and the steps followed to select the proper technique for the analysis of problems.

2.2 Multivariate Techniques

Multivariate techniques can be classified into two types, (Table 2.1) dependence techniques and interdependence techniques [1].

Table 2.1 Multivariate Techniques

Dependence	Interdependence
Structural Equation Modeling	Factor Analysis
Canonical Correlation Analysis	Confirmatory Factor Analysis
Multivariate Analysis of Variance	Cluster Analysis
Multiple Regression	Multidimensional Scaling
Conjoint Analysis	Correspondence Analysis
Multiple Discriminant/Logistic	

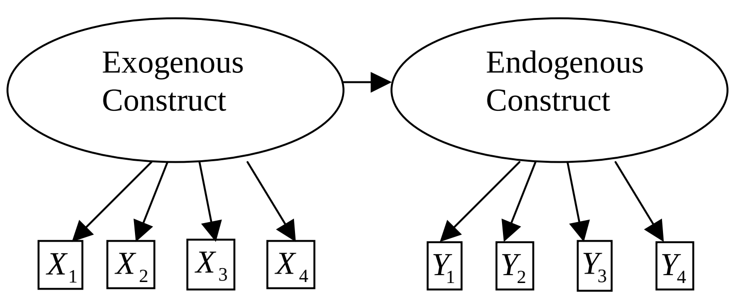
2.2.1 Dependence Techniques

The dependence technique is classified as such because it has a variable or set of variables, as the dependent variable(s) and the remaining variables as independent. The classification of dependence is further divided depending on the number of variables and the type of measurement scale, metric or non-metric, used by the variable.

2.2.1.1 Structural Equation Modeling

Structural Equation Modeling (SEM) is a technique that tries to explain the relationship among multiple variables. SEM has two basic components: the measurement model, which uses several variables or indicators for a single independent or dependent variable; the structural model, which relates the independent variables to the dependent [2,3]. Figures 2.1 a and b show a simple representation of a measurement and structural model. In the measurement model, the arrow between the exogenous and the endogenous means there is a dependence relationship between both constructs. Each construct has four indicators or variables assigned, for this specific example. The curved arrow in the structural model represents a co relational relationship or the strength of the association between variables.

(a) Measurement Model



(b) Structural Model

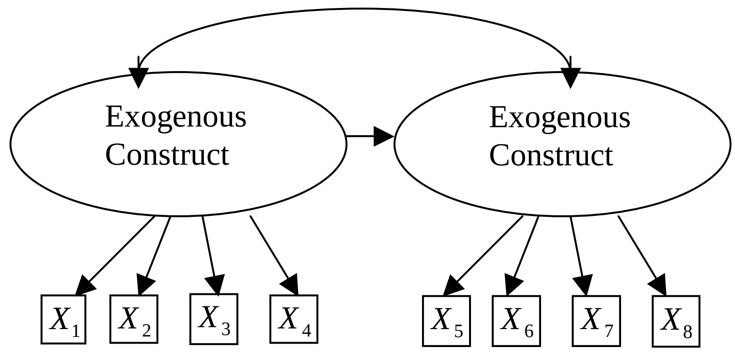


Figure 2.1 Visual Representation of a Measurement and Structural Model in SEM

2.2.1.2 Canonical Correlation

The objective of Canonical Correlation analysis is to correlate simultaneously several metric dependent variables and independent variables. Equation 2.1 represents the relationship between the dependent (metric or non-metric) and the independent (metric or non-metric) variables. It is important to notice that each equation differs depending on the type of variable being used as the dependent or independent.

$$Y_1 + Y_2 + Y_3 + ... + Y_n = F(X_1 + X_2 + X_3 + ... + X_n) \quad (2.1)$$

2.2.1.3 Multivariate Analysis of Variance

Multivariate Analysis of Variance or MANOVA can be used to find the relationship between several categorical independent variables or treatments and two or more metric independent variables [4].

Multivariate Analysis of Variance (MANOVA)

$$Y_1 + Y_2 + Y_3 + ... + Y_n = F(X_1 + X_2 + X_3 + ... + X_n) \quad (2.2)$$

Where Y variables are metric and X variables are non-metric. Comparing equation 2.2 to equation 2.1, it is clear that the independent variables in a Canonical Correlation can be either metric or non-metric.

2.2.1.3 Multiple Regression

Multiple Regression is a statistical technique used to analyze the relationship between a single Y dependent metric variable and several X independent metric variables [5,6].

$$Y_1 = F(X_1 + X_2 + X_3 + ... + X_n) \tag{2.3}$$

2.2.1.5 Conjoint Analysis

Conjoint Analysis is a family of techniques and methods developed to understand individual preferences that share a theoretical foundation based on the models of information integration and functional measurement [7]. It analyzes the factors that are controlled (independent variables) which are qualitatively specified [8].

$$Y_1 = F(X_1 + X_2 + X_3 + ... + X_n) \tag{2.4}$$

Where Y_1 can be non-metric or metric and the X are non-metric

2.2.1.6 Multiple Discriminant Analysis and Logistic Regression

The purpose of Multiple Discriminant Analysis and Logistic Regression is to identify the group to which an object belongs. Basically it estimates the relationship between a single non-metric dependent variable and a set of metric independent variables. Logistic Regression is limited to a two group dependent measure [9,10].

$$Y_1 = F(X_1 + X_2 + X_3 + ... + X_n) \tag{2.5}$$

Where Y_1 is non-metric and the X are metric. This is the difference between equation 2.4 and 2.5.

2.2.2 Interdependence Techniques

In the interdependence technique, variables are analyzed as a single set. Variables are neither classified as dependent or interdependent. The interdependence group is also divided further depending if the relationship is between variables, cases/respondents or objects.

2.2.2.1 Factor Analysis

Factor analysis is a statistical technique that can be used to analyze the interrelationships among large numbers of variables in terms of their common factors. Factor analysis is divided into Common Factor and Principal Components Analysis. Common Factor Analysis is used to describe the covariance among variables in terms of a few underlying factors. In Principal Component Analysis, the data is reduced into smaller number of components, which explain the maximum amount of variance [11,12].

As part of obtaining an interpretable factor solution it may be useful to implement a factor rotation method, which may simplify the factor matrix structure (simplification of rows and columns). The values of the rows and columns are made as close to zero as possible. In factor rotation the reference axes of the factors are turned about the origin until some other position has been reached. In Orthogonal Factor Rotation the axes are rotated, but are maintained at 90 degrees (Figure 2.2). The X_1 and X_2 variables represent the first factor and second factor, respectively, extracted from the factor analysis and represent the most significant factors. The Y_1 and Y_2 are the rotated factors

X_1 and X_2 , where the θ represent the angle of the rotated factors with respect to the original axis. The main purpose of this is to help visualize which variables are highly correlated with each factor.

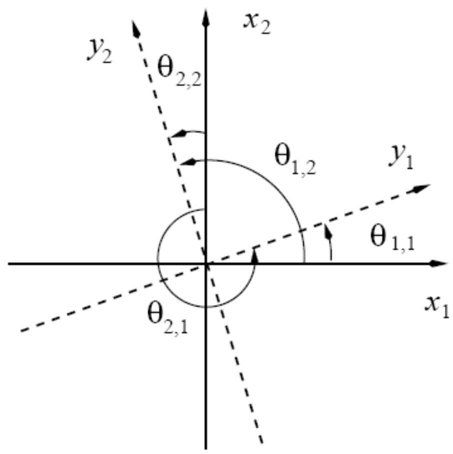


Figure 2.2 Orthogonal Factor Rotation

There exists three Orthogonal Rotation Methods: Quartimax, Variamax and Equimax. Two of the most used are Quartimax and Varimax. In the Quartimax rotation, simplification is based on the rotation of the initial factor such that a variable loads high (highly correlated with) on one factor and as low as possible on another factor. In the Variamax Criterion, loadings should be close to 1 (+1 or –1) or 0. Equimax is a combination of Quartimax and Variamax [13]. The purpose of this is to eliminate having the same variable repeat itself as a significant variable for each factor.

2.2.2.2 Confirmatory Factor Analysis

Confirmatory factor Analysis is used to test how well measured variables represent a smaller number of constructs. It may be used with structural equation modeling. The difference with this technique compared to other multivariate techniques is that with confirmatory factor analysis one must specify the number of factors that exist within a set of variables and state, which factors will load highly on before the computation of the results [14].

2.2.2.3 Cluster Analysis

Cluster analysis can be considered as an exploratory technique, which groups individuals or objects into clusters so that objects in the same cluster have similar characteristics than objects in other clusters, see figure 2.3 [15].

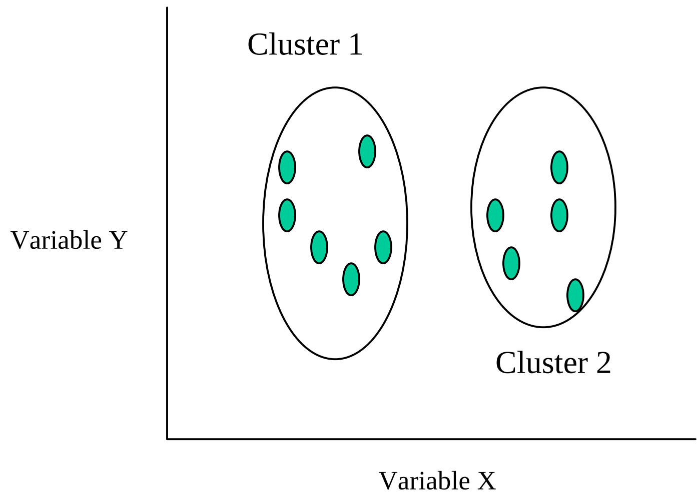


Figure 2.3 Observations based on Two Clustering Variables (X & Y)

2.2.2.4 Multidimensional Scaling and Correspondence Analysis

Multidimensional scaling or perceptual mapping is a technique that determines the perceived relative image of a set of objects. It uses a single measure of similarity across the entire set of objects. Figure 2.4 shows an example of the perception of 5 candy manufacturers. Manufacturers A and B have been judged to be the most similar if comparing to other possible pairs such as A and C or B and D. The purpose of multidimensional scaling is to transform judgments into distances in a multidimensional space [16]. In correspondence analysis, perceptual maps are created with the variables and observations plotted simultaneously [17]. Figure 2.5 shows a hypothetical example of a product based on the region where it is used.

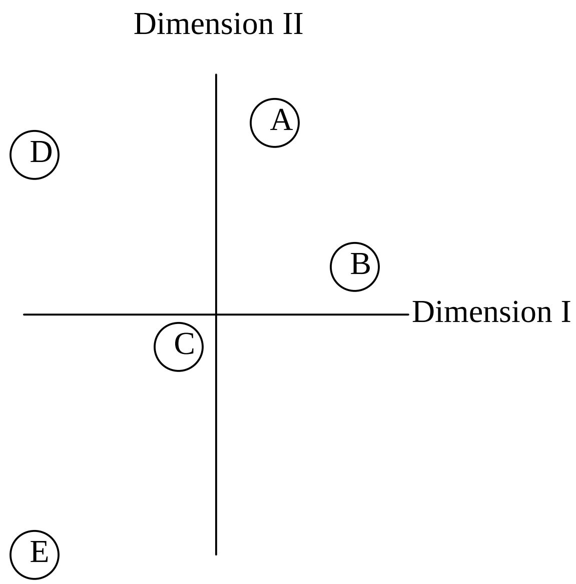


Figure 2.4 Multidimensional Map of Perceptions of 5 Candy Manufacturers

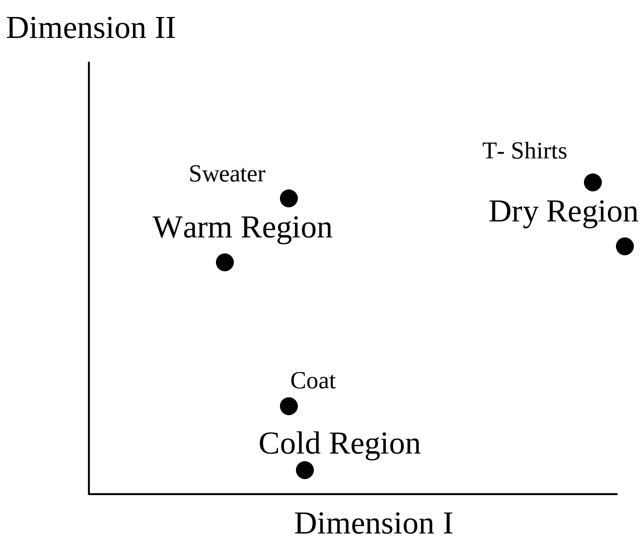
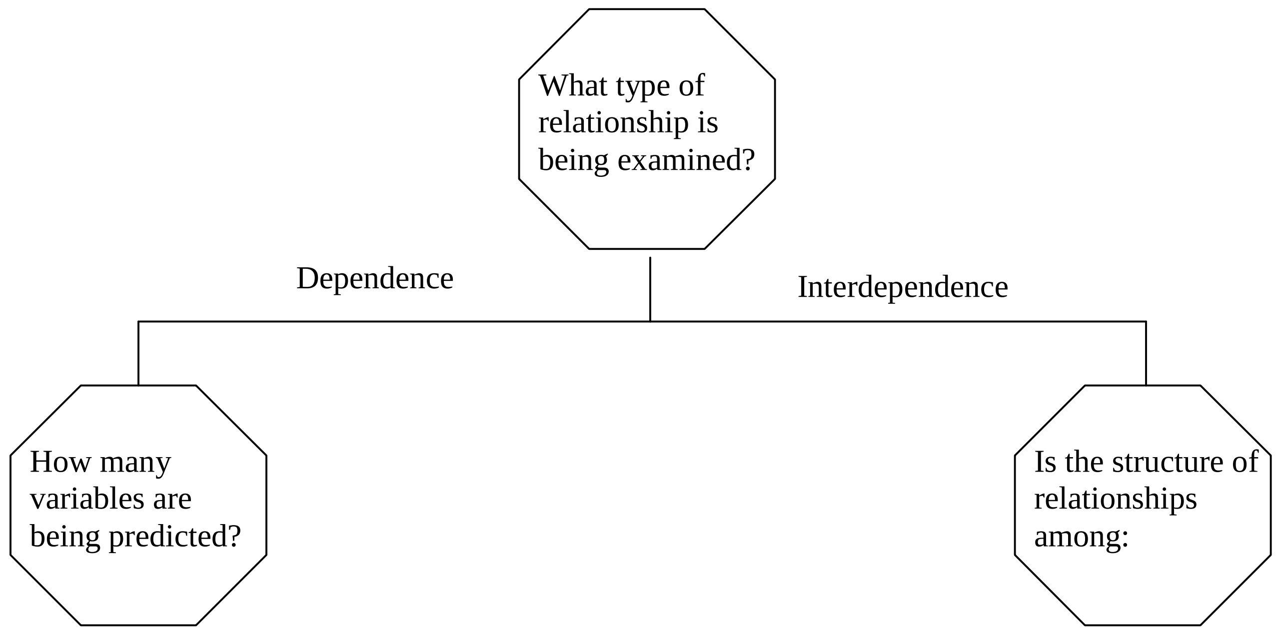


Figure 2.5 Perceptual Map From Correspondence Analysis of Product Type and Region

2.2.3 Guide for the Selection of A Multivariate Technique

Hair et al [1] provides a decision diagram (Figure 2.6 thru 2.8) for the selection of a multivariate technique depending on the variables that are going to be analyzed. These diagrams are useful because they serve as a guideline for the selection of the multivariate technique most appropriate for any case study under evaluation. For example, if there were a case study, which consists of variables that will be used to predict another variable or set of variables, then a dependence technique (Figure 2.6 and 2.7) would be selected. The specific technique used will depend if there is only one dependent variable to be predicted or various dependent variables. This is further divided on the classification of the variable as being metric or non-metric. Metric variables are defined as those variables, which are quantitative and Non-metric variables are qualitative. Examples of metric variables could be age, weight, temperature, pressure and height. Non-metric variables could be sex (female or male) and occupations (doctors or engineers). If the relationship among the variables is unknown and a structure is to be found between these variables then an interdependence technique is used (Figure 2.8). These are also broken down depending if the variables are metric or non-metric. Examples of these have been presented in section 2.2.2.3 Cluster Analysis and 2.2.2.4 Multidimensional Scaling and Correspondence Analysis, where formations or patterns among variables are analyzed or relationships are established between variables such as in Factor Analysis. The technique selected for this research will be explained in chapter 5.

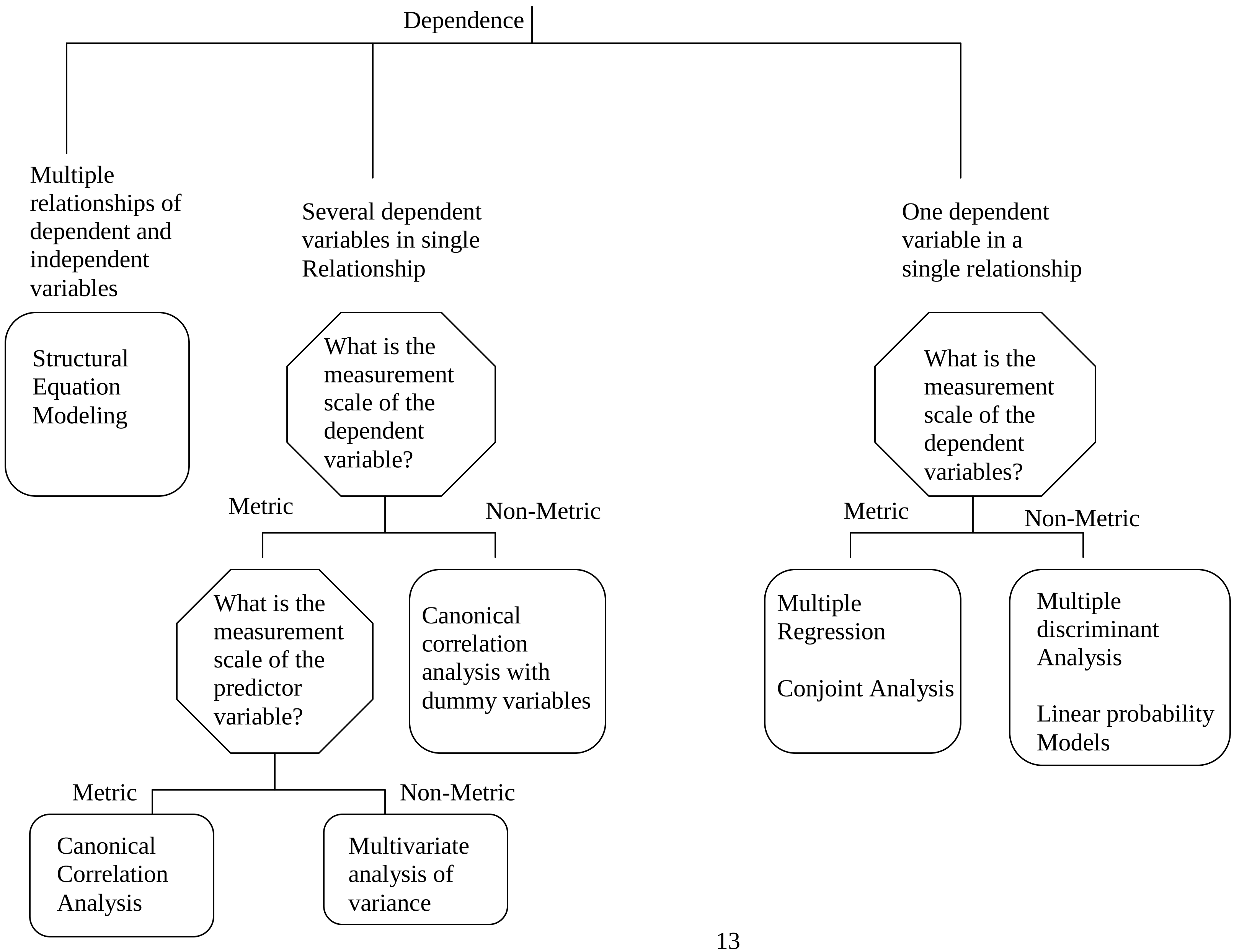


See diagram 2

See diagram 3

Figure 2.6 Decision Diagram 1 (from Hair et al "Multivariate data Analysis", page 14-15)

Figure 2.7 Decision Diagram 2 (from Hair et al "Multivariate data Analysis", page 14-15)



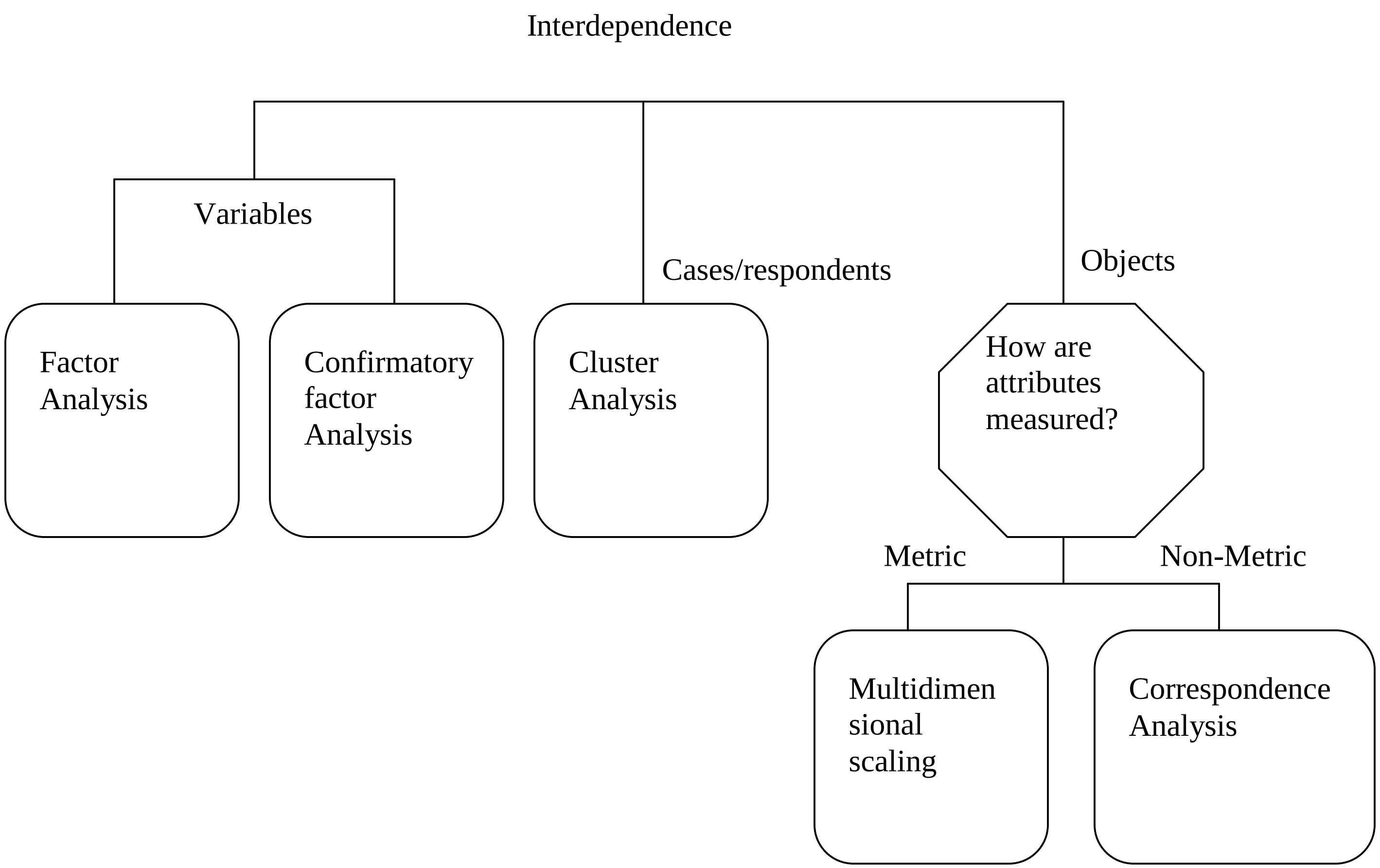


Figure 2.8 Decision Diagram 3 (from Hair et al "Multivariate data Analysis", page 14-15)

Chapter 3 Literature Review

It has been the goal of many researchers and industries to provide methods of maintaining control of processes. These processes may include chemical processing, molding, and extrusion, mixing of resins among others. Maintaining control of the operation of a process translates into savings, since an efficient use of resources and equipment reduces wastes in material and time. Any deviation from the established operating ranges during the processing or production of a product may lead to the introduction of erroneous quantities of solutions, improper mixing or defective molded products that may cause problems to the end user or the process itself.

Comparing the actual results to the predicted results when a mechanistic model, such as a linear regression model is used can monitor a process performance. Statistical process control charts such as the Shewart [18], Cumulative Sum (CUSUM) [19], or Exponentially Weighted Moving Average (EWMA) [20] can be used to compare the actual state of the process of interest to the normal operating conditions. The setback to these control charts is that they were developed for the monitoring of uni-variate processes [21].

Multivariate statistical analysis, such as Principal Component Analysis and Partial Least Squares have been used in many areas such as the pulp and paper, chemical processing, socio-economic and psychology [22,23]. Yacoub and MacGregor used Principal Component Analysis (PCA) and Partial Least Squares (PLS) to understand the spatial variation in the manufacture of polyurethane foam insulation panels by reaction injection molding process, to correct the causes of variation and optimize the quality variables by using response surface modeling [24].

Kresta et al proposed multivariate statistical process control procedures for a fluidized bed reactor and an extractive distillation column. Using PCA and PLS methods they were able to recognize that the product space should be restricted to variables of interest in the monitoring procedure, scaling should be performed in such a way that the variances reflect their relative importance and loading vectors help identify possible causes to product abnormalities [25]. Only simulations were used for this analysis.

Nomikos, MacGregor and Kourti emphasized on historical data modeling to monitor the progress of styrene-butadiene batch reactor process based on multi-way principal component analysis. The future behavior of the process was monitored by comparing it against that observed in the past when the process was in a state of statistical control [26,27]. They were able to detect simulated faults in the process.

Multivariate statistical methods have been used to analyze data from an industrial batch drying process. PLS methods were able to isolate the group of variables in the chemistry, in the timing of the various stages of the batch and in the shape of the time-varying trajectories of the process variables and how they were related to a poor quality product [28].

Multivariate methods have also been able to provide a more efficient and reliable optimization procedure for the derivation of mass spectrometric analysis of a semi-synthetic amino-glycoside anti-biotic used in food-animal production by incorporating designed experiments in each of which the values for several parameters are changed at the same time [29].

Bashir, Khokhar and Schonfeld presented a modeling scheme for object motion trajectory based analysis and recognition, where Principal Component Analysis was used to reduce the dimensionality of the feature space denoted as CDF-Centroid Distance Function. Object motion trajectories were segmented and PCA coefficients were used for trajectory classification and activity recognition [30].

Principal Component Analysis and Partial Least Squares have also been used in the classification of olive oils by cultivars and geographical region by using Nuclear Magentic Resonance enhanced signals of ^{13}C spectra [31] and in the analysis of metal concentrations in coastal sediments by tracing anthropogenic pollutant sources and for characterizing various processes related to pollution [32].

Cho and Kim [33] proposed a method for predicting future observations in the monitoring of a batch process by using an extensive batch historical library and multi-way Principal Component Analysis. The current batch was compared to the historical library and the most similar trajectory was used for the prediction of future observations.

This research will propose the use of a multivariate method and data collection methodology, which will enable the monitoring of a process with high number of variables. The main goal is to be able to determine, which methodology provides the best results for the detection of process deviation or product defect. Table 3.1 outlines the various methodologies that have been used along with the multivariate method.

Table 3.1 Multivariate Technique and Methodology Utilized in Various Research Areas

	Methodology			
Contributors	Designed Experiment	Batch Historical Data	PCA	PLS
Yacoub/MacGregor [24]	X	X	X	X
Kresta [25]		X	X	X
Nomikos [26]		X	X	
Garcia/Kourti/MacGregor [28]		X	X	X
Cho/Kim [33]		X	X	

The multivariate technique selected and methodology proposed for this research will be explained in chapters 5 and 6.

Chapter 4 Research Problem and Methodology

4.1 Research Problem Description

Most processes are of multivariate nature. Monitoring the process becomes an arduous task when various factors contribute to the variation of the process. These factors may include untrained personnel, changes in raw material properties, equipment or tooling malfunction. Researchers have used various multivariate techniques and data collection methods that have provided positive results. Material resources, machine availability and implementation time are factors that also have to be considered when proposing a statistical technique and data collection methodology, which has to be implemented real time, since these factors translate into savings or losses to any given industry.

4.2 Methodology

The following items a-g will provide a description of the steps that will be followed during this research:

a. Definition of the process.

b. Selection of the multivariate technique following guideline of Figure 2.6-2.8

c. Definition of the modeling methodology being proposed as part of the research contributions.

d. Establishment of the modeling evaluation criteria.

e. Case study selection.

f. Implementation of methodology.

g. Evaluation of model performance.

Chapter 5 Multivariate Process Description and Technique Selection

5.1 Multivariate Process Description:

The Figure 5.1 illustrates the type of process variables that are present in the multivariate process. The non-measurable variables are described as those variables such as thickness or humidity, which could be measured if there was a sensor or measuring device available, but are not being monitored. The measurable variables are those described as having the means of being measured every machine cycle, for example pressure, velocity, temperature or voltage. A cycle is defined as a time period in which a product is created. The metric output variables are those that can be measured from the final product, but are not measured such that one can associate a specific product with a specific cycle. In other words if there existed a link between the process signals and the resulting product attributes, such as dimension taken by a vision system, then one can associate the process conditions with the final product. Non-metric variables are those that describe the appearance of the product such as burned, incomplete part or part with excessive material or missing components.

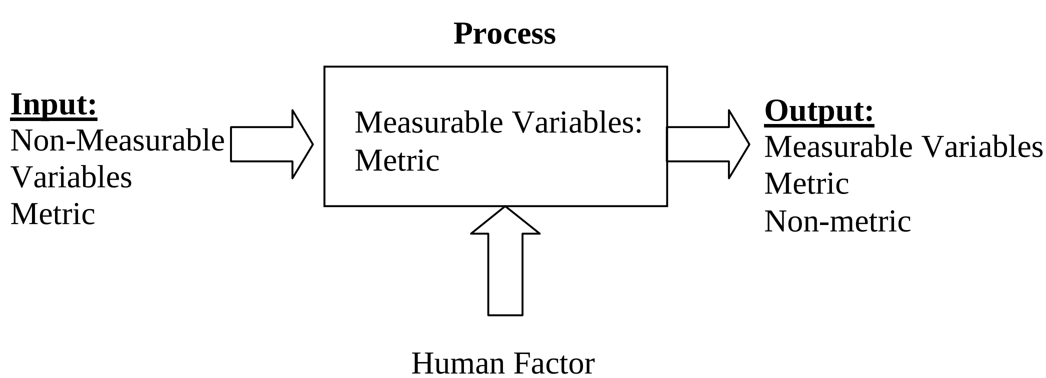


Figure 5.1 Process Flow Chart

The human factor is another critical variable, which at times cannot be completely controlled. This variable will not be measured as part of the process variables, which have an effect during the product creation.

5.2 Variable Selection and Classification

The variables of interest are those that can be measured for every cycle of the process. These would be metric variables describing parameters such as pressure and temperature, which can be compared at any moment in the process. The metric variables and non-metric variables at the end of the process (output) will not be utilized for the mathematical analysis, but will be used for the data collection and modeling methodology evaluation.

5.3 Selection of Multivariate Technique

Using the multivariate technique selection diagram presented in figures 2.6-2.8 a technique will be selected. First the type of relationship must be determined. The relationship between the variables in the process is unknown and these variables will not be used to predict other variables in the process. So to begin, the structure of the relationship between the variables is of interest. The techniques that can be used for this type of situation fall under the Interdependence section in the tree diagram. There are three branches that may be chosen: variables, cases/respondents or objects. The ultimate goal of process control is to be able to maintain the process as stable as possible while achieving a quality product. Variations in process parameters are to be controlled or at least minimized. Also the variables are quantitative. That means they will have a way of measuring them. So variables have two options for analysis: Factor Analysis and Confirmatory Factor Analysis

The Factor Analysis was selected as the multivariate technique most appropriate for the process since variables will be analyzed. There are still two approaches, Common Factor Analysis and Principal Component Analysis, within Factor Analysis, which have to be considered. To determine which type of analysis is appropriate it is important to understand what is being measured. There exist three types of variances: common variance, unique variance, and error variance. Common variance is defined as variance shared with other variables in the factor analysis. Unique variance is variance of each variable unique to that variable and not explained or associated with other variables and error variance is variance of a variable due to errors in data collection or measurement. Common Factor Analysis focuses on the common variance and is not interested in the structure of the variables. Principal Component Analysis focuses on the combination of all the three types of variances and the goal is to reduce the variables of interest. Looking at it from this point of view Principal Component Analysis would be the approach, which would help identify those parameters or variables that have the most variation in the process. Table 5.1 shows the path towards the selection of the multivariate technique by utilizing the steps presented above.

Table 5.1 Selection of Multivariate Technique

Interdependence			
Structure	Variables	Factor Analysis	Ratio Scales
		Confirmatory Factor Analysis	Use of summated scales
	Cases/Respondents	Cluster Analysis	Metric
	Objects	Metric	Multidimensional Scaling
		Nonmetric	Corresponence Analysis

5.4 Principal Component Analysis

Principal Components are the linear combinations of the original variables calculated with the maximum variance criterion and are characteristic vectors of the covariance matrix Σ. The purpose of Principal Component Analysis is to reduce the number of variables to be considered for further study by discarding the linear combinations, which have small variances.

Assumptions

1. All variables used in the multivariate technique must have some degree of measurement error (noise).
2. An underlying structure exists
3. The factor analysis should be of independent or dependent, but not both. This means that all the variables are either all independent X or all dependent Y, but not X and Y together.
4. The sample is homogeneous.
5. Normality is desirable, but not necessary since normality for each individual variable does not guarantee multivariate normality.
6. Multi-collinearity-the extent to which a variable can be explained by the other variables in the analysis.

The following derivation has been presented by T.W. Anderson in his book "An Introduction to Multivariate Statistical Analysis" 3rd edition pages 459-464 [34].

Let β be a p-component column vector such that $\beta'\beta = 1$ where β' is the transpose of β.
X is a random vector of p components
Σ is the covariance matrix, singular, positive semi-definite with multiple roots
ε is the variance

The variance of $\beta\ 'X$ is

$$\varepsilon(\beta' X)^2 = \varepsilon\beta' XX'\beta = \beta'\Sigma\beta \qquad (5.1)$$

Determine the normalized linear combination $\beta' X$ with maximum variance by finding a vector β, which satisfies $\beta'\beta = 1$ and maximizes equation 5.1.

Let

$$\phi = \beta'\Sigma\beta - \lambda(\beta'\beta - 1) = \sum_{i,j} \beta_i \sigma_{ij} - \lambda(\sum_i \beta_i^2 - 1) \qquad (5.2)$$

where λ is the Lagrange Multiplier.

The partial derivative of equation 5.2

is:

$$\frac{\partial\phi}{\partial\beta} = 2\Sigma\beta - 2\lambda\beta \qquad (5.3)$$

$\beta'\Sigma\beta$ and $\beta'\beta$ have derivatives everywhere in a region containing $\beta'\beta = 1$.

A vector β maximizing $\beta'\Sigma\beta$ must satisfy equation 5.3 where the equation is simplified

to $(\Sigma - \lambda I)\beta = 0$.

To obtain a solution to equation 5.3 with $\beta'\beta = 1$, λ must satisfy $|\Sigma - \lambda I| = 0$ must be singular.

$|\Sigma - \lambda I|$ is a polynomial in λ of degree p, where p has roots $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p$.

By multiplying $(\Sigma - \lambda I)\beta = 0$ on the left by β' the following is obtained:

$$\beta^{'}\Sigma\beta = \lambda\beta'\beta = \lambda \tag{5.4}$$

The variance of $\beta' X$ is λ. The maximum variance in $(\Sigma - \lambda I)\beta = 0$ corresponds to the largest λ. Let $\beta^{(1)}$ be a normalized solution of $(\Sigma - \lambda I)\beta = 0$, then $U_1 = \beta^{(1)'} X$ is a normalized linear combination with maximum variance. Let the p-component random vector X have $\varepsilon X = 0$ and $\varepsilon XX' = \Sigma$. Then there exists an orthogonal linear transformation U=**β**'X, where U is defined as the vector of principal components of X, such that the covariance matrix of U is $\varepsilon UU' = \lambda$ and

$$\boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & \ldots & 0 \\ . & . & & . \\ . & . & & . \\ . & . & & . \\ 0 & 0 & \ldots & \lambda_p \end{bmatrix}$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p$ are the roots of $\left|\Sigma - \lambda I\right| = 0$. These roots are also called the Eigen-values and are used to determine the maximum amount of components to be extracted. Principal Components with Eigen-values equal to or greater than 1, also known as the Kaiser Method, are maintained in the models. Figure 5.2 shows an example of observations in three dimensions and the corresponding principal components. The first principal component corresponds to the direction of most variance in the data. Each following principal component is perpendicular to the last component derived and corresponds to the next direction of most variance in the data.

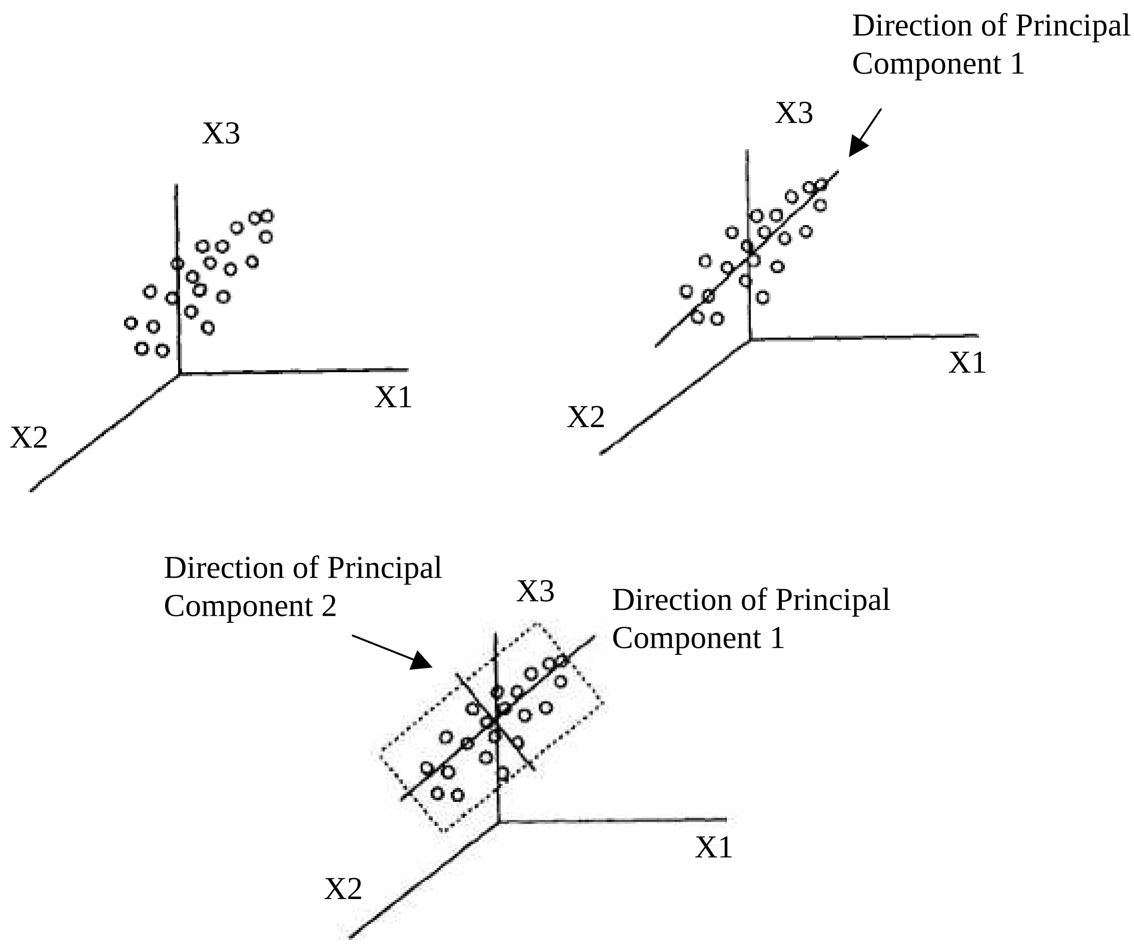


Figure 5.2 Observations in 3-dimensional Space and Principal Components

The basic Principal Component model or variate has the form:

$$PC = w_1 x_1 + w_2 x_2 + \ldots + w_n x_n \tag{5.5}$$

where w_n is the weight determined by the multivariate technique and x_n is the observed variable. The purpose of the variate is to separate the variables contribution to the overall variate effect, w_n also know as the loading.

Chapter 6 Modeling Methodology

6.1 Introduction

One of the main purposes of this research is to propose and validate a data collection methodology to be used with the multivariate technique. The data collection methodology is essential for the creation of the data matrix β used for the derivation of the principal components in the factor analysis. The data collection requires an understanding of the process under investigation, although most analyses start out as an exploratory test.

In the literature (Table 6.1), the data collection methodologies found were historical batch data and designed experiments using the Principal Component Analysis or Projected Latent Structures (PLS). Projected latent Structure or Partial Least Squares is a regression technique, which is used with Principal Component Analysis. Partial Least Squares analysis is beyond the scope of this research since dependent variables will not be measured for every set of observations. The multivariate techniques provide the form of the mathematical models to be used and these models require a data collection methodology. The methodologies presented in the literature have not shown to be able to accommodate themselves to the changing conditions of the process. Two modeling methodologies will be proposed which can help solve this problem. The Continuous Modeling Methodology utilizes process data at three levels (low parameter setting, medium parameter setting and high parameter setting) to create sub-matrices and the Combination Methodology, which utilizes gradual changes to critical variables to the process or product defect. This is the primary contribution to this research.

Table 6.1 Data Collection Methodologies and Factor Analysis Proposed

	Methodology				
Contributors	**3-Level Batch Analysis/Critical Factors**	**Designed Experiment**	**Batch Historical Data**	**PCA**	**PLS**
Yacoub/MacGregor [24]		X	X	X	X
Kresta [25]			X	X	X
Nomikos [26]			X	X	
Garcia/Kourti/MacGregor [27,28]			X	X	X
Cho/Kim [33]			X	X	
V.Diaz	X	X	X	X	

6.2 Continuous Modeling

The process shown in Figure 6.1 can be considered as a three-dimensional problem in which there are variables (parameters) that have a measurable value (observations) and are changing with respect to time. In the literature Wold et al and Nomikos [26] used multi-way principal component analysis to examine batches throughout time. Batches are basically defined as a group of objects with a common origin. These objects can be raw materials or products manufactured in a certain period of time under the same conditions. The methodology proposed in this thesis as the continuous methodology uses the concept of taking these batches with respect to time and adding three levels of operation to each batch. The levels are the low, medium and high settings for the parameters (variables) that are being monitored in the process. These define the operational ranges in which good product is manufactured.

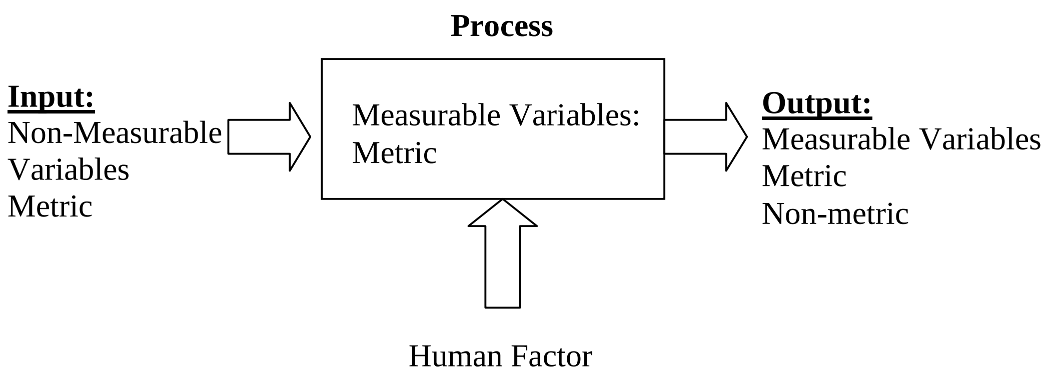


Figure 6.1 Process Flowchart

The Continuous Methodology constitutes of first obtaining the limits for each variable being monitored. The process is set to the low parameter settings. The process starts and observations at this low level setting are obtained. This is repeated for the medium and high parameter settings.

Let

$l_{b,o}$ = Low limit parameter setting

$m_{b,r}$ = Medium limit parameter setting

$h_{b,u}$ = High limit parameter setting

where,

b=1…n is batch number

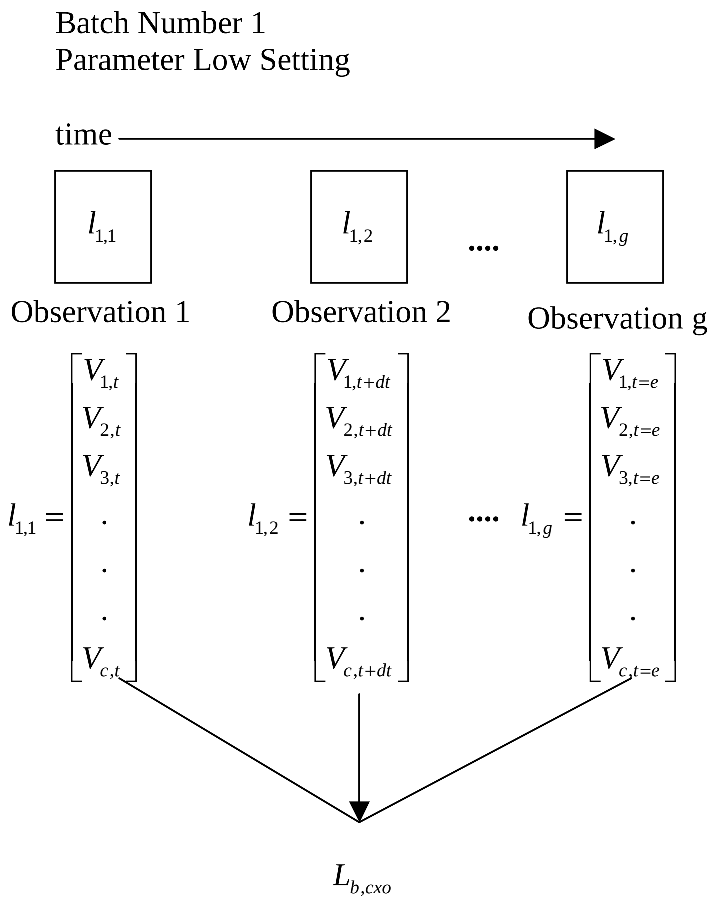
o=1…g is the observation for low parameter

r=1…h is the observation for the medium parameter setting

u=1…q is the observation for the high parameter setting

$l_{b,o}$, $m_{b,r}$ and $h_{b,u}$ are column vectors having all the observations for each variable V_a, where a=1…c is the amount of variables being monitored, at a particular setting at a time t (Figure 6.2 (a) and (b) for $l_{b,o}$). For the example Batch number 1 in Figure 6.2 a each box represents an observation at the low level setting. Each column vector contains the value of each variable for that specific observation at time t. After these observations are obtained they are used to create a matrix, which represents all these observations at the low level (Figure 6.2 b). Time t goes from the time process starts (s) and the time the process ends (e) in Figure 6.2 a and b.

(a)



(b)

$$L_{1,cxo} = \begin{bmatrix} V_{1,t=s} & V_{1,t+dt} & . & . & V_{1,t=e} \\ V_{2,t=s} & V_{2,t+dt} & . & . & V_{2,t=e} \\ V_{3,t=s} & V_{3,t+dt} & . & . & V_{3,t=e} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ V_{c,t=s} & V_{c,t+dt} & . & . & V_{c,t=e} \end{bmatrix}$$

Figure 6.2 Column Vectors and Matrix for low parameter settings

Let $L_{b,cxo}$, $M_{b,cxr}$ and $H_{b,cxu}$, respectively be c x o, c x r and c x u matrices containing all of the observations from a specific batch in a specified time for that setting (Figure 6.2 b for batch 1 low setting). Where b is the batch number, c is the total amount of variables being monitored and o, r and u are the amount of observations obtained to create each matrix $L_{b,cxo}$, $M_{b,cxr}$ and $H_{b,cxu}$. For example, if a matrix is being created for the first batch with the low setting, where there are 15 parameters (variables) being monitored for a time period providing 150 observations then the matrix would be $L_{1,15x150}$.

Let $S_{b,cxz}$ be the data sub-matrix, which contains $L_{b,cxo}$, $M_{b,cxr}$ and $H_{b,cxs}$ such that $z = \sum_{t=s}^{t=e} o + \sum_{t=s}^{t=e} r + \sum_{t=s}^{t=e} u$ (Figure 6.3). For example, if each matrix $L_{b,cxo}$, $M_{b,cxr}$ and $H_{b,cxs}$ for the first batch contained the same 15 parameters and 150 observations each, $S_{b,cxz}$ would be $S_{1,15x450}$. Figure 6.3 shows all the observations from each level used to create $S_{b,cxz}$.

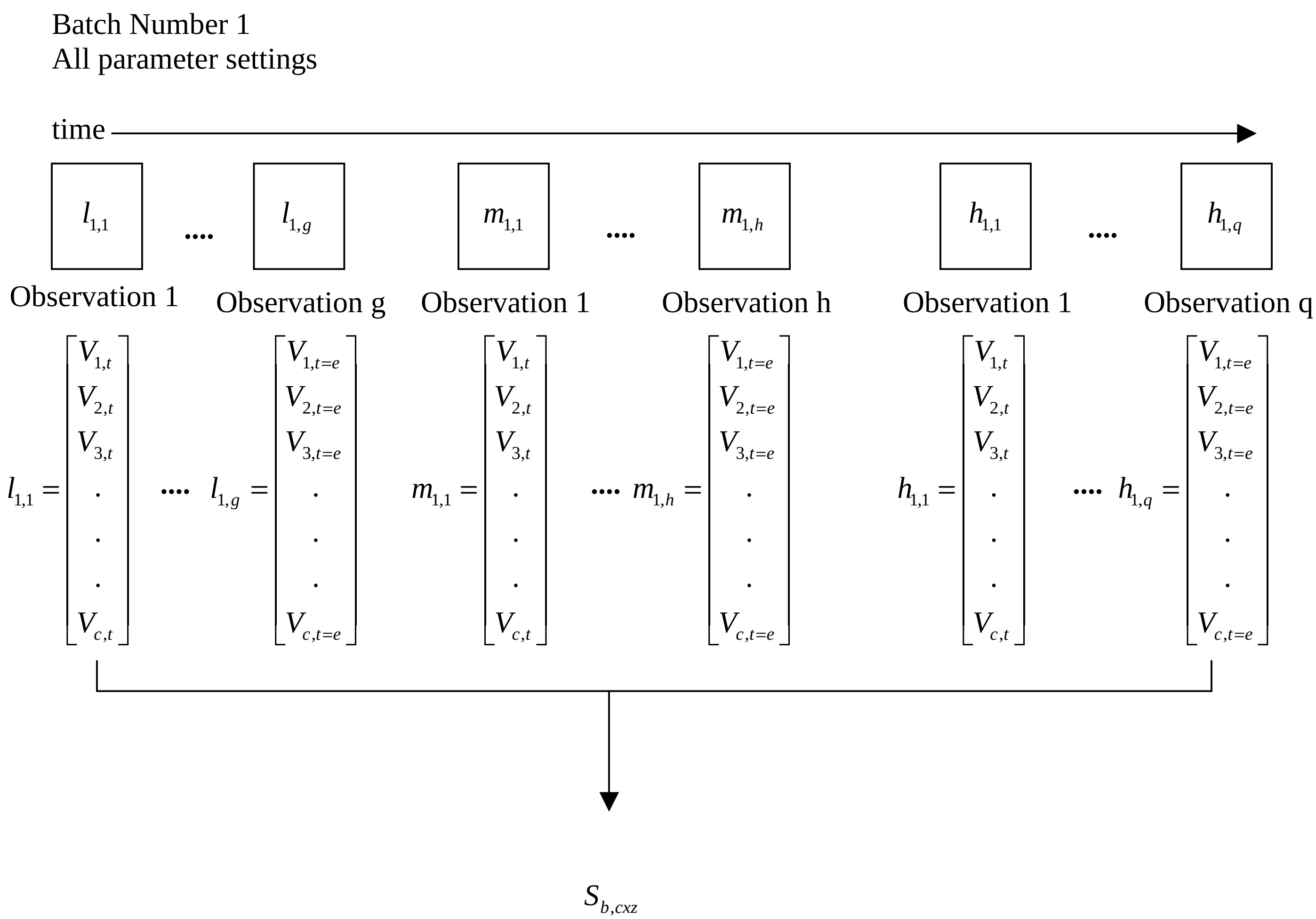


Figure 6.3 Sub-Matrix Creation for Low, Medium and High Parameters

Using sub-matrix $S_{b,cxz}$ (β) for the analysis, the eigen-values λ or roots are calculated to determine the maximum amount of components to be extracted. The model created using $S_{b,cxz}$ must be evaluated before continuing with the methodology being proposed. This is to have a baseline from which to evaluate the methodology as it is being developed. The evaluation criteria are explained in section 6.3 of this chapter. The idea of developing the Continuous Methodology came from the fact that there will always be changes in batch behavior either due to controllable or uncontrollable factors. If the uncontrollable factors are within limits and the controllable factors are acceptable then the Continuous Methodology proposes to proceed with the creation of a new data matrix, which includes the previous sub-matrix and the sub-matrix under the current state conditions. Figure 6.4 demonstrates the concept of the Continuous Methodology. If these conditions are not met than the process must be evaluated to determine the cause for this out of control state, either it being material related, machine related or any other factor that affects the process and may not be monitored. Figure 6.4 shows the observations for each level setting at the left. All the observations for each level are combined to create $L_{b,cxo}$, $M_{b,cxr}$ and $H_{b,cxu}$, respectively. $L_{b,cxo}$, $M_{b,cxr}$ and $H_{b,cxu}$ are used to create $S_{b,cxz}$ for each batch. All sub-matrices representing the process at the different batch conditions are used to create the data matrix or the continuous model. This data matrix is used for the Principal Component Analysis and has all the observations in column format for each variable being monitored. X1 represents the first variable and Xc represents the last variable or total amount of parameters c.

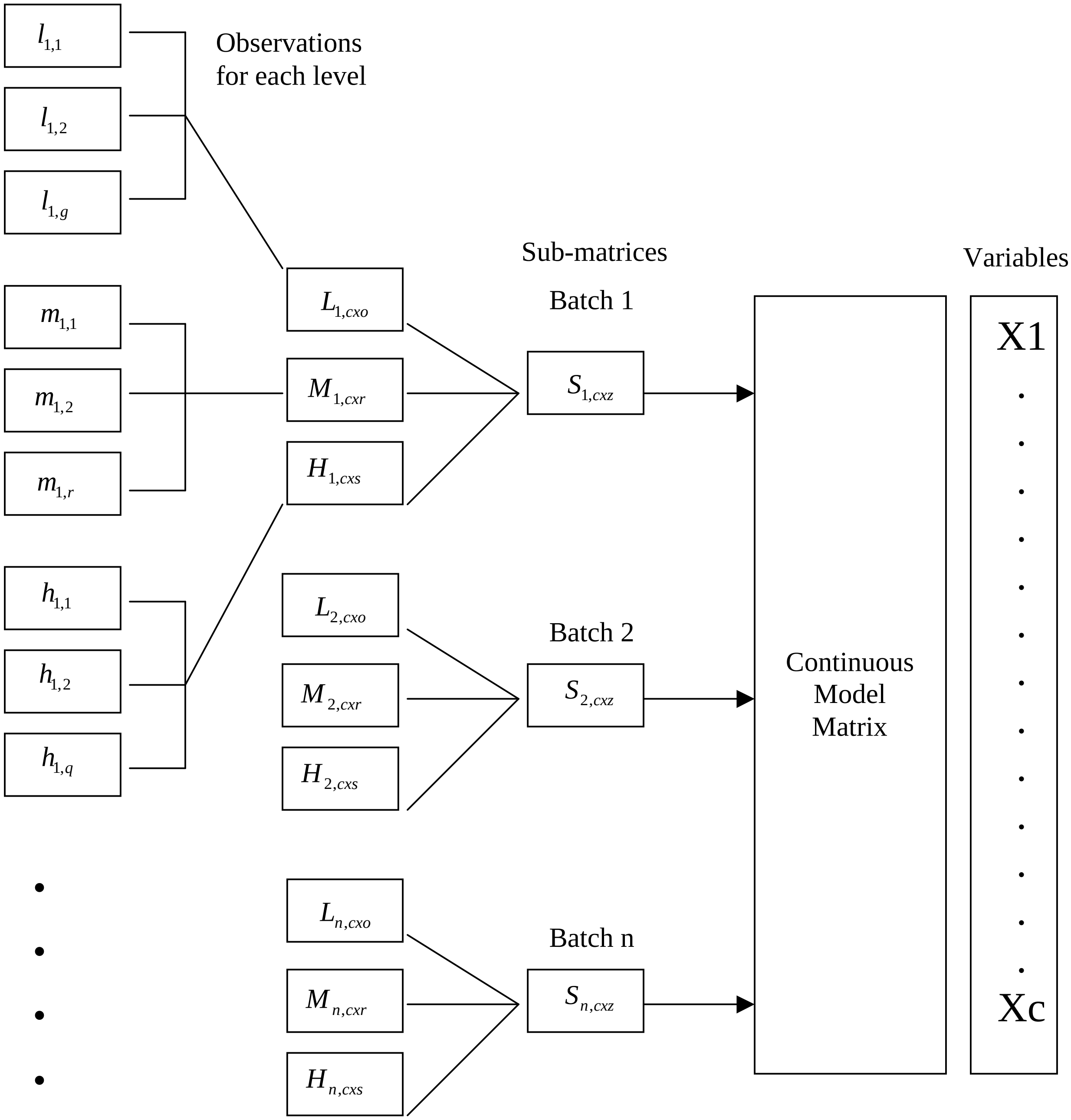


Figure 6.4 Continuous Modeling Methodology

6.3 Combination Methodology

The Combination Methodology which is the second methodology being proposed as part of this research is an extension to the Continuous Methodology in which variables critical to the process or the product are selected and gradually changed until the desired state of process is no longer found. In other words, changes in the variables are made until a defect is found in the product being created. These observations, while still in the acceptable range, are included into the continuous model. These changes may be a one factor at a time change or various factors depending on the adjustments required based on process limitations such as machine speeds or pressure as an example.

6.4 Evaluation Criteria

The following criteria will be used to evaluate the performance of the Continuous and Combination data collection methodology being proposed.

1. **Principal Components extracted**: there exist three methods of determining how many principal components to extract.
    a. The Kaiser Method retains those components with Eigen-values greater than 1.
    b. The Scree test is a graphical form of determining the amounts of components to maintain by selecting the point before the curve begins the line trend (Figure 6.5). For example, in Figure 6.5 the line seems to straighten out as it reaches the sixth component, which is close to having an eigen-value close to 1.

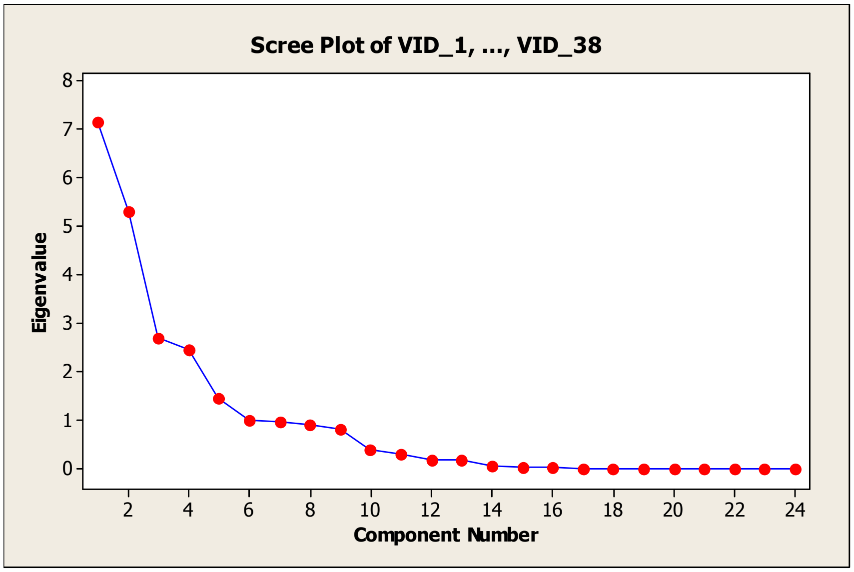


Figure 6.5 The Scree Test for Principal Component Selection

c. The Percent Variation Explained can also be used. In the percent variation method, the components that cumulatively (the variation calculated is summed up for each component) explain a certain percent of the variation, R^2>.5 goodness of fit, are retained.

2. Hotelling's T^2: is the multivariate analog to the uni-variate statistic t^2.

$$T^2 = N(\bar{x} - \mu)' S^{-1} (\bar{x} - \mu) \tag{6.1}$$

delineates a confidence region for the mean vector, μ, in the shape of an ellipsoid (Figure 6-6). Values within and on the ellipsoid are considered to be within the confidence interval:

Confidence 1-α, $N(\bar{x} - m)' S^{-1} (\bar{x} - m) \le T^2_{p,N-1}(\alpha)$

Where N=sample, $\bar{x}$=mean, S=covariance matrix.

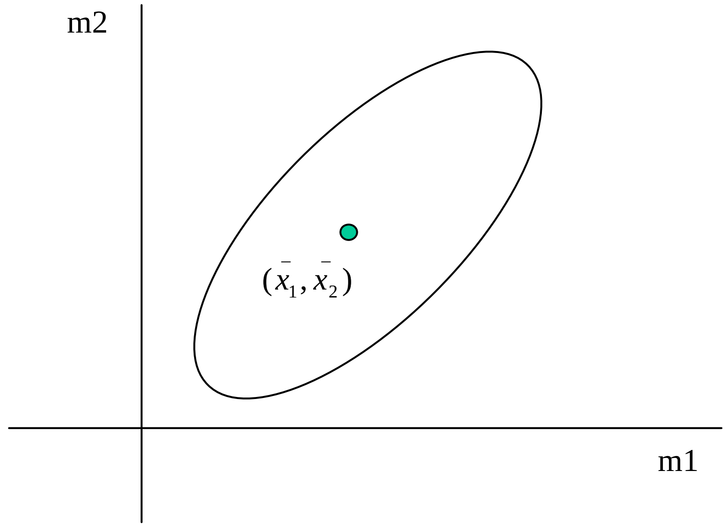


Figure 6.6 Confidence Ellipse P-dimensional space of m

3. Q^2 -Goodness of Prediction: evaluates the predictive ability of the model with increasing number of components.

4. $R^2 - Q^2 \leq .3$

5. Sample Size Guide for Multivariate Analysis found in the literature and reference books:

   Guide 1:

N	ADEQUACY
50	VERY POOR
100	POOR
200	FAIR
300	GOOD
500	VERY GOOD
1000	EXCELLENT

   Guide 2: Using best model fit R^2

6. Hypothesis Testing Type I and Type II error:
    a. α Type I error: when the null hypothesis (Ho) is rejected when in fact it is true and should not be rejected. Calculates the amount of good parts rejected as bad when is actually good.
    b. β Type II error: when the null hypothesis (Ho) is not rejected when in fact it is false and should be rejected. Calculates the amount of bad parts accepted as good when is actually bad.

These criteria are used after the modeling is implemented and product is inspected. Each product, which represents an observation, is evaluated and classified as being a good or bad part according to the part specifications. This is used to evaluate if the model implemented will create excessive scrap or allow bad product out to the customers.

Chapter 7 Experiment Process Description

7.1 Introduction

To validate the continuous and combination methodologies proposed, two distinct manufacturing processes will be used as case studies. This chapter will cover the following topics:

a. Description of the manufacturing process of each case study.

b. List of variables under consideration in each case study.

The injection molding process of a polycarbonate medical part and welding of PVC film by means of radio frequency will be used as case studies to test the data collection methodologies proposed. A signal monitoring system is used for the variables under study and the multivariate data analysis software, SIMCA-P+ 12 from the UMETRICS Company is used for the analysis of the data matrices. Variables used for the analysis in the injection molding process and the RF processes are common variables for each process. Table 7.1 provides a brief description of the differences between each process.

Table 7.1 Differences between Injection Molding and RF Welding Affecting Modeling Strategy

	Injection Molding	**RF Welding**
Variables	22	36
Production	175 cycles/hr	562.5 cycles/hr
Process	Single batch raw material during trials	Multiple batches-raw material
	Humidity or pellet size Difference	Difference between sheeting in same batch
	If faulty equipment is found it is usually replaced immediately	Life of specific equipment decreases with time; adjusted gradually to make up for losses until replaced.

7.2 Injection Molding Process

Injection molding technology is a method of processing used for thermoplastic polymers. It consists of heating thermoplastic material until it melts, then forcing this melted plastic into a steel mold, where it cools and solidifies [35]. A thermoplastic material is that which requires heat to make it formable and after cooling, retains the shape it was formed into. Frequently used thermoplastics are ABS, Polycarbonate, Polyvinylchloride, Polyethylene and Polyester.

In the injection molding cycle, resin pellets are placed within a hopper, (Figure 7.1), which is placed on top of the molding machine barrel. The pellets then enter the barrel through the feed throat and are pushed forward by a rotating screw. The rotation of the screw forces the pellets against the walls of the barrel causing them to melt due to the heat of compression and friction and the barrel walls own heat [36]. The melted material is pushed into the mold and held at a pre-defined pressure for a period of time until the material solidifies and cools.

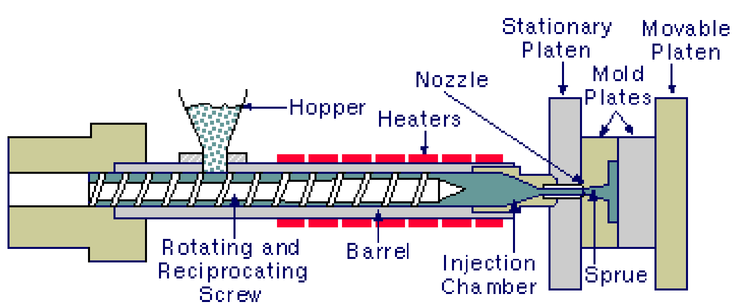


Figure 7.1 Injection Molding Machine Components [37]

A 110 ton electric injection molding machine (Figure 7.2) is used to mold a Polycarbonate plastic part in an eight cavity semi-hot runner mold.

Figure 7.2 Injection Molding Machine [38]

The part is created using Polycarbonate resin material which is melted to a temperature of 580 F and injected into the mold at a speed of approximately 4.50 in/s. The part is a basic component of an assembly that is used to control the flow of fluid through an intravenous set. The medical part can present various defects depending on the conditions that are created in the injection molding process. The most common types of defects (see figure 7.3 a and b) that affect the part are Sinks and Short Shots. A sink mark can be considered as a depression caused in thick regions of a plastic component due to slow cooling. A short shot is basically missing material, so the part is incomplete when ejected from the mold. The short shots are usually detected by visual inspection so as the sink mark, but in a process that produces nearly 32,000 parts per day visual inspection becomes arduous and costly. Apart from this aspect the customer satisfaction is affected severely since they will be receiving a defective product that will affect the production schedules, assembly machines and functionality of the product, if for example the sink mark is present.

(a) Sample Part with short shot

(b) Part with sink mark

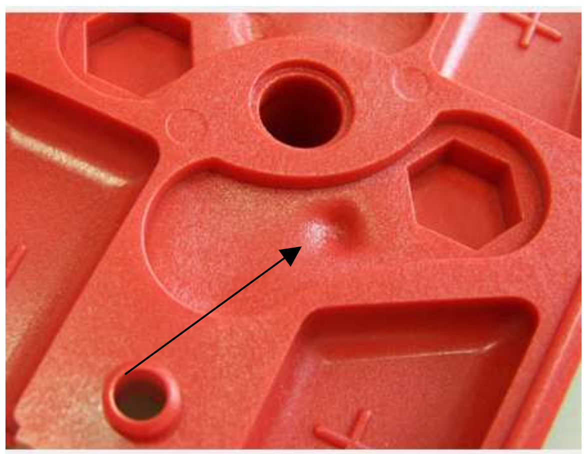


Figure 7.3 Sinks and Short shots [39]

The following list (Table 7.2), gives a description of each variable used for the analysis of the injection molding process.

Table 7.2 Injection Molding Process Variables

Variable Name	**Description**
X1	FILL TIME
X2	PACK TIME
X3	COOLING TIME
X4	CYCLE TIME
X5	SCREW DISPLACEMENT
X6	SCREW VELOCITY
X7	INJECTION PRESSURE
X8	NOZZLE TEMPERATURE
X9	BARRELTEMPERATURE ZONE 1
X10	BARREL TEMPERATURE ZONE 2
X11	BARREL TEMPERATURE ZONE 3
X12	CUSHION
X13	SHOT SIZE

Some of these parameters are established through a methodology called Scientific Molding or Decoupled Molding. Scientific molding or decoupled molding was developed by RJG, Inc as a methodology to achieve process repeatability and minimize shot to shot variation. Previously, molded parts were created by injecting the molten material into the mold as fast as possible, holding the material within the mold and then releasing the part from the mold after it was solidified. The methodology proposed by RJG separated or decoupled (partially decoupled, fully decoupled, totally decoupled) the process into fill, pack and hold.

In partially decoupled process, fill and pack is partially separated and pack is mainly controlled by kinetic energy. Fully decoupled separates fill and pack completely. The pressure is controlled by first controlling it by means of a velocity to a constant value of pressure applied by the screw when a pre-defined position is reached known as the velocity to pressure transfer position. In totally decoupled, fill, pack and hold are completely separated and packing is controlled by means of a pressure sensor placed within a cavity.

The purpose of the Scientific Molding method is to obtain three main parameters: Pack Pressure, Mold Temperature and Cooling Time. The pack pressure is the pressure exerted by the screw on the melt, which helps maintain the plastic already within the mold inside, prohibiting the back flow of material. This pressure is maintained for a specific amount of time required for the sealing of the gate and the solidification of the part within the mold. The mold also has to be maintained at a certain temperature to facilitate the flow of the melt into the mold.

In the stage of filling, the optimum fill time and shot size is determined by creating a machine rheologic curve. The machine rheologic curve is used to determine when the changes in the viscosity of the melt are minimal. The graph of the relative viscosity of the melt versus the shear rate (Figure 7.4) is created by setting the injection-molding machine to various injection velocities. The fill time and hydraulic pressure (hydraulic machines) is obtained from the molding machine. The plastic pressure, an approximate shear rate and relative viscosity are calculated. The following figure is data collected for a Co-Polyester injection molded part produced in a 32-cavity mold.

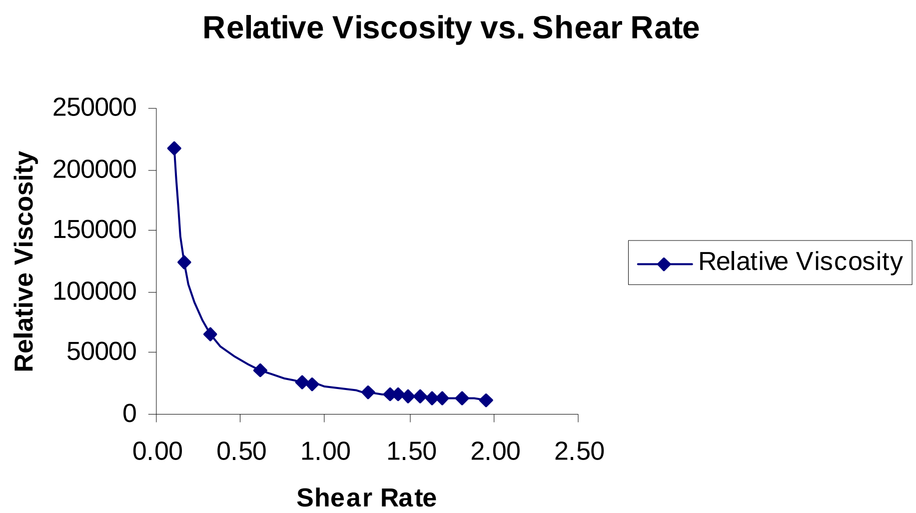


Figure 7.4: Rheologic Curve Relative Viscosity vs. Shear rate

During the packing stage, the hold time and hold pressure is determined. A gate seal test is used to obtain the optimum hold time or minimum time after the injection to seal the gate of the part. Parts are produced where the sum of the cooling time and hold time is maintained constant are carried out. The cooling time and hold time are changed simultaneously and shots are produced and weighed. This procedure is stopped when the shot weight is constant (Figure 7.5).

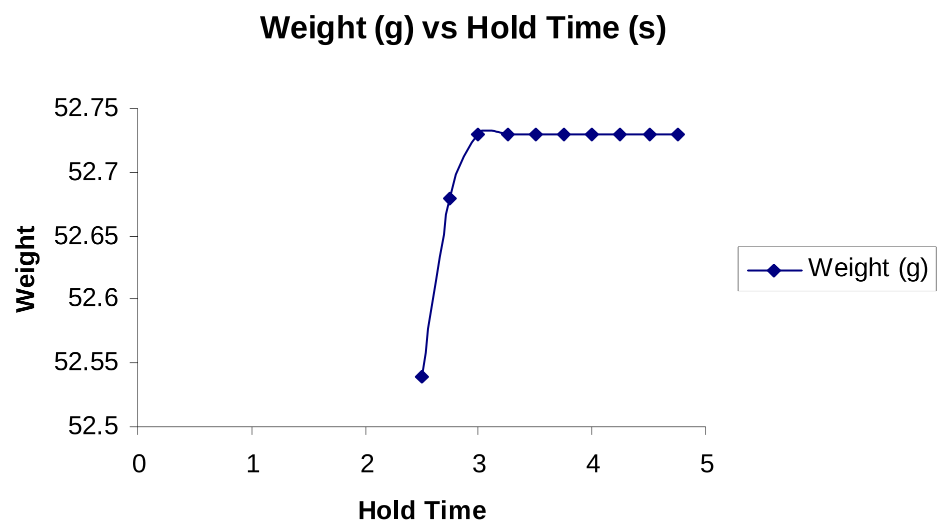


Figure 7.5 Shot size vs. Holding time

Using the fill time, shot size and hold time; various trials at different pack pressures are made. Plastic parts produced are examined for visual defects and dimensional discrepancies. A range for pack pressure is selected. Using this range and the previously determined parameters the mold temperature range is proposed and selected. Again visual and dimensional inspections are made. Finally, the cooling time, time after fill to finish the cooling of the part until it reaches the desired dimensions is also selected.

This procedure is the one normally carried out during the validation of a mold and has been previously established. What is useful from this procedure is that it provides a basis from where to start when creating the Combination Model that will be created for this process. The creation of the Combination Model will be covered in Chapter 8.

7.3 Welding by Radio Frequency Process

Radio frequency welding, also known as dielectric or high frequency welding, is the process of fusing materials together by applying radio frequency energy to the area to be joined. The area to be welded is placed within the electromagnetic alternating field (Figure 7.6), which changes its polarity from positive to negative and vice versa at a set frequency.

An electromagnetic alternating field can be found between two capacitor plates. The molecular movement of materials with a polar molecular structure can be influenced. If a material with a polar molecular structure, such as PVC (Figure 7.7), Polyurethane and PETG, is placed in an electromagnetic alternating field whose polarity changes rapidly, its molecules try to adapt themselves according to the constantly changing field. The thermoplastic can be brought to its melting temperature. If this takes place under a certain joining pressure the molecules mix with one another. Once the dielectric energy is switched off and the joining pressure maintained the materials returns to its solid state. This produces high strengths, which often come close to the inherent strength of the weld material. Since only partial areas have to be joined when welding films, the material only heats up in those areas where the electrodes are applied. In Figure 7.8 a welding tool/die is shown. This tool fuses the material in the area where both sides of the tool make contact. The hole present in the tool provides a space for the seal around cylindrical tubing.

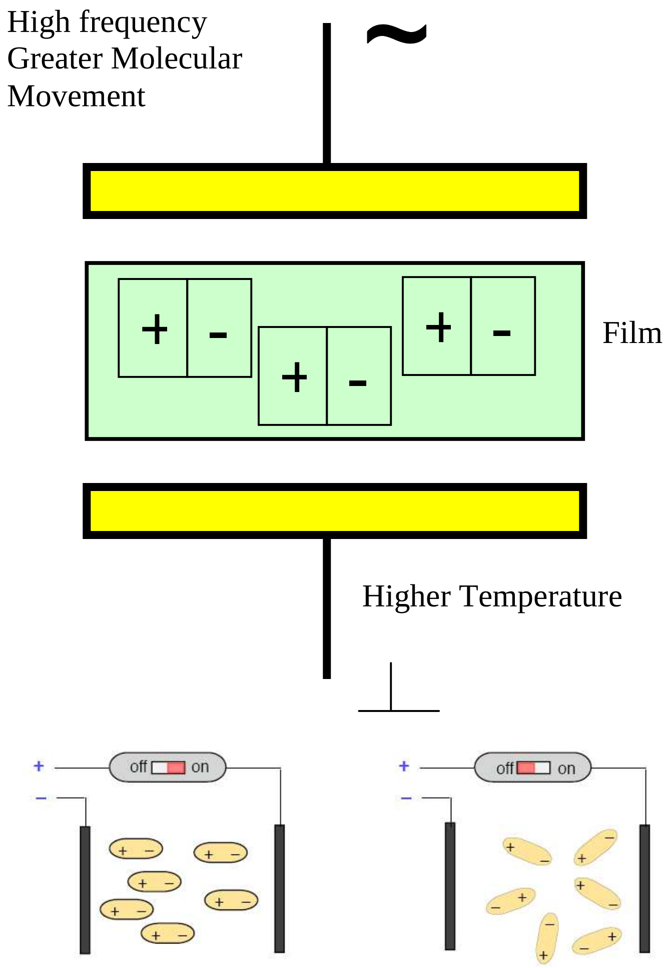


Figure 7.6 Electromagnetic alternating field

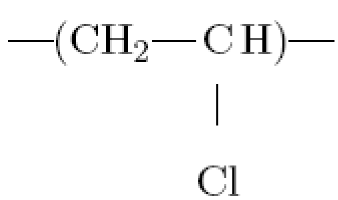


Figure 7.7 PVC Structural Bonding

Figure 7.8 Tool for port seal

A dielectric system (Figure 7.9) has a high frequency generator, which produces electromagnetic energy; a low pass filter, installed between the generator and the welding press allowing the basic, approved industrial frequency of 27.12 MHz to pass. The building out section is a variable capacitor, which allows the re-adjustment of the frequency in the press to accommodate for various joining tasks, tooling sizes and different material thicknesses. The welding press task is to fuse the materials together to create a homogeneous bond [40].

Figure 7.9 RF Welding System [41]

In this experiment a double press welding by radio frequency machine is used to create patterns of 10 fluid bags per cycle index. The first press creates the port seal and the second press creates the main seal (Figure 7.10). The product consists of two films made of PVC, which are fused together by radio frequency. The bag contains two cylindrical tubing which are fused inside and to the film and are formed by the port tool in press 1. Then the machine indexes or moves to the next station where the main seal weld is formed by the main seal tool. The defects that have been encountered during the manufacture of the bags are leaks and missing tubing.

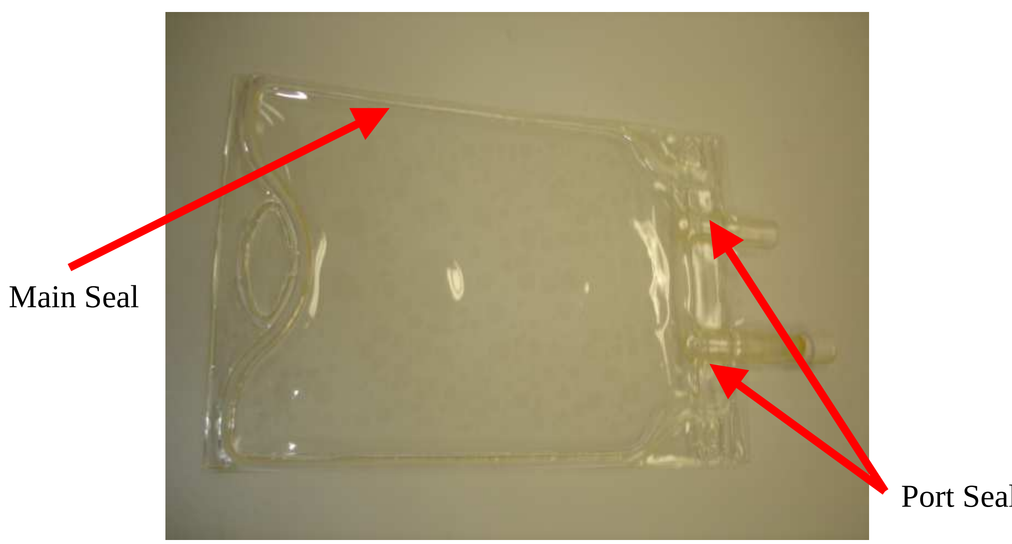


Figure 7.10 Solution bag with welded areas

The following list (Table 7.3), gives a description of each variable commonly used for the welding process.

Table 7.3 Welding by Radio Frequency Process Variables

Variable Name	Description
X1	PORT CYCLE TIME
X2	PORT SEAL TIME
X3	FLAT SEAL TIME
X4	PRE-SEAL TIME PORT
X5	COOL TIME PORT
X6	ANODE PORT
X7	ANODE FLAT
X8	SOLL PORT
X9	SOLL FLAT
X10	POSITION PORT
X11	POSITION FLAT
X12	HF PORT
X13	FLAT
X14	GRID CURRENT PORT
X15	GRID CURRENT FLAT
X16	PRESSURE PORT
X17	PRESSURE FLAT
X18	DIE COOLANT
X19	MAIN CYCLE TIME
X20	MAIN SEAL TIME
X21	PRE-SEAL TIME MAIN
X22	COOL TIME MAIN
X23	ANODE MAIN
X24	SOLL MAIN
X25	POSITION MAIN
X26	HF MAIN
X27	GRID CURRENT MAIN
X28	PRESSURE MAIN

The values for each one of these parameters are based on a one factor at a time change and are carried out in a validation protocol for the following parameters: RF Power Port, RF Power Flat, Welding Pressure Flat, Welding Pressure Port, Tempering Temperature Port/Flat, Seal Time Port, Seal Time Flat, Temperature Main Top Plate, Temperature Main Bottom Plate, Welding Pressure Main, RF Power Main and Seal Time Main. The parameters used for the Combination Model are the RF Power, Seal times and Welding pressure, which have been identified as being critical to the process, since any changes in these may cause leaks.

Chapter 8 Continuous and Combination Methodology In Injection Molding Process

8.1 Introduction

In this section the following will be covered:

1. Creation and evaluation of the preliminary sub-matrix $S_{1,cxz}$ (β) .
2. Creation and evaluation of the continuous model.
3. Creation and evaluation of the combination model.
4. Determination of: Eigen-values, principal components extracted, R^2, Q^2, T^2, Type I and II error for each model created.

8.2 Analysis and Results for the Continuous Modeling Methodology

The sub-matrix, $S_{1,cxz}$, for batch number 1 is created by obtaining data at the low, medium and high parameters for this batch. Twenty-one variables are being monitored for this process, therefore c=21. The total amount of observations for batch 1, which contains the low, medium and high parameter runs, is z=456 (sample size). The sub-matrix model is $S_{1,21x456}$. The multivariate data analysis software SIMCA-P+ is used to analyze the data matrix $S_{1,21x456}$ and obtain the data found in table 8.1. The requirements that must be satisfied are: eigen-values λ>1, R^2>.5, R^2-$Q^2 \leq$ .3. The table presents the minimum value of the eigen-value for the amount of principal components being extracted. In this evaluation, the Kaiser criterion of accepting eigen-values greater than one for the selection of principal components is utilized.

Table 8.1 Multivariate Data Analysis of Sub-matrix $S_{1,21x456}$ Using SIMCA-P+12 for Injection Molding Process

Sub-matrix Model $S_{1,21x456}$								
Minimum Eigenvalues	5.62	4.180	2.140	1.790	1.280	1.040	1	0.95
Principal Components	1	2	3	4	5	6	7	8
R2	0.268	0.467	0.569	0.654	0.715	0.765	0.812	0.858
Q2	0.116	0.308	0.369	0.392	0.426	0.368	0.305	0.236
R2-Q2	0.152	0.159	0.200	0.262	0.289	0.397	0.507	0.622
T2	3.870	6.057	7.925	9.651	11.293	12.881	14.431	15.952

The following results were obtained when implemented in the monitoring system. Parts that were created and accepted or rejected were evaluated for defects such as short shots, sink marks, burns and flash according to the part specification and acceptance guidelines. This model provided a high rate of false rejects (α -Alpha=1) and no false accepts (β -Beta=0). It was considered at this time that the model created using sub-matrix $S_{1,21x456}$ required some improvement since the false rejects were high, equivalent to 9% of what was produced (Table 8.2).

Table 8.2 Performance Criteria for $S_{1,21x456}$

Performance Criteria	
Machine Cycles	924
Machine Cycles Rejected	85
Total Parts Produced	7392
Parts Accepted	6712
Parts Rejected	680
Scrap %	9%
Alpha	1
Beta	0

A second sub-matrix model, $S_{2,21x1216}$, was created to include observations from another batch. Table 8.3 shows the results of the analysis for this new matrix.

Table 8.3 Multivariate Data Analysis of Sub-matrix $S_{2,21x1216}$ Using SIMCA-P+12 for Injection Molding Process

Sub-matrix Model $S_{2,21x1216}$							
Minimum Eigenvalues	7.06	4.070	2.790	2.250	1.380	1.020	0.734
Principal Components	1	2	3	4	5	6	7
R2	0.336	0.530	0.662	0.770	0.835	0.884	0.919
Q2	0.263	0.392	0.435	0.566	0.583	0.665	0.668
R2-Q2	0.073	0.138	0.227	0.204	0.252	0.219	0.251
T2	3.852	6.010	7.856	9.548	11.153	12.699	14.201

The model created with sub-matrix $S_{2,21x1216}$ was implemented in the monitoring system and was found to achieve a decrease in the scrap rate as well as the probability of making a Type I error (α) by decreasing from 1 to .59 (Table 8.4).

Table 8.4 Performance Criteria for $S_{2,21x1216}$

Performance Criteria	
Machine Cycles	64,890
Machine Cycles Rejected	659
Total Parts Produced	519,120
Parts Accepted	513,848
Parts Rejected	5,272
Scrap %	1%
Alpha	.59
Beta	0

8.3 Analysis and Results for the Combination Modeling Methodology

To use the combination methodology in injection molding a one factor at a time change is used for those parameters that are considered as critical to the defects, such as short shot and sink marks. In this section the machine rheologic curve (Table 8.5) and the gate seal test are used to establish the limits of the injection speed and the pack time. The following procedure was conducted:

1. Using the gate seal test the minimum hold time is obtained. The maximum time can be anything above the minimum, but this will increase the cycle time.

2. The minimum and maximum injection speed is obtained from the machine rheologic curve.

Table 8.5 Values used for the creation of the Rheologic Curve

Trial	Injection Velocity (in/s)	Fill Time (s)	Hydraulic Pressure (psi)
1	5.50	0.60	22170
2	5.00	0.65	21046
3	4.75	0.68	20350
4	4.50	0.72	19655
5	4.00	0.80	18209
6	3.25	1.03	17615
7	2.75	1.21	16681
8	2.50	1.35	16205
9	2.00	1.65	15248
10	1.50	2.19	13987
11	1.25	2.62	13458
12	1.00	3.27	12922
13	0.75	4.34	12488
14	0.50	6.51	13244
15	0.25	13.26	16883

For example, if the injection speed selected during the decoupled molding phase is 1.25 (Table 8.5) then the minimum injection speed used is 1.00 and the maximum is 1.50. It is convenient to use the same tools that are used during decoupled molding for the selection of the minimum and maximum values since this information is always provided when the decoupled methodology is used. This would standardize the procedure for all other molds being evaluated. Ten trial runs were carried out using a one factor at a time change. Ten trial runs were required because there were 5 parameters with low and high setting to be determined. These trials are included in the model created using continuous modeling to form the combination model. The position of the screw for shot size was increased until a permissible amount of flash was found and decreased until a short shot was achieved. The temperatures of the barrel were kept within manufacturers recommended range and depending on the material and mold can vary between 20-50 degrees above and below the nominal temperature used during the initial validation. The trials for the temperatures were changed for all zones at the same time. The extruder rpm was increased and decreased taking into consideration the residence time of the material in the barrel and the machine capacity. Table 8.6 provides a list of all the parameters that were changed for the creation of the new model using the combination methodology.

Table 8.6 Parameters used for the Creation of The Combination Model

PARAMETERS
PACK TIME
INJECTION VELOCITY
SHOT SIZE
RPM
NOZZLE TEMP
ZONE 1 TEMP
ZONE 2 TEMP
ZONE 3 TEMP

The combination matrix consists of 1246 observations, which include those from the continuous model. Table 8.7 presents the results of the multivariate analysis and Table 8.8 presents the results of the effectiveness of the model implemented. The scrap rate is reduced to less than 1% and the type I error has been decreased to .027. This means that there were more defective parts correctly rejected.

Table 8.7 Multivariate Data Analysis of Combination Matrix Using SIMCA-P+12 for Injection Molding Process

Combination Model							
Minimum Eigenvalues	6.33	4.78	3.37	2.22	1.98	1.14	0.651
Principal Components	1	2	3	4	5	6	7
R2	0.288	0.505	0.658	0.759	0.849	0.901	0.93
Q2	0.217	0.402	0.48	0.46	0.585	0.574	0.642
R2-Q2	0.071	0.103	0.178	0.299	0.264	0.327	0.288
T2	3.852	6.015	7.855	9.547	11.151	12.696	14.198

Table 8.8 Performance Criteria For the Combination Model for Injection Molding

Performance Criteria	
Machine Cycles	67,569
Machine Cycles Rejected	597
Total Parts Produced	540,552
Parts Accepted	535,776
Parts Rejected	4,776
Scrap %	0.88%
Alpha	.027
Beta	0

The Continuous and Combination Methodology implemented in the injection molding case study provided excellent results as was seen in the reduction of type I error from 1 to .27 and a reduction of the scrap rate from 9% to .88%.

Chapter 9 Continuous and Combination Methodology In Welding by RF Process

9.1 Introduction

In this section the following will be covered:

1. Creation and evaluation of the continuous model for the main seal and port/flat seal.
2. Creation and evaluation of the combination model for the main seal and port/flat seal.
3. Determination of: Eigen-values, principal components extracted, R^2, Q^2, T^2, Type I and II error for each methodology.

9.2 Analysis and Results for the Continuous Modeling Methodology

One of the differences between the injection molding process and the welding by Radio Frequency is that in the injection molding process parts are made in the mold in one step, while in the RF process the welding is done in two different steps, first the port and flat seal is made and then the main seal. Therefore, one continuous model has to be created for each type of seal. The solution bags evaluated at the end of the process are destructively tested and checked for leaks by filling each solution bag with pressurized air to separate the films. These solution bags are placed in an oven and heated to 118 degrees Fahrenheit for a period of 15 minutes. Afterwards each solution bag is submersed into a water bath and is visually inspected for leaks. This procedure has been previously established in the product specifications for testing of the solution bags.

The model created using the $S_{2,25x2653}$ and $S_{2,14x2649}$ sub-matrix is implemented in the monitoring system that is available for the experiment in the machine, which produces the solution bags. Tables 9.1, 9.2, 9.3 and 9.4 present the multivariate analysis results for the variables for press 1 and press 2. Due to limited time and resources for the experiment the data collected for both batches were tested under sub-matrix $S_{2,25x2653}$ for press 1 and $S_{2,14x2649}$ for press 2.

Table 9.1 Multivariate Data Analysis of Sub-matrix $S_{1,25x144}$ Using SIMCA-P+12 for RF Welding Press 1

Sub-matrix Model $S_{1,25x144}$					
Minimum Eigenvalues	15.4	3.51	1.43	1.17	0.853
Principal Components	1	2	3	4	5
R2	0.615	0.755	0.812	0.859	0.893
Q2	0.598	0.721	0.693	0.663	0.629
R2-Q2	0.017	0.034	0.119	0.196	0.264
T2	3.924	6.205	8.176	10.023	11.806

Table 9.2 Multivariate Data Analysis of Sub-matrix $S_{2,25x2653}$ Using SIMCA-P+12 for RF Welding Press 1

Sub-matrix Model $S_{2,25x2653}$						
Minimum Eigenvalues	6.88	5.18	1.17	1.07	1	0.794
Principal Components	1	2	3	4	5	6
R2	0.362	0.635	0.696	0.753	0.805	0.847
Q2	0.311	0.578	0.553	0.508	0.488	0.451
R2-Q2	0.051	0.057	0.143	0.245	0.317	0.396
T2	3.846	6.003	7.834	9.515	11.108	12.641

Table 9.3 Multivariate Data Analysis of Sub-matrix $S_{1,14x135}$ Using SIMCA-P+12 for RF Welding Press 2

Sub-matrix Model $S_{1,14x135}$			
Minimum Eigenvalues	10.1	1.4	0.994
Principal Components	1	2	3
R2	0.723	0.823	0.894
Q2	0.698	0.743	0.717
R2-Q2	0.025	0.08	0.177
T2	3.94	6.22	8.201

Table 9.4 Multivariate Data Analysis of Sub-matrix $S_{1,14x2649}$ Using SIMCA-P+12 for RF Welding Press 2

Sub-matrix Model $S_{2,14x2649}$					
Minimum Eigenvalues	3.41	2.4	1.15	1	0.971
Principal Components	1	2	3	4	5
R2	0.31	0.528	0.633	0.724	0.812
Q2	0.114	0.275	0.221	0.143	0.057
R2-Q2	0.196	0.253	0.412	0.581	0.755
T2	3.845	6.001	7.832	9.514	11.107

The following results were obtained for press 1 and 2 using the continuous methodology: A total of 744 units were produced, where 8 of these units were accepted and 736 units were rejected. Of the 736 units rejected, 12 units were actually bad and 724 were actually good. All the units accepted were actually good. In other words with this model a type I error of .98 and type II of 0 is achieved with a scrap rate of 98%.

9.3 Analysis and Results for the Combination Methodology

The parameters used for the Combination Model are the RF Power, Seal times and Welding pressure, which have been identified as being critical to the process during past process validations, since any changes in these may cause leaks. Tables 9.5 and 9.6 provide the multivariate analysis for the data matrices used for this methodology. The press 1 model had a total of 3133 observations and press 2 had 3129 observations.

Table 9.5 Multivariate Data Analysis of Combination Matrix Using SIMCA-P+12 for RF Welding Press 1

Combination Model					
Minimum Eigenvalues	8.94	2.81	1.14	1.05	0.902
Principal Components	1	2	3	4	5
R2	0.497	0.653	0.716	0.774	0.824
Q2	0.472	0.573	0.542	0.498	0.447
R2-Q2	0.025	0.08	0.174	0.276	0.377
T2	3.846	6.001	7.831	9.512	11.103

Table 9.6 Multivariate Data Analysis of Combination Matrix Using SIMCA-P+12 for RF Welding Press 2

Combination Model					
Minimum Eigenvalues	4.05	1.92	1.26	1.04	0.992
Principal Components	1	2	3	4	5
R2	0.368	0.542	0.657	0.752	0.842
Q2	0.229	0.295	0.39	0.329	0.261
R2-Q2	0.139	0.247	0.267	0.423	0.581
T2	3.845	6	7.83	9.51	11.101

The combination models implemented for press 1 and 2 provided the following results: A total of 2564 units were produced where 601 units were rejected. Out of the 601 units, 11units were actually bad and 590 were actually good. 1963 units were accepted and out of these 1945 were actually good and 18 were actually bad. This methodology provided for a type I error of .98 and a type II error of .009, with a scrap rate of 23%.

The Continuous and Combination Methodology implemented in the RF welding case study provided moderate results as the scrap was reduced from 98% to 23%, but the type II error went from 0 to .009 and type I stayed at .98.

Chapter 10 Findings, Conclusions and Recommendations

10.1 Overview

In this research two methodologies were proposed for the creation of the data matrices used in multivariate data analysis using principal components. The Continuous Modeling Methodology proposed the use of process data at three levels to create sub-matrices and the Combination Methodology utilized gradual changes to critical variables to the process or product defect. Two processes were evaluated in this research to validate the methodologies proposed, the injection molding process and welding by radio frequency.

10.2 Conclusions for the Injection Molding Experiment

Table 10.1 summarizes the results obtained for the injection molding process using the two methodologies. It was demonstrated that the addition of the sub-matrix, $S_{2,21x1216}$, to the preliminary data matrix , $S_{1,21x456}$, contributed to the improvement of type I error and the reduction of scrap. By including the critical factors to the models the combination model was created and proved to have a significant improvement by reducing the Type I error to .027. These results are valid for the time period of the six months in which the modeling was implemented.

Table 10.1 Comparison Between Continuous and Combination Methodologies Results for Injection Molding

Comparison Between Continuous and Combination Modeling			
Criteria	Preliminary Model	Continuous Model	Combination Model
Sample Size	456	1216	1246
Number of Components	3	4	5
R2	0.569	0.77	0.849
Q2	0.369	0.566	0.585
R2-Q2	0.2	0.204	0.264
Type I Error	1	0.59	0.027
Type II Error	0	0	0
Scrap Rate	9%	1%	0.88%

The following observations are made based on situations that happened during the experiments. The Combination Methodology has been helpful with these observations since this methodology included the critical variables shot size, barrel and nozzle temperatures and injection speed, which have been related to various problems found in the process.

1. Screw displacement and cushion are parameters that have been significant in the detection of problems with drooling (leak of resin during the injection). If there exists drooling there is an insufficient amount of material used to maintain pressure on the melt already injected in the mold. The screw displacement is affected because the screw moves forward more than the established amount. Sink marks and short shots were found in production rejected when these parameters changed.

2. Changes in barrel temperatures of more than 50 degrees have been associated with faulty thermocouples when comparing the values obtained by an external monitoring system and that of the injection-molding machine.

3. Increasing moisture content in polyester resin was seen as a drop in injection pressure and can help in the detection of cracks in parts. This defect is critical since a micro crack can be present in the part and not detectable by visual inspection. Cracks can lead to leaks and failure of the device during use.

10.3 Conclusions for the RF Welding Experiment

Table 10.2 summarizes the results obtained for the welding by radio frequency process. Like in the injection molding experiment, a decrease in the scrap rate was seen when the combination methodology was implemented. The type I error was maintained at .98. It is concluded that this may be due to the fact that not enough observations were obtained for the modeling, for this transition to be seen. A slight increase in the type II error indicated that faulty product was being accepted as good. This may be due to the data collected for the modeling. If borderline data is used as part of the sub-matrix or during the creation of the combination model, then the implemented model may accept product that could fail.

Table 10.2 Comparison Between Continuous and Combination Methodologies Results for RF Welding Process

Comparison Between Continuous and Combination Modeling				
	Continuous Model		Combination Model	
Criteria	Press 1	Press 2	Press 1	Press 2
Sample Size	2653	2649	3133	3129
Number of Components	2	2	2	3
R2	0.635	0.528	0.653	0.657
Q2	0.578	0.275	0.573	0.39
R2-Q2	0.057	0.253	0.08	0.267
Type I Error	0.98		0.98	
Type II Error	0		0.009	
Scrap Rate	98%		23%	

The following observations were also made during the experiment for the RF welding process:

1. If a tube was removed before the seal was made an arc was created. The pattern was rejected. The signal that was affected was the maximum position of the port press (Figure 10.1), and the maximum grid current (Figure 10.2). Both signals decreased to zero.

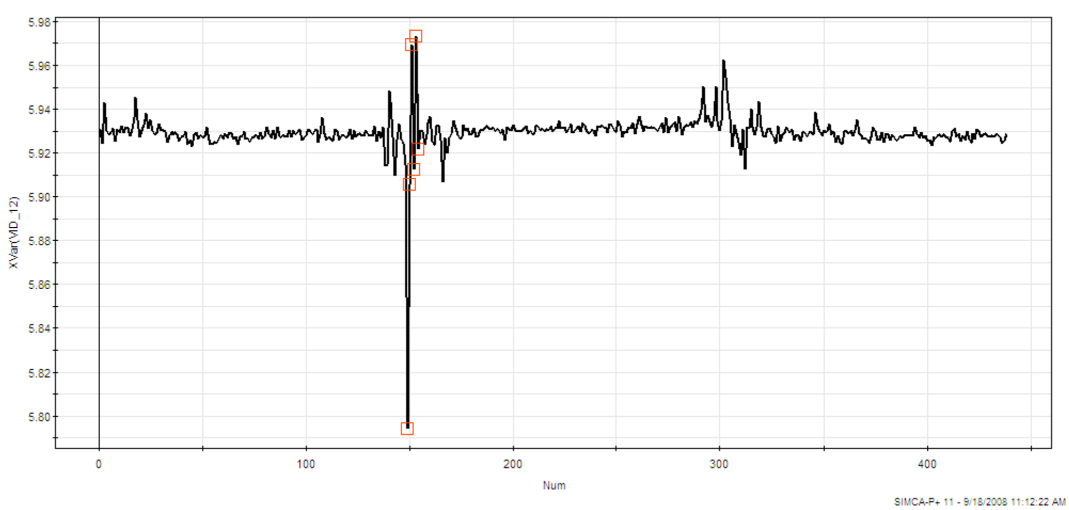


Figure 10.1 Maximum Position of the Port with Respect to the Observations

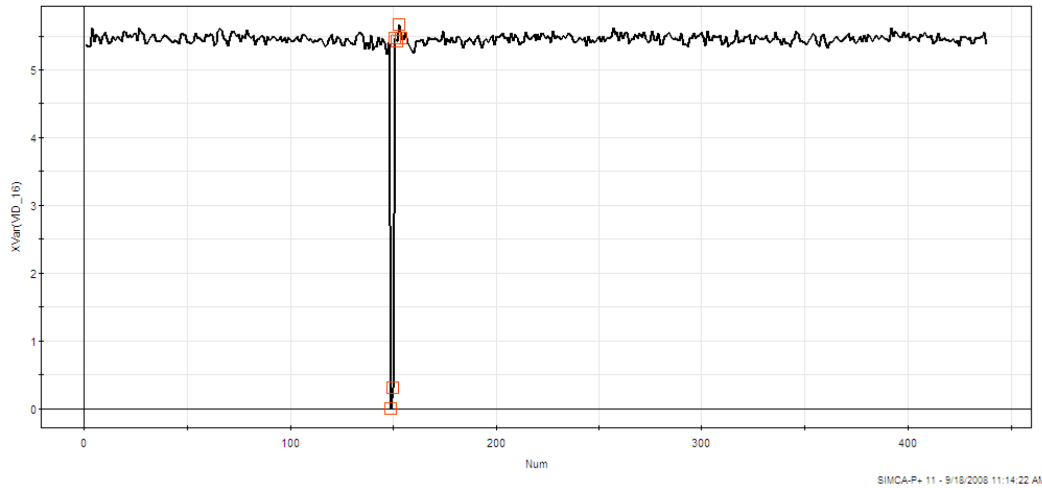


Figure 10.2 Maximum Grid Current with Respect to the Observations

2. If a tube was removed before the seal was made an arc was not created. The pattern was rejected. The signal affected was the pressure (Figure 10.3).

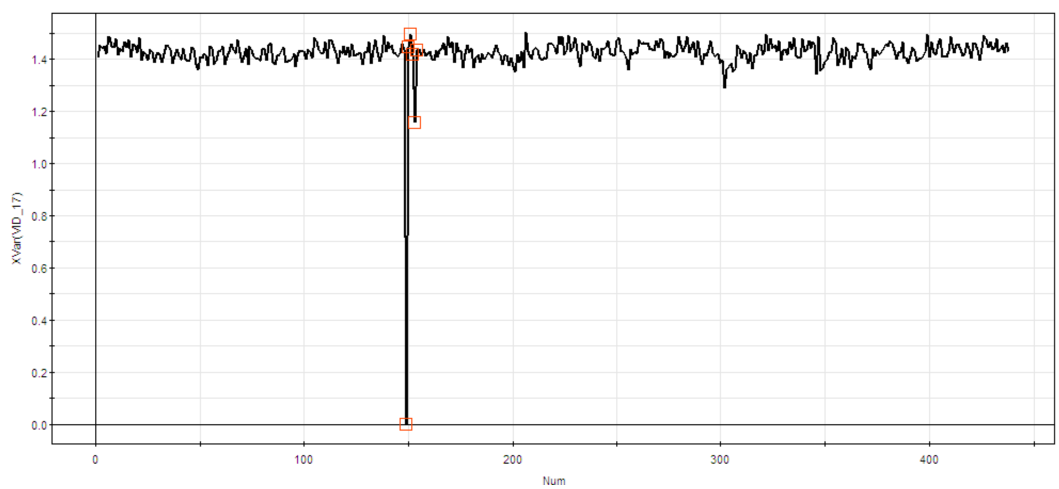


Figure 10.3 Pressure with Respect to the Observations

These findings are important because this indicates that a defect of missing tube can be detected. Usually this defect may escape the visual inspections and reach the customer if there is only one tube missing from twenty and there are about 5625 solution bags being produced per hour. For this experiment it would be recommended to include more sub-matrices into the models and an exhaustive evaluation of the signals, which may be on the borderline compared to the other observations. The difficulty in this process, which is not found in the injection molding as much, is the ability to trace a solution bag back to the variable observations if a system where the patterns are immediately identified and associated with a specific set of observations is not in place.

This research proposed the Continuous and Combination Methodology where the goal was to provide a methodology, which could accommodate itself to the changing conditions of the process. Using the Continuous Methodology, in the injection molding case study, the goal of obtaining the most information from the process as changes arose was achieved with acceptable results. After using the Combination Methodology many problems that occurred, such as problems with faulty equipment or product defects could be detected. So an additional benefit was found that was not considered initially. In the RF Welding case study the results were not as marked as in the injection molding. Even though the scrap rate was decreased an increase in type II error was measured. This is not attributed to the methodology; instead it is the use of observations that were borderline and included in the data matrix used for the modeling. Identifying these borderline observations and removing them from the data matrix can correct this matter. Additional data could be added in the future to make the model more robust. A benefit of the Combination Modeling used in the RF Welding was the detection of missing tubing, which greatly benefits in the inspection of solution bags.

Future applications of these multivariate techniques and methodologies can be used in the detection of epileptic seizures, characterization of materials and failure detection through image analysis.

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