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An Integrated Probability-Based Approach for Multiple Response Surface Optimization

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AN INTEGRATED PROBABILITY-BASED APPROACH FOR MULTIPLE RESPONSE SURFACE OPTIMIZATION

by

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ABSTRACT

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Nearly all real life systems have multiple quality characteristics where individual modeling and optimization approaches can not provide a balanced compromising solution. Since performance, cost, schedule, and consistency remain the basics of any design process, design configurations are expected to meet several conflicting requirements at the same time. Correlation between responses and model parameter uncertainty demands extra scrutiny and prevents practitioners from studying responses in isolation. Like any other multi-objective problem, multi-response optimization problem requires trade-offs and compromises, which in turn makes the available algorithms difficult to generalize for all design problems. Although multiple modeling and optimization approaches have been highly utilized in different industries, and several software applications are available, there is no perfect solution to date and this is likely to remain so in the future. Therefore, problem specific structure, diversity, and the complexity of the available approaches require careful consideration by the quality engineers in their applications.

The purpose of this dissertation is to suggest strategies in order to improve the quality of processes and products with multiple quality characteristics. An integrated

probability-based approach will be applied in the modeling and optimization of the problem, which will utilize strengths of probability-based and desirability approaches. A conformance probability metric is the most commonly used optimization criterion for probability-based approaches and it will be shown that particularly when conformance probability is high it can prematurely stop the search process and give biased solutions in mean response values. Another concern is when the number of responses increases a feasible solution set may not exist due to the response constraints. Therefore, penalization of infeasible solutions can help to identify near feasible solutions and also help decision makers articulate their preference information efficiently in order to find compromising solutions.

The proposed approach is coded in MATLAB by the help of readily available tools in the MATLAB Toolbox. Several cases from published literature are implemented and simulations are conducted to show the quality of proposed and existing methodologies. The results showed that, operating conditions obtained by the proposed approach are always superior in terms of mean targets, and almost equally good in terms of conformance probability.

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TABLE OF CONTENTS

LIST OF TABLES

Table

LIST OF FIGURES

Figure

1 INTRODUCTION

1.1 BACKGROUND

Response Surface Methodology (RSM) is a collection of statistical and mathematical techniques useful for empirically developing, improving, and optimizing processes. It also has important applications in the design, development, and formulation of new products, as well as in the improvement of existing product designs (Myers and Montgomery, 2002). RSM, first developed by Box and Wilson in 1951 has been successfully utilized in many industries for the design and improvement of systems where efficient design characteristics are sought.

RSM can be generalized in three sequential steps:

1. Designing an optimal experimentation plan that encompasses adequate and reliable information for the modeling and optimization of responses;
2. Determining a mathematical model that best fits the data collected from the design chosen; and,
3. Determining the optimal settings of input factors that produce the best settings of response.

Much of the RSM studies, particularly in recent years focus on multiple responses where several characteristics of a system are of interest. Nearly all systems have multiple quality characteristics and one direction of improvement for a response might give poorer performances for the others (as shown in Figure 1.1). Simultaneous optimization of

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multiple quality characteristics of a system emanates from the need to consider different, conflicting, and often correlated responses which use the same resources in a system.

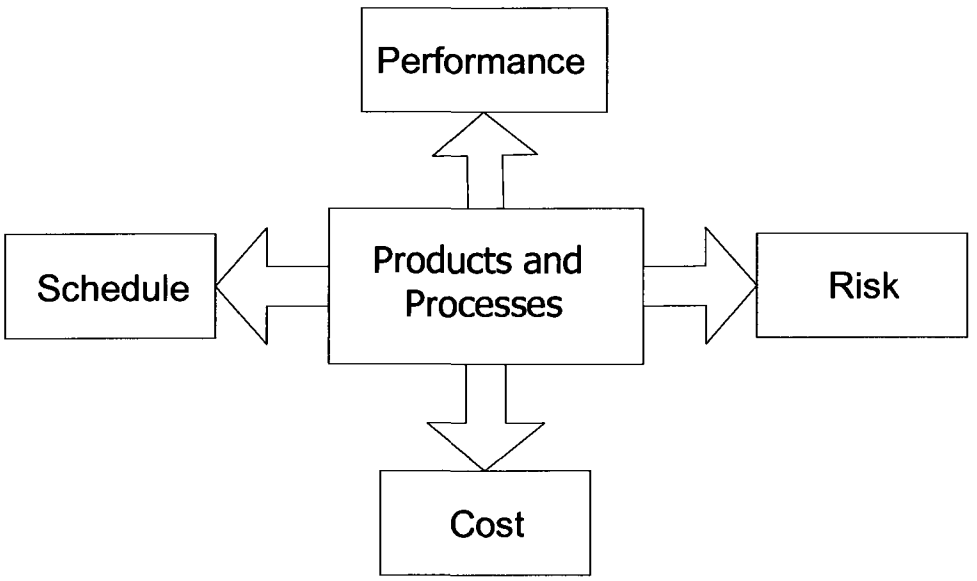


Figure 1.1 Multiple and Conflicting Quality Characteristics of a Product or a Process

However, it is not easy to maintain a balance among responses when they have different measurement units, correlations, and when the types of responses are of different variety. Therefore, solution procedures which will efficiently lead decision makers (DM) to compromising solutions are of great importance.

1.2 PROBLEM DEFINITION AND DISSERTATION OUTLINE

Although considerable attention is given to the multiresponse surface optimization field, complexity of both the problem and proposed solutions leave room for further research in order to help practitioners test the validity and confidence of applied procedures. Moreover, there are several statistical properties that should be considered when establishing sound procedures in both modeling and the optimization of procedures. These properties help in the classification of available approaches and with diversifying

the production of new approaches for problems. These statistical properties can be summarized as follows:

- Correlation structure among responses
- Robustness of responses
    - Robustness to uncontrollable (noise) factors
- Quality of response models
    - Quality of description (R^2)
    - Quality of prediction ($R^2_{\text{Prediction}}$)

Moreover, typically of any multi-criteria optimization problem, decision makers preferences need to be considered as well as and how preference information is articulated during the optimization process. In a multiple response problem when the number of factors or responses grows moderately high and the responses are strictly constrained, relative weighting of responses can be cumbersome and, in most cases, a common set of input variables satisfying all the responses may not be possible. Hence, a procedure that defines efficient DM involvement to find compromising solutions with the least number of iterations should be a required characteristic of any multiple response surface optimization technique.

Since Harrington (1965), the *desirability approach* has been highly utilized by several researches due to its flexibility in the DM articulation process and its applicability to different response types. However when the desirability approach is used in the optimization, correlation among responses, which is the primary characteristic of multiple responses, can not be incorporated and there is little or no study in this regard. Another important and new emerging paradigm is the *probability-based approaches* which are

able to account satisfactorily for statistical considerations. However there is still a need for exploiting its applicability in the optimization of multiple responses and several improvements are possible when these methods are used in unison.

The main focus of this research will be on the second (mathematical modeling) and third step (optimization) of response surface methodology when multiple responses are considered. In Chapter 2, the basics of regression formulations used in the calculation of response surface model parameters for single and multiple response cases will be given. In Chapter 3, a brief summary of existing work on multiple response surface methodology (MRSM) will be given regarding statistical properties and DM involvement issues. Then the research effort will be mapped as to how an integrated approach can help to overcome limitations in previous studies, along with what would be the possible contributions to the body of knowledge with the intended study. In Chapter 4, the proposed approach will be formulated and its applicability will be shown with an example. In Chapter 5, in order to test the performance of the proposed approach, several examples from published literature will be studied regarding response types, optimization method, and number and type of responses used in the study.

The conclusion and directions for future research are discussed in Chapter 6.

2 RESPONSE MODELING AND OPTIMIZATION

In this chapter, the basics of regression formulations used in the calculation of response surface model parameters for single and multiple response cases will be given. A response is an empirically obtained approximation for the actual quality characteristic. Therefore, it is important to understand the limitations and the underlying assumptions while developing response functions as well as finding optimum operating conditions with the help of these functions.

Correlation structure between responses were also emphasized as well as why individual optimization strategies are not sufficient for multiple responses. As the multiple criteria nature of the problem necessitates, the DM preference articulation process is an important characteristic of MRS and several alternatives were discussed regarding their pros and cons that will be used in the proposed methodology.

2.1 RESPONSE SURFACE METHODOLOGY (RSM)

As the second stage in RSM, building trusted regression models for responses is very important since results in the optimization stage cannot be trusted unless the established models approximate the true responses well. A response is generally an empirically obtained approximation on a quality characteristic of interest defined as:

$$y = f(x_1, x_2, ..., x_k) + \varepsilon \tag{2.1}$$

where $\boldsymbol{x}$ forms a set of controllable factors, and ε is the unexplained variation by f, which is assumed to have a normal distribution with mean 0 and variance $Var(\varepsilon)$. If the mean of ε is zero, the expectation of (1) is:

$$\begin{aligned} E(y_i) &= E[f_i(x_1, x_2, ..., x_k)] + E(\varepsilon_i) \\ &= \eta_i \\ &= f_i(x_1, x_2, ..., x_k) \end{aligned} \tag{2.2}$$

Since the true response function f_i is usually unknown, it is approximated by employing mathematical modeling techniques to experimentally obtained data. If the true response η_i depends on a set of controllable factors $x_1, x_2, ..., x_k$ (i.e., $\eta_i = f(x)$, and $x = (x_1, x_2, ..., x_k)^T$), it is possible to approximate it locally to any degree of accuracy with a Taylor Series Expansion around some arbitrary point x_0 as follows:

$$\eta_i \cong f(x_0) + \nabla f_i(x_0)^T (x - x_0) + \frac{1}{2}(x - x_0)^T \mathbf{H}_i(x_0)(x - x_0) + ..., \tag{2.3}$$

where $\mathbf{H}_i(x_0)$ is the Hessian of f_i at x_0.

Neglecting higher-order terms in (2.3), the expansion reduces to polynomial function of the form:

$$\eta_i = f_i(x) \cong \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{j=1}^{k} \beta_{jj} x_j^2 + \sum_{j=1}^{k-1} \sum_{<l=2,}^{k} \beta_{jl} x_j x_l, \tag{2.4}$$

where $\beta_0, \beta_j, \beta_{jj}$ and β_{lj} are called the parameters or regression coefficients. The second order model is widely used in RSM for several reasons. First, it is flexible and can take a wide variety of functional forms. Second, it is easy to estimate the parameters with the least squares method. Finally, there is considerable practical experience indicating that second-order models work well solving real life problems. For example, if the controllable variables are standardized to have a zero mean and equal standard deviations

(see Box and Wilson, 1951), the resulting experimental region can be interpreted easily as some geometric figure with the center point as the origin. Thus, a radial constraint $(x^T x \leq \rho^2)$ is appropriate for optimization purposes when the region of experimentation is spherical or near spherical.

2.2 ORDINARY LEAST SQUARES ESTIMATION

In order to estimate β parameters with the method of least squares, Equation (2.4) can be written as (Myers and Montgomery, 2002):

$$\boldsymbol{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \tag{2.5}$$

Where

$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots x_{1k} \\ 1 & x_{21} & x_{22} & \cdots x_{2k} \\ \vdots & \vdots & \vdots & \ddots \ \vdots \\ 1 & x_{n1} & x_{n2} & \cdots x_{nk} \end{bmatrix},$$

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \quad \text{and} \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

We wish to find the vector of least squares estimators, $\boldsymbol{\beta}$, that minimizes:

$$L = \sum_{i=1}^{n} \varepsilon_i^2 = \varepsilon^T \varepsilon = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Note that L may be expressed as:

$$\begin{aligned} L &= \boldsymbol{y}^T \boldsymbol{y} - \boldsymbol{\beta}^T \mathbf{X}^T \boldsymbol{y} - \boldsymbol{y}^T \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\beta} \\ &= \boldsymbol{y}^T \boldsymbol{y} - 2\boldsymbol{\beta}^T \mathbf{X}^T \boldsymbol{y} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X}\boldsymbol{\beta} \end{aligned}$$

since $\boldsymbol{\beta}^T\mathbf{X}^T\boldsymbol{y}$ is a scalar, and its transpose $(\boldsymbol{\beta}^T\mathbf{X}^T\boldsymbol{y})^{\mathrm{T}} = \boldsymbol{y}^T\mathbf{X}\boldsymbol{\beta}$ is the same scalar. The least squares estimators must satisfy:

$$\frac{dL}{d\boldsymbol{\beta}}\Big|_{\mathbf{b}} = 2\mathbf{X}^T\boldsymbol{y} + 2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} = \mathbf{0}$$

which simplifies to:

$$\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} = \mathbf{X}^T\boldsymbol{y} \tag{2.6}$$

In order to solve (2.6), we multiply both sides with the inverse of $\mathbf{X}^T\mathbf{X}$. Thus the least squares estimator of $\boldsymbol{\beta}$ is:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{y}$$

The vector of fitted values $\hat{y}_i$ corresponding to the observed values y_i is:

$$\hat{\boldsymbol{y}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{y}$$

For a quadratic model like in Equation (2.4), if we decompose $\boldsymbol{\beta}$ into its linear and quadratic terms we get:

$$\hat{\boldsymbol{y}} = b_0 + \mathbf{x}^T\mathbf{b} + \mathbf{x}^T\hat{\mathbf{B}}\mathbf{x}$$

where b_0, $\mathbf{b}$ and $\hat{\mathbf{B}}$ are the estimates of the intercept, linear, and second order coefficients respectively. For a single response, optimum settings of $\mathbf{x}$, $\mathbf{x}_s$, can be calculated differentiating $\hat{y}$ in the direction of $\mathbf{x}$.

$$\frac{\partial\hat{y}}{\partial\mathbf{x}} = \mathbf{b} + 2\hat{\mathbf{B}}\mathbf{x}$$

Setting the derivative to $\mathbf{0}$, one can find the optimum (stationary) point of the system:

$$\mathbf{x}_s = -\frac{1}{2}\hat{\mathbf{B}}^{-1}\mathbf{b}.$$

The predicted response for any design point can now be estimated, for the stationary point:

$$\begin{aligned}\hat{y} &= b_0 + \mathbf{x}'_s\mathbf{b} + \mathbf{x}'_s\hat{\mathbf{B}}\mathbf{x}_s \\ &= b_0 + \frac{1}{2}\mathbf{x}'_s\mathbf{b}\end{aligned}.$$

Since the $\hat{\mathbf{B}}$ coefficients are estimates, based on normality assumption, the confidence interval information may account for the parameter uncertainty.

2.3 ESTIMATION OF A MULTIRESPONSE SYSTEM

"Simultaneous consideration of multiple responses involves first building an appropriate response surface model for each response and then trying to find a set of operating conditions that in some sense optimizes all responses or at least keeps them in desired ranges" (Myers, R., Montgomery D. 2002).

Let $y_1, y_2, \ldots, y_m$ be a set of responses which can be measured at each of N settings for a group of k coded controllable factors, $x_1, x_2, \ldots, x_k$. Hence, the ith response model can be written in vector form (Khuri and Cornell 1996):

$$\boldsymbol{y}_i = \mathbf{X}_i\boldsymbol{\beta}_i + \boldsymbol{\varepsilon}_i, \qquad i = 1, 2, \ldots, m, \tag{2.7}$$

where $\boldsymbol{y}_i$ is an $N \times 1$ vector of observations on the ith response, $\mathbf{X}_i$ is an $N \times p$ matrix of the levels of the independent variables, $\boldsymbol{\beta}_i$ is a $p \times 1$ is the vector of the unknown regression coefficients, and ε_i is an $N \times 1$ random error vector associated with the ith response. It is assumed that:

$$\begin{aligned}&E(\boldsymbol{\varepsilon}_i) = 0, \qquad i = 1, 2, \ldots, m \\ &\Rightarrow E(\boldsymbol{y}_i) = \mathbf{X}_i\boldsymbol{\beta}_i \\ &\mathrm{Var}(\boldsymbol{\varepsilon}_i) = \boldsymbol{\sigma}_{ii}\mathbf{I}_n, \quad i = 1, 2, \ldots, m \\ &\mathrm{Cov}(\boldsymbol{\varepsilon}_i, \boldsymbol{\varepsilon}_j) = \boldsymbol{\sigma}_{ij}\mathbf{I}_n, \quad i \neq j.\end{aligned} \tag{2.8}$$

The $m \times m$ variance-covariance matrix whose $(i,j)^{th}$ element is $\sigma_{ij}(i \neq j, and\ i,j = 1,2,...,m)$ and $(i,i)^{th}$ element is $\sigma_{ii}(i = 1,2,...,m)$ and denoted by Σ. To the extent of the unknown matrix Σ, homogenity for each component σ_{ij} is assumed herein (homogenity implies that the within-group variances and covariances are similar, and can therefore be pooled together to create a common variance-covariance matrix for the multiple groups). An unbiased estimator of Σ is $\hat{\Sigma}$, given by the formula:

$$\hat{\Sigma} = \frac{\mathbf{Y}^T[\mathbf{I}_N - \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}]\mathbf{Y}}{N-p} \tag{2.9}$$

where $\mathbf{I}_N$ is an identity matrix of order $N \times N$. With $m \leq N - p$, $\hat{\Sigma}$ will be nonsingular provided that $\mathbf{Y}$ is of rank m. Therefore, detecting linear dependencies among response data is crucial. Box et al. (1973) showed that with r many linearly independent relationships must exist among the multiresponse data if and only if the matrix $\mathbf{DD}^T$ has a zero eigenvalue of multiplicity r, where $D = (d_{ij})$ is a matrix of order $m \times N$ whose (i,j)th element is $d_{ij} = y_{ij} - \bar{y}_i$, where y_{ij} is the jth component of y_i and $\bar{y}_i = \sum_{j=1}^{N} y_{ij} / N, i = 1,2,...,m;\ j = 1,2,...,N$. In matrix form $\mathbf{D}$ is written as:

$$\mathbf{D} = \mathbf{Y}^T(\mathbf{I}_n - \mathbf{1}_n\mathbf{1}_n^T / N),$$

where $\mathbf{1}_N$ is a vector of ones of dimension N. If q is the multiplicity of the zero eigenvalue of $\mathbf{DD}^T$, then it is possible to find a set of $m - q$ responses among which no linear functional relationships exist. This necessitates the dropping of q responses that are linear functions of the remaining $m - q$ responses.

The m equations in (2.7) can be written as a single linear multi-response model of the form:

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_2 & \cdots & \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{X}_m \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_m \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_m \end{bmatrix} \tag{2.10}$$
$$\Rightarrow \boldsymbol{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where $\boldsymbol{Y} = [\boldsymbol{y}_1^T\ \boldsymbol{y}_2^T \ldots \boldsymbol{y}_m^T]^T, \boldsymbol{\beta} = [\boldsymbol{\beta}_1^T\ \boldsymbol{\beta}_2^T \ldots \boldsymbol{\beta}_m^T]^T, \boldsymbol{\varepsilon} = [\boldsymbol{\varepsilon}_1^T\ \boldsymbol{\varepsilon}_2^T \ldots \boldsymbol{\varepsilon}_m^T]^T$, and $\mathbf{X}$ is the block diagonal matrix. Percy (1992) called this the *seemingly unrelated regressions* (SUR) *model.* His choice of name reflects the fact that model (2.10) may be written as m separate multiple linear regressions which contains different parameters and are thus seemingly unrelated. However, they are connected because the responses in the different regressions are correlated with each other. It is common practice to assume $\mathbf{X}_1 = \mathbf{X}_2 = \ldots = \mathbf{X}_m = \mathbf{X}_0$, $\mathbf{X}_0$ has full rank and all responses can be approximated with the same function (i.e., quadratic) :

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1k} & x_{11}^2 & \cdots & x_{k1}^2 & x_{11}x_{12} & \cdots & x_{1k-1}x_{1k} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & & \cdots & & & \cdots & & & \cdots & x_{nk-1}x_{nk} \\ & \underbrace{\qquad\qquad}_{\text{linear terms}} & & & \underbrace{\qquad\qquad}_{\text{pure quadratic terms}} & & & \underbrace{\qquad\qquad}_{\text{interaction terms}} & & \end{bmatrix}$$

then model (2.10) called traditional multivariate regression model and

$$\hat{\boldsymbol{\beta}}_i = (\mathbf{X}_0^T\mathbf{X}_0)^{-1}\mathbf{X}_0^T\boldsymbol{y}_i \tag{2.11}$$

can be estimated using ordinary least squares (OLS) method. As common to almost all multiple response optimization schemes proposed so far, the assumption is that all response functions in the system depend on the same set of controllable variables and that they can be represented by polynomial regression models of the same degree within a certain region of interest.

2.4 SIGNIFICANCE OF CORRELATION STRUCTURE AND THE NEED FOR MULTIVARIATE MONITORING

Correlation structure, mostly dealing with linear correlations, is one of the most important issues that necessitates simultaneous treatment of multiple responses, and also has not been considered in many of the proposed methods. As a graphical explanation, Figure 2.1 presents comparisons of two bivariate response distributions with different $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ parameters (Chiao and Hamada 2001). The square in the middle of each graph is the specification region given for two responses. The 95% contours for **Y** indicate the shape of the distribution and gives an idea of the likeliness that the product will meet specifications. In Figure 2.1 (a), we see two responses having independent distribution (i.e. $\sigma_{ij} = 0$ and $\sigma_{ii} = \sigma_{jj}$). Only the means of both Y_1 and Y_2 are different, and case a_1 is better since (a_1) and (a_2) have proportions of conformance of 0.366 and 0.119 respectively. In Figure 2.1 (b) only the variance values for Y_2 changes. Case (b_2) is preferred because the variance for Y_2 for this case is smaller. Proportions of conformance are 0.366 and 0.911 respectively. These proportions can be calculated with MATLAB's "mvncdf" command provided the parameters of the bivariate normal distribution. In Figure 2.1 (c), Y_1 and Y_2 have significant negative correlation ($\sigma_{ij} = -0.9$) revealing that they are not independently distributed. Case (c_2) is preferred because it has proportion of conformance 0.501, which is 0.366 in case (c_1). As expected, accumulation inside the specification region is due to the tilted cigar shape distribution that is higher in c_2 case.

A conclusion can be made that the correlation structure may have a significant effect on quality of the product or process when quality characteristics are correlated. In order to improve quality or make quality robust, one needs to first identify what

controllable variables impact the mean and variances (σ_{ii}^2) of responses as well as the correlations ($\sigma_{ij}^2 / \sigma_{ii}\sigma_{jj}$) between responses. Therefore, an optimization algorithm should take these distributional parameters into consideration and then find the values of controllable variables that make quality goals achievable.

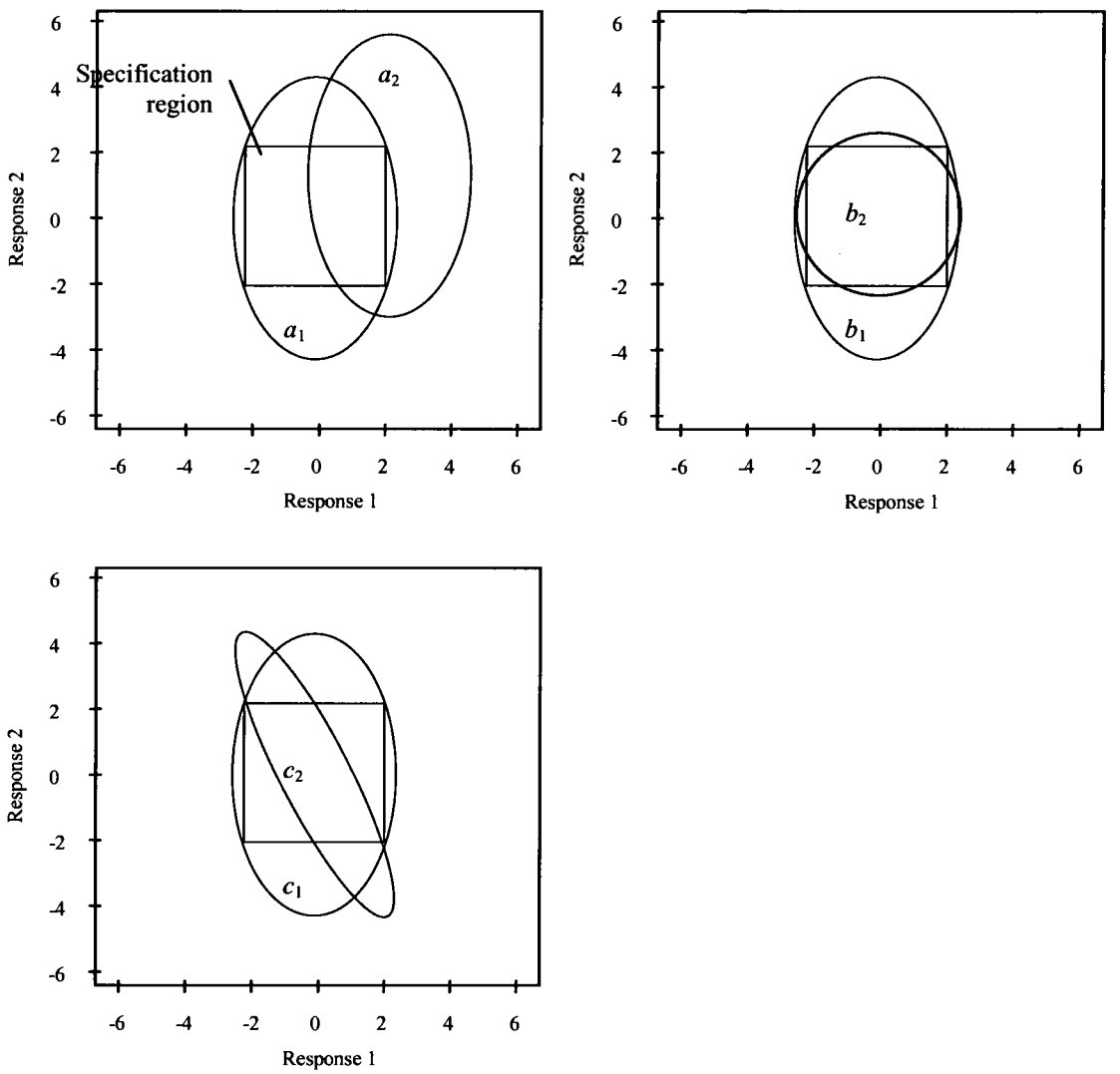


Figure 2.1 Some 95% Contours and Specification Region for Bivariate Responses.

2.5 MODEL ADEQUACY CHECKING

It is always necessary to (a) examine the fitted model to ensure that it provides an adequate approximation to the true system and (b) verify that none of the least squares regression assumptions are violated in (2.8) (Myers and Montgomery, 2002). For this purpose, nearly all mathematical software packages provide ANOVA tables to check the significance of regression model as shown in Table 2.1.

Table 2.1 Analysis of Variance for Significance of Regression

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Regression	SS_R	$p-1$	$MS_R = SS_R/(p-1)$	MS_R/MS_E
Residual	SS_E	$N-p$	$MS_E = SS_E/(N-p)$	
Total	SS_T	$N-1$		

The entries in the table represent measures of information concerning the separate sources of variation in the data. The total variation in a set of data is called the total sum of squares (SS_T). It is calculated summing squared deviations of individual response values from their mean value:

$$SS_T = \sum_{j=1}^{N}(y_j - \bar{y})^2$$

The total sum of squares can be decomposed into two parts, the sum of squares that can be explained by regression model (SS_R) and the sum of squares of error or residuals (SS_E). SS_R can be computed as:

$$SS_R = \sum_{j=1}^{N}(\hat{y}_j - \bar{y})^2$$

and SS_E can be computed as:

$$SS_E = \sum_{j=1}^{N} (y_j - \hat{y}_j)^2$$

Using the above statistics, the hypothesis H_0 can be tested. All β_i parameters (except β_0) are equal to zero, against the null hypothesis H_0: at least one β_i parameter (except β_0) is not equal to zero. Assuming normality of the errors, F_0 statistics in the table follows an F distribution with $p - 1$ and $N - p$ degrees of freedom. The null hypothesis can be rejected at α level if F_0 exceeds $F_{\alpha, p-1, N-p}$, revealing that variation accounted by the model is significantly greater than the unexplained variation.

An ancillary statistic to the F statistic is the coefficient of determination which is the ratio of the regression sum of squares to the total sum of squares:

$$R^2 = \frac{SS_R}{SS_T}$$

The value of R^2 is a measure of the amount of reduction in the variability of y when x_1, x_2, ..., x_k are used in the model. However by artificially increasing the number of β_i parameters in the model, R^2 can be inflated. A more realistic statistic is the adjusted R^2 which will not increase with the addition of insignificant model parameters, as follows (Myers and Montgomery 2002):

$$R^2_{Adj.} = 1 - \frac{SS_E / (N-p)}{SS_T / (N-1)} = 1 - (1 - R^2)\left(\frac{N-1}{N-p}\right).$$

Therefore, R^2 and $R^2_{Adj.}$ values would be very close to each other when only significant terms are used in the model.

PRESS (prediction error sum of squares) is another useful method which is indicative of predictive power of a regression model. To calculate PRESS, with N runs in

the data set, the model equation $\hat{y}_{(i)}$ is fitted to $N-1$ runs and a prediction is taken from this model for the remaining one. The difference between the recorded data value and the value given by the model (at the value of the omitted run) is called a prediction residual, $e_{(i)}$:

$$PRESS = \sum_{i=1}^{N} e_{(i)}^2 = \sum_{i=1}^{N} \left[y_i - \hat{y}_{(i)} \right]. \tag{2.12}$$

PRESS is the sum of squares of the prediction residuals. Over fitting problems can be eliminated when PRESS is minimized in the calculation of the second order models. It is useful to compare PRESS RMSE with RMSE as this may indicate problems with over fitting. RMSE is minimized when the model gets very close to each data point; 'chasing' the data will therefore improve RMSE. However chasing the data can sometimes lead to strong oscillations in the model between the data points; this behavior can give good values of RMSE but is not representative of the data and will not give reliable prediction values where you do not already have data. The PRESS RMSE statistic guards against this by testing how well the current model will predict each of the points in the data set (in turn) if they were not included in the regression. A small PRESS RMSE usually indicates that the model is not overly sensitive to any single data point.

2.6 ARTICULATION OF THE DECISION MAKER'S PREFERENCE INFORMATION

"Human intervention in the solution process is one of the characteristics that distinguish the methods of multiple criteria optimization from those of single criterion optimization" (Steuer, 1986). The problem of optimizing multiple response models is

similar to the problems addressed in multi-criteria or multi-objective mathematical programming algorithms. A DM can articulate his\her preference information by imposing relative weights or using a utility function. Another need arises when the responses are strictly constrained; a common set of input variables satisfying all the responses may not be possible. Hence, the DM's involvement may be required throughout the optimization process to find a compromising solution.

When a feasible solution does not exist, the DM's involvement may be needed to relax the constraints on responses. This can be done by either changing the target values of responses or allowed ranges of responses. Various multi-objective optimization methods are classified into three major categories by the timing of a DM's preference information articulation into the model including prior preference articulation, progressive preference articulation, and posterior preference articulation methods (Jeong and Kim, 2005). Prior preference articulation methods require that all the preference information of a DM be extracted prior to solving the problem. The preference of the DM is specified through interviews between the DM and an analyst. The major disadvantage of such methods is the difficulty a DM has in specifying the required preference information. The optimization process, however, is usually relatively simple since the problem has typically been reduced to a single objective.

Progressive preference articulation methods (interactive methods) require that a DM input his/her preference information into a model during the problem solving process. These methods are initiated through the finding of a solution for examination. As a result of the examination, the DM provides some information concerning his/her preference structure on outcomes arising from this solution. This process is repeated until

the DM either converges toward a best-compromise solution or terminates the process prior to reaching this point. Compared with the prior preference articulation methods, progressive preference articulation methods have the advantages that:

- show initial preference information may be enough and the DM may not be required to provide redundant information or answer hypothetical questions.
- provide an opportunity for a DM to learn his/her own tradeoff space is given, and,
- garner an obtained solution that has a better prospect of being implemented.

There are some shortcomings that

- for some cases it is not guaranteed that the preferred solution can be obtained within a limited number of iterations,
- have considerable cognitive effort is required of a DM, and
- have an extra computational load for solving the problem at each iteration is required.

The first progressive preference articulation method STEM (Step Method) was proposed by Benayoun, et al in 1971. Mollaghasemi and Evans (1994) developed a modified STEM in order to reduce the cognitive burden on the DM in the sense that s/he needs only to identify the least satisfactory performance measure value. Jeong and Kim (2005) proposed D-STEM that utilizes the desirability function approach, which can also be useful in modeling nonlinear preference information of a DM.

Posterior preference articulation methods do not need any substantial DM involvement before or during the problem solving process. They first find all (or most) of the efficient solutions. The DM then chooses the best one from the set of efficient

solutions. The main advantage of the posterior method is that no explicit preference of a DM is required to generate all the efficient solutions. However the number of efficient solutions generated may be too large to analyze.

Jeong and Kim (2007) proposed a posterior articulation process where the desirability approach is used for a dual response problem. They first generate several non-dominated solutions (Pareto optimal) with different weights of estimated mean and variance values of a single response. A solution to a multi-objective problem (call it A) is Pareto optimal if no other feasible solution is at least as good as A with respect to every objective and strictly better than A with respect to at least one objective (Winston, 2003). Hence, a non-dominated solution cannot be improved at the expense of other objective functions. Then, they let DM communicate with a set of alternative non-dominated solutions to accomplish the DM's best compromise solution.

3 OVERVIEW OF PREVIOUS AND RELATED RESEARCH

In this chapter, an extended overview of existing methodologies for computing optimum point in a MRSM study is presented. One of the primary objectives of a RSM is the determination of operating conditions on a set of input variables that results in an optimum response. In a multiresponse situation however, several response variables are considered and the optimization problem is more complex than in single response cases. Only rarely do all response variables achieve their respective optima with the same set of conditions (Khuri and Cornell, 1996). Moreover, a DM may have different priorities on responses and the optimization process should consider statistical properties that were mentioned before.

In this Chapter, cited literature will be criticized considering, correlation, robustness, quality of response models, the DM's preference articulation, and the applicability to different response types. Then, a brief summary of literature and a gap analysis will be provided in order to map the research effort and signify the contribution of the expected results. A formal research hypothesis will be formulated and the specific research directions to test the hypothesis will be presented.

3.1 PRIORITY-BASED APPROACH (DUAL RESPONSE APPROACH)

Myers and Carter (1973) considered a multiresponse optimization problem with only two responses (dual response optimization). One is taken as the primary and the

other is taken as the secondary response. They attempt to solve dual response problems analytically. The same approach can be generalized for more than two responses. Suppose there are m responses $\boldsymbol{y} = (y_1, y_2, \ldots, y_m)$ which are determined by a set of input variables $\boldsymbol{x} = (x_1, x_2, \ldots, x_k)$. If one of the responses has priority on others and the others can be tolerated with upper and lower specification limits, a multiresponse problem can be defined as:

$$\begin{aligned} &\text{Optimize} && \hat{y}_1 \\ &\text{Subject to} && l_i \le \hat{y}_i \le u_i, \quad i = 2,3,\ldots,m \\ & && \mathbf{x} \in R^k, \end{aligned} \tag{3.1}$$

where $\hat{y}_1$ denotes the primary response and l_i and u_i are lower and upper specifications of remaining responses. In cases where these specifications are not known *a priori*, these specifications can be obtained by optimizing each response function individually. The last constraint represents the solution set $\boldsymbol{x}$ that must be in the experimental region R. For cubodial designs, this constraint usually takes the form $-\mathbf{1} \le \boldsymbol{x} \le \mathbf{1}$ and for spherical designs, the constraint is $\boldsymbol{x}^T\boldsymbol{x} \le r^2$, where r is the design radius.

The priority-based approach, that consists of formulating the multiple-response problem to a constrained optimization problem, utilizes the ideas in the multi-criteria optimization literature and several arrangements can be made for the model above including giving different weights to responses. Without any transformation on responses, such as a desirability function, this strategy could be used when the primary quality characteristic is a large-is-better (LTB) or small-is-better (STB) while the secondary characteristics are nominal: the best (NTB), LTB, or STB variety. Minimum and maximum specifications would need to be stated for the LTB and STB

characteristics, respectively. These specification limits serve as the constraints that are to be satisfied at the optimal **x**.

In Model (3.1), one of the responses might be a process mean and the other might be a process variance that can be referred as response surface approach to Robust Parameter Design (RPD). Myers and Montgomery (2002) showed how control and noise factor interactions can be modeled with response surfaces, particularly with combined arrays. Del Castillo (1996) found confidence limits for the solution set of the above constrained problem both for linear and quadratic responses that can be generalized to RPD case.

The key issue in formulating the multiresponse problem is the choice of the optimization criterion. In practice there is no absolute need to rely solely on a single-number criterion; it would also be informative to separately study the mean and variance of each response, as provided, for example, by the Dual Response Model (Romano, 2004). However, applicability of these approaches becomes difficult as the number of responses increases. Other disadvantages for the priority-based approach are:

- that it does not consider the correlation structure between responses, and,
- for some cases, it might be difficult to prioritize the responses.

3.2 OVERLAYING CONTOUR PLOTS APPROACH

When a small number of responses and input variables, say two or three, included in the problem, overlaying contour plots can be used to find a "sweet spot" where responses meet their respective requirements. "The collection of such depictions could be helpful in identifying new regions to explore for possible quality improvement and may

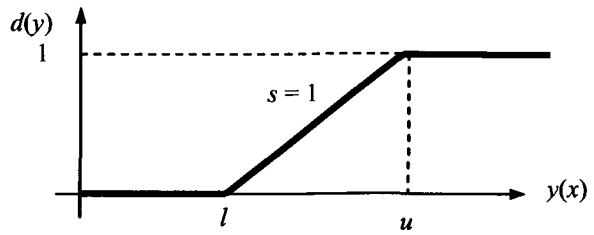
yield further insight into the relationships between the controllable variables and the quality characteristics and between the quality characteristics themselves" (Pignatiello, 1993). Application of graphical approaches is limited if the number of responses and input variables grows higher. Besides, it does not produce a certain solution and understanding the correlation structure is not easy through visual inspection of response graphs, which may also complicate the DM's involvement.

3.3 DESIRABILITY APPROACH

The desirability approach, first introduced by Harrington (1965), allows the involvement of the DM in the optimization process to incorporate economic information through the definition of the individual desirability functions. Since Harrington, this approach has been highly utilized and improved in the multiple response optimization field by several authors (Derringer and Suich, 1980; Kim and Lin, 2000; Ribardo and Allen, 2003; Kim and Lin, 2006; Lee and Kim, 2007).

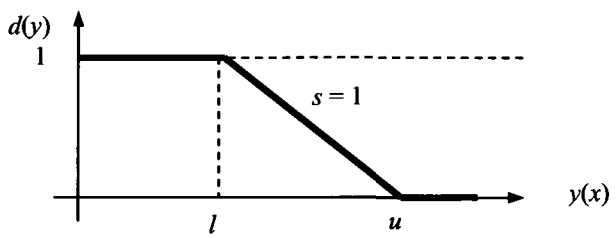
In the desirability approach, response functions, usually obtained via least square regression, are transformed into an individual desirability function d that varies over the range $0 \le d(y_j) \le 1,\ j = 1,...,m$. The transformation in a unit interval might be linear or nonlinear depending on the response type and the decision maker preferences as follows in Figure 3.1:

$$d(y_j)=\begin{cases}0 & y_j<l_j\\ \left(\dfrac{y_j-l_j}{u_j-l_j}\right)^{s_j} & l_j\le y_j\le u_j\\ 1 & y_j>u_j\end{cases}$$



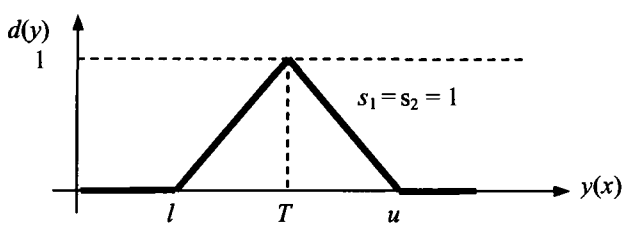
(a) Larger the Better Type (LTB) Response

$$d(y_j)=\begin{cases}1 & y_j<l_j\\ \left(\dfrac{u_j-y_j}{u_j-l_j}\right)^{s} & l_j\le y_j\le u_j\\ 0 & y_j>u_j\end{cases}$$



(b) Smaller the Better Type (STB) Response

$$d(y_j)=\begin{cases}0 & y_j<l_j\\ \left(\dfrac{y_j-l_j}{T_j-l_j}\right)^{s_1} & l_j\le y_j\le T_j\\ \left(\dfrac{u-y_j}{u-T_j}\right)^{s_2} & T_j\le y_j\le u\\ 0 & y_j>T_j\end{cases}$$



(c) Nominal the Best Type (NTB) Response

Figure 3.1 Desirability Function Transformations for Different Types of Responses

When the shape parameter $s = 1$, the desirability function is linear. Choosing $s > 1$ places more emphasis on being close to the target value, and choosing $0 < s < 1$ makes

this less important. For asymmetric responses around a target s_1 and s_2 parameters can be chosen unequal in the NTB type.

These individual desirability functions can be aggregated into a single overall desirability function which should be maximized.

$$D(\boldsymbol{x}) = \left[d(\hat{y}_1)d(\hat{y}_2)...d(\hat{y}_m)\right]^{1/m} \tag{3.2}$$

This is the most commonly used desirability metric (Derringer and Suich, 1980). The rationale behind using the geometric mean is that if any quality characteristic has an undesirable value (i.e., $d(\hat{y}_i) = 0$) at some operating conditions, $\boldsymbol{x} = \boldsymbol{x}_0$, then the overall result is 0 regardless of the values taken by the other responses (Del Castillo et al., 1996). Moreover, it provides a better balance between responses. For example, the arithmetic mean is indifferent for an overall desirability value composed of 2 responses, such as $D_1 = (.9 + .1)/2 = .5$ and $D_2 = (.5 + .5)/2 = .5$. Geometric mean on the other hand would prefer $D_2 = \sqrt{.5(.5)} = .5$ to $D_1 = \sqrt{.1(.9)} = .3$. Therefore, it is superior to arithmetic mean in the optimization process.

Several modifications have been proposed for Equation (3.2). Kim and Lin (2000) proposed modifications for transformation functions in order to incorporate predictive capability of response functions. Kim and Lin (2006) proposed dual response optimization for robustness.

Ortiz et al. (2004) made an important step by incorporating a penalty component to Equation (3.2) that can be very helpful when the number of responses is high and the problem is infeasible due to the tight constraints of responses. This idea is used in conjunction with the probability-based approach which will be detailed in the "Proposed

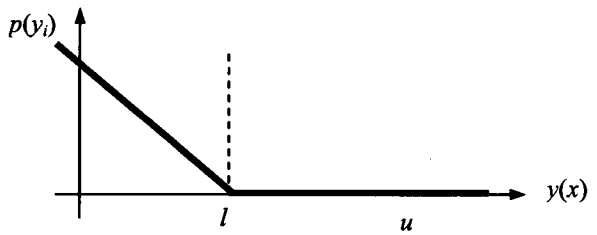
Approach" section of this study. A summary of the penalized desirability approach will now be provided.

The Penalized Desirability Function, $PD(\boldsymbol{x})$, includes an overall desirability component and an overall penalty component. The overall penalty function $P(\boldsymbol{x})$, which is also a combined function of the individual fitted responses, is particularly important because it reflects the overall severity of the infeasibility. The overall penalty function for the ith design setting is:

$$P(\boldsymbol{x}_i) = \left[\left(p(\hat{y}_1) p(\hat{y}_2) \ldots p(\hat{y}_m) \right)^{1/m} - c \right]^2 \tag{3.3}$$

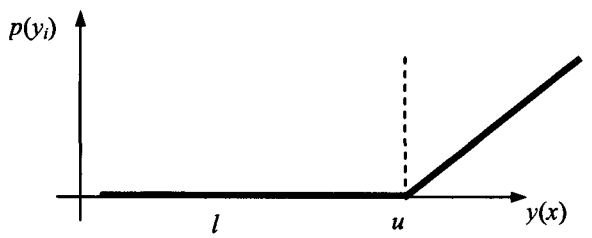
where the corresponding individual penalties $p(\hat{y}_i)$ are found again by similar transformations, as shown in Figure 3.2:

$$p(y_i)=\begin{cases} c+\left|\dfrac{y_i-l_i}{T_i-l_i}\right|, & y_i<l_i \\ c, & l_i\le y_i \end{cases}$$



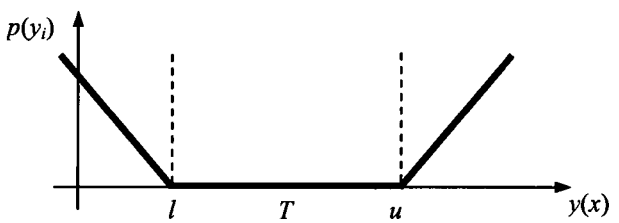
(a) Penalization for Larger the Better Type (LTB) Response

$$p(y_i)=\begin{cases} c, & y_i<u_i \\ c+\left|\dfrac{y_i-u_i}{u_i-l_i}\right|, & u_i\le y_i \end{cases}$$



(b) Penalization for Small the Better Type (STB) Response

$$p(y_i)=\begin{cases} c+\left|\dfrac{y_i-l_i}{T_i-l_i}\right|, & -\infty\le y_i<l_i \\ c, & l_i\le y_i\le u_i \\ c+\left|\dfrac{y_i-u_i}{T_i-u_i}\right|, & u_i<\hat{y}_i\le+\infty \end{cases}$$



(c) Penalization for Nominal the Best Type (NTB) Response

Figure 3.2 Penalization for Different Types of Responses

where c is a relatively small constant used to force $p(\hat{y}_i)>0$. Requiring a nonzero $p(\hat{y}_i)$ ensures that some nonzero overall penalty $P(\boldsymbol{x})$ is assessed for each infeasible solution. Smaller or larger values of c may be used according to the DM's understanding of penalization beyond the lower and upper values of responses. Incorporating this overall penalty function into a combined fitted response metric, the proposed overall desirability function for ith design setting can be estimated as:

$$PD(\boldsymbol{x}_i)=\left[d(\hat{y}_1)d(\hat{y}_2)...d(\hat{y}_m)\right]^{1/m}-\left[\left(p(\hat{y}_1)...p(\hat{y}_m)\right)^{1/m}-c\right]^2. \qquad (3.4)$$

The purpose accomplished by the overall penalty function is to ensure design space locations $\boldsymbol{x}$ are appropriately ranked relative to each other based on their degree of infeasibility. Once feasible solutions are found, their associated penalty function becomes $P(\boldsymbol{x}) = 0$, removing any penalty function influence from $PD(\boldsymbol{x})$. Therefore, $PD(\boldsymbol{x})$ reduces to Derringer and Suich's (1980) $D(\boldsymbol{x})$ metric when there is no infeasibility in the responses.

A penalized desirability metric can be particularly important when a feasible solution cannot be found through optimization efforts. Infeasibility may occur due to inconsistent constraints of design variables or due to inconsistent constraints of responses. The first case may result from false selection of ranges of controllable variables or an important factor in the screening experiments may be assumed as insignificant. Either way, a more comprehensive study is required to resolve that kind of infeasibility and this problem was excluded from the research as it is more related to design phase of the RSM.

For the later case however, a compromise may be achieved with DM involvement by relaxing the constraints on responses. Prioritization of infeasible points according to their degree of infeasibility helps progressive articulation of DM preferences with minimum number of iterations.

The desirability approach is very effective when incorporating a DM's preferences through an optimization process. It aggregates the overall utility of a product into a single desirability metric, which can be defined as a measure of overall quality of a product or a process. This is particularly important when comparing different operating conditions in the optimization process. Harrington (1965) developed a scale relating the

overall desirability of a product to its perceived quality. Harrington's (1965) scale is shown in Table 3.1.

Table 3.1 Harrington's Rating System for Interpreting the Desirability, $D(x)$ (adapted from Ribardo and Allen (2003)

Rating	Description
1.00	The ultimate in satisfaction and quality (an improvement beyond this point would have no appreciable value)
1.00–0.80	Acceptable and excellent (represents unusual quality or performance well beyond anything commercially available)
0.80–0.63	Acceptable and good (represents an improvement over the best commercial quality)
0.63–0.40	Acceptable but poor (quality is acceptable to the specification limits but improvement is desired)
0.40–0.30	Borderline (if specification exists, then some of the product quality lies exactly on the specification maximum or minimum)
0.30–0.00	Unacceptable (materials of this quality would lead to failure)
0.00	Completely unacceptable

Moreover, desirability approach can handle any type of responses (LTB, STB and NTB) efficiently. Jeong (2005) proposed an interactive desirability approach for the progressive articulation of a DM's preference information where shape, target, and bound parameters update during the optimization process. The basic weaknesses of desirability function approach are:

- Correlation structure between responses cannot be incorporated.
- It is not straightforward to account for model parameter uncertainty.
- Selection of bounds, target values and also the shape of the desirability function may not be straightforward.
- Commonly used individual desirability functions are discontinuous; hence gradient-base algorithms may have difficulty finding the optimum. Cahya (2002)

provided continuous desirability functions that provide good approximations for all response types.

3.4 SQUARED ERROR LOSS APPROACH (QUADRATIC LOSS APPROACH)

The squared error loss approach, or quadratic loss approach, is the multivariate analog of Taguchi's loss function approach. In a multiresponse case, loss is defined as:

$$L = \left[\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta}\right]^T \mathbf{C}\left[\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta}\right]$$

where $\mathbf{C}$ is a positive definite matrix of weights or costs, $\boldsymbol{\theta}$ is the vector of target values for each response (Pignatiello 1993). Vinning (1998) proposes minimizing estimated expected loss of above function:

$$\widehat{E[L]} = \left[\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta}\right]^T \mathbf{C}\left[\hat{\mathbf{y}}(\mathbf{x}) - \boldsymbol{\theta}\right] + trace\left[\mathbf{C}\Sigma_{\hat{\mathbf{y}}(\mathbf{x})}\right] \tag{3.5}$$

where

$$\Sigma_{\hat{\mathbf{y}}(\mathbf{x})} = \boldsymbol{x}_0^T (\mathbf{X}^T\mathbf{X})^{-1} \boldsymbol{x}_0 \hat{\Sigma}. \tag{3.6}$$

The first part of the right hand side of (3.5) shows the penalty or loss due to the deviance from the target values and the second half represents the penalty imposed by the quality of the prediction or penalty due to the uncertainty in the predicted responses. Vinning (1998) demonstrates several alternatives for the C matrix. For the case $\mathbf{C} = \mathbf{K}\Sigma^{-1}$, a correlation structure can be incorporated into the optimization. Here, $\mathbf{K}$ is a diagonal matrix with the diagonal elements reflecting the relative economic importance of quality characteristics.

The squared error loss approach has several advantages. First of all, it regards the correlation structure between responses. Second, the DM's preference information and

tradeoffs can be carried through the **C** matrix: and finally, it considers the penalty imposed by the prediction error. Romano et al. (2004) used the Finite Element simulation tool for the design of an elastic element of a force transducer. Their methodology decomposed the scalar value of loss into two different components as consumer loss and producer loss and they successfully and comprehensively applied most of the response surface arguments in the multiresponse case, such as handling robustness, response correlations, DM preferences, and model parameter uncertainty.

On the other hand, the multivariate squared error loss function is designed to model NTB type of responses and is not suitable for STB and LTB type of responses (Seshadri and Savage, 2002). In particular, a finite target does not exist for STB or LTB type responses and forcing target values for responses and trying to minimize deviations from those hypothetical targets may cause bias from the optimum. Maghsoodlo and Huang (1997) studied necessary calculations to estimate loss functions for mixed type of responses for bivariate cases and their results showed that even for bivariate cases loss function calculations might be cumbersome and each combination (i.e., LTB-NTB or STB-LTB) leads to a different loss function formulation. Therefore, for large number of responses, a general loss function formulation is difficult and has yet to be proposed. Calculation of the **K** matrix can also pose problems for the DM.

3.5 PROBABILITY-BASED (BAYESIAN PREDICTIVE) APPROACH

Chiao and Hamada (2001) proposed a very novel approach to MRSM called the probability-based,or Bayesian predictive, approach for replicated experiments. This approach is also followed by Peterson (2000 and 2004) and Miro-Quesada, et al. (2004)

later for unreplicated experiments. Generally speaking, Bayesian data analysis essentially involves:

1. Setting up a probability model that posits a distribution for observables (measurements or attributes) conditional on unobservables (parameters) where functions of some or all of the unobservables and observables (target quantities) is the object of inference,

2. A prior distribution that summarizes *a priori* uncertainty about the likely values of the parameters, and

3. Computing and interpreting the posterior distribution of the target quantities of interest (Raghunathan 2000).

These steps also constitute the basics of probability-based approaches for the multiple response surface optimizations developed so far. In a multivariate optimization problem, the probability of multiple responses simultaneously meeting their corresponding specifications provides an intuitive and easily interpreted statistic. Given the experimentally acquired data, that can also be named observables, a multivariate distribution can be posited, which is a function of design settings for the quality characteristics of interest. Then the cumulative distribution function (cdf) of this probability distribution can be maximized over the entire design space in order to find the design setting that gives the optimized quality characteristics. In other words, the Bayesian approach utilizes the posterior predictive distribution of the multiple responses in order to compute the probability that a future multivariate response will satisfy specified quality conditions.

As an example, Chiao and Hamada (2001) address the assessment and optimization of a replicated multiresponse experiment. Consider m responses $\boldsymbol{Y} = (Y_1, Y_2, \ldots, Y_m)$, each having a lower and upper specification region that can be represented by (l_i, u_i). In a multivariate setting, these individual bounds construct a common specification region, an m dimensional hypercube, S, whose sides are individual specifications. Then, a measure of quality, m, can be infered with responses being simultaneously in that specification region:

$$P(\boldsymbol{Y} \in S). \tag{3.7}$$

The above metric can be estimated and optimized by several methods. Chiao and Hamada (2001) assumed that $\boldsymbol{Y}$ follows an m dimensional multivariate normal distribution for each design setting, such as;:

$$f(\boldsymbol{Y};\boldsymbol{\mu},\boldsymbol{\Sigma}) = (2\pi)^{-(m/2)}\left|\boldsymbol{\Sigma}\right|^{-1/2} \times \exp\left[-\frac{1}{2}(\boldsymbol{Y}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{Y}-\boldsymbol{\mu})\right]. \tag{3.8}$$

After estimating $\hat{\boldsymbol{\Sigma}}$ and $\hat{\boldsymbol{\mu}}$ parameters, and integrating the pdf in (3.8) over the specification region, the proportion of conformance can be estimated for different design settings. However, $\hat{\boldsymbol{\Sigma}}$ and $\hat{\boldsymbol{\mu}}$ first need to be estimated for the settings that were not included in the experimental design (unobservables). This can be achieved by fitting regression functions to the estimates of variance-covariance matrix $\hat{\boldsymbol{\Sigma}}$ and mean responses $\hat{\boldsymbol{\mu}}$. Chiao and Hamada (2001) fit first order regression models for $\hat{\boldsymbol{\Sigma}}$ and $\hat{\boldsymbol{\mu}}$, where logarithmic transformations are used for the estimated variance-covariance matrix, for it to be positive definite.

Using regression models, conformance probability can be optimized applying an extended design grid, and the calculating $P(\boldsymbol{Y} \in S)$ value for each point in the grid. The

optimum design setting should be the one giving the maximum conformance probability. The integration can be done using a cdf of the multivariate normal distribution, which is provided as a built-in function in many programming packages such as MATLAB.

Parallel to Chiao and Hamada (2001), Peterson (2000, 2004) and Miro-Quesada et al. (2004) developed a probability-based approach for unreplicated experiments. They proposed multivariate-*t* distribution for responses and rather than using cdf function they used simulation to estimate the conformance probabilities. Their approach has the advantage of applying different performance metrics in the optimization process which this research intends to expand in the research methodology section.

A serious drawback of the probability-based approach is that it does not consider different degrees of satisfaction within the acceptable region. As an example, in desirability approach terms, two operating conditions, say $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, having an overall desirability D^1, $D^2 > 0$ and $D^1 \neq D^2$ are assumed to be equally satisfactory as long as all the responses lie within their specifications. In reality however, the DM may have differing degrees of satisfaction for the two operating conditions.

Moreover, Chiao and Hamada (2001) do not take into account the uncertainty of the model parameters. The model parameters are simply replaced by their point estimates. This study's verification study showed that, for some design settings, probability measures can be noticeably higher than they should be, revealing that the normality assumption may not be a good approximation. Another issue is that in order to estimate $\hat{\Sigma}$ and $\hat{\boldsymbol{\mu}}$ replicates are required, hence the costs of experimentation for this approach may be expensive.

3.6 LITERATURE SUMMARY – GAP ANALYSIS

In this section, this research aimed to provide a snapshot of what was previously done for each optimization approach regarding statistical properties and DM involvement issues that were presented in the previous section. Table 3.2 summarizes previous research on multiple response surface optimization with respect to the authors' contributions to the problem space.

The synopsis and findings on the literature are as follows:

- The desirability based approach is the most studied approach due to its flexibility to handle DM involvement. However, none of the desirability approaches in Table 3.2 have considered correlation structure among responses. The quality of response models can not be incorporated with desirability method either.
- Correlation among responses can be captured more efficiently with the squared error loss approach and probability-based approach. The squared error loss approach is designed to handle NTB-type responses only.
- Robustness to noise variables is the most considered statistical property.
- The quality of response models is least considered statistical property. This may lead to an incorrect prediction and bias at the optimum operating conditions.
- All approaches prefer prior articulation of the DM except the desirability approach. Posterior articulation is never used.

Table 3.2 Literature Summary and Research Mapping.

Authors	M	P_1	P_2	P_3	P_4	P_5
MIRO-QUESADA and DEL CASTILLO (2004)	1	X	X	X	1	
MYERS and CARTER (1973)	1				1	X
BENAYOUN et al (1971)	2				1	X
DEL CASTILLO et al. (1996)	2				1	X
DERRINGER and SUICH (1980)	2		X		1	X
HARRINGTON (1965)	2		X		1	X
JEONG (2005)	2		X		2	X
JEONG and KIM (2005)	2				2	X
KIM and LIN (2000)	2		X	X	1	X
KIM and LIN (2006)	2		X	X	1	X
LEE and KIM (2007)	2		X		1	X
ORTIZ et al. (2004)	2		X		1	X
RIBARDO and ALLEN (2003)	2		X		1	X
AMES et al. (1997)	3				1	
KHURI and CONLON (1981)	3	X			1	
KO et al. (2004)	3	X	X	X	1	X
KOKSOY and YALCINOZ (2006)	3	X	X	X	1	
LAMGHABBAR et al. (2004)	3		X		2	
MAGHSOODLO and HUANG (1997)	3	X	X		1	X
PIGNATIELLO (1993)	3	X	X		1	
ROMANO et al. (2004)	3	X	X	X	1	
VINING (1998)	3	X		X	1	
CHIAO and HAMADA (2001)	4	X			1	X
MIRO-QUESADA et al. (2004)	4	X	X	X	1	
PETERSON (2000)	4	X	X	X	1	
PETERSON (2004)	4	X		X	1	X
ISIK (2008)	4+2	X	X	X	2	X

Key:
M: Optimization Method
- 1: Priority-based approach
- 2: Desirability approach
- 3: Squared error loss approach
- 4: Probability-based approach

P_1: Correlation
P_2: Robustness of responses
P_3: Quality of response models
P_4: DM's preference articulation:
- 1: Prior articulation
- 2: Progressive articulation
- 3: Posterior articulation

P_5: Applicability to all response types

- Although probability-based approaches can handle any type of response, all of the proposed studies used conformance probability as an optimization metric. Conformance probability assumes response estimates are equally good as long as they lie between the specifications. This may provide serious bias in the optimization process and high conformance does not imply high quality responses all the time. This issue will be further explained in the research question and motivation section.

In this study, an integrated approach will be developed, that will utilize the strengths of probability-based and desirability approaches in a unique algorithm. The proposed approach will use the penalized desirability metric in order to avoid bias in the optimization process and to also efficiently consider the statistical properties through the use of a probability-based approach.

3.7 RESEARH QUESTIONS AND MOTIVATION

For an effective compromise among the responses, the analyst wishes to find the optimal setting with three desirable properties, namely, small bias, high robustness, and high quality of predictions. That is, it is desired that the expected responses be close to their targets, and the variances of the true and predicted responses be small at the optimal setting (Ko et.al. 2005). Probability-based approaches, or Bayesian predictive approaches, use conformance probability as an optimization metric, which is a function of response specifications, experimental design, and correlations among responses. Therefore, it is highly intuitive and seriously takes into account the statistical properties of multiple responses.

However, as an optimization criterion, conformance probability does not incorporate a degree of satisfaction throughout the optimization process. This can create a bias in terms of response targets that is explained through the following example. Suppose that design settings x_1 and x_2 provide a good balance between bivariate responses Y_1 and Y_2, and have equally large conformance probabilities $p_1 = P(Y \in S|x_1) \cong 1$, $p_2 = P(Y \in S|x_2) \cong 1$ over the specification region, as depicted in Figure 3. Let us further assume that each ellipsoid represents the 99% contour plots for multivariate normal distributions having similar Σ but having different μ parameters.

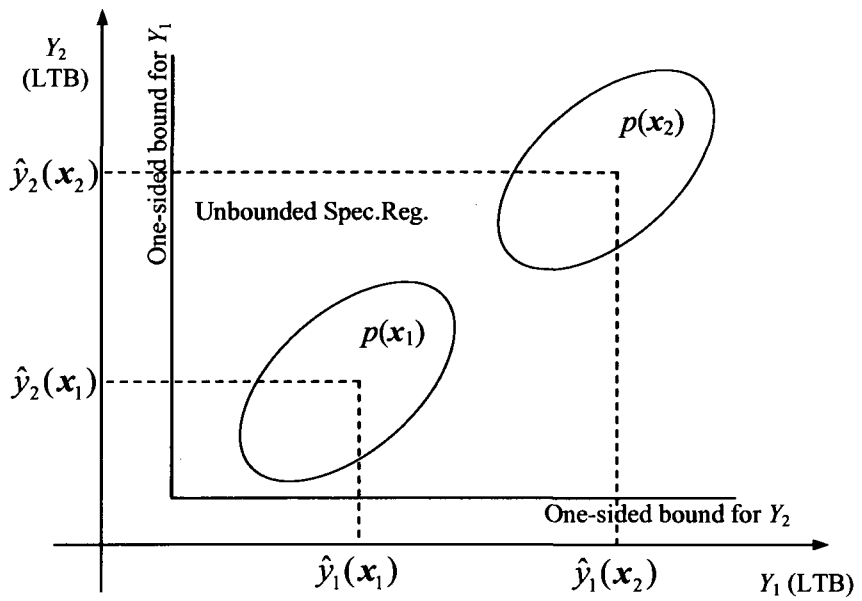


Figure 3.3 Two Different Operating Conditions Having the Same Conformance Probability and Different Mean Response Value for Bivariate Responses

In Figure 3.3, the shaded area shows the specification region for two LTB type responses, Y_1 and Y_2. Two operating conditions x_1 and x_2 provide almost equal conformance probabilities but different mean responses. According to conformance

probability criteria both operating conditions are equally good. However, in reality, the DM or customer would observe a significantly higher quality with x_2 on the average.

Therefore, the assumption of higher conformance implies that higher quality should be checked carefully for multiresponse surface optimization. In this study, a penalized desirability function was incorporated to probability-based approach which forces the search procedure through highly desirable values within the specification region. PD(x) is the penalized desirability function and by sampling from a posterior predictive distribution of $\boldsymbol{Y}$ for a given $\boldsymbol{x}$ value, it is possible to average $PD(\boldsymbol{x})$ over the solution space. The optimum value for $PD(\boldsymbol{x})$ should have an equal conformance probability but a higher desirability with respect to the optimum which is obtained by conformance probability. This is known as the integrated probability-based approach, and it compares the performance by means of validation runs for each solution obtained by this research's proposed approach with those obtained via the probability-based approach. The details of the simulation will be explained in the "Proposed Approach" section.

A formal hypothesis can be constructed with the following scenario. Let us assume $\boldsymbol{x}_1$* represents an optimum operating condition found by the probability-based approach, and $\boldsymbol{x}_2$* represents an optimum operating condition found by the integrated probability-based approach $PD(\boldsymbol{x})$. By means of validation runs it will be found provided that $p(\boldsymbol{x}_1^*) \cong p(\boldsymbol{x}_2^*)$

$$\begin{aligned} H_0 &: PD(\boldsymbol{x}_1) \geq PD(\boldsymbol{x}_2) \\ H_1 &: PD(\boldsymbol{x}_1) < PD(\boldsymbol{x}_2) \end{aligned} . \tag{3.9}$$

We can reject the null hypothesis if, on the average, the operating condition x_2 produces higher quality responses. Since the distributional properties of multiple responses is a function of:

- experimental design,
- number of controllable factors,
- number of responses, and
- number of experimental runs

the above hypothesis should be checked for different levels of these factors. Therefore, several examples will be studied from recently published literature to develop a generalized integrated approach that can be applicable to broad range of multiresponse problems.

Another concern is the articulation of the DM's preference information through an optimization process. DM involvement is particularly needed when a feasible compromising solution cannot be obtained with the first optimization attempt. The DM requires an informative procedure while encompassing his/her trade offs on the parameters (targets, bounds, and shapes) of different responses. A progressive articulation process will be followed in conjunction with the desirability approach in the proposed method section as well.

3.8 RESEARCH OBJECTIVES

The specific goal of this research is to develop computational methods for multiresponse modeling and optimization that will account for statistical properties and also allow for efficient DM involvement. This goal will be accomplished by integrating

the desirability approach and the probability-based approach by considering the following specific objectives.

- To develop an extended probability-based approach by studying different optimization schemes with the penalized desirability approach, that can be applied to a mixed type of responses.
- To assess the performance of the proposed approach by making comparisons with the probability-based approach; by studying several examples in the published literature.
- To apply Bayesian analysis methods using Monte Carlo simulation in order to:
    - Check the reliability of solutions found in terms of conformance probabilities, and
    - Identify response model quality issues by estimating uncertainty in response models.
- To develop a user-friendly computer code for the intended approach that is capable of modeling and optimizing any type of multiresponse optimization problem.

4 PROPOSED APPROACH

4.1 INTRODUCTION

The strength of the desirability approach is in its flexibility for DM involvement through an adjustment of a set of parameters. However, transforming individual responses to desirability functions does not consider correlations among responses. On the other hand, a probability-based approach can incorporate correlations as well as parameter uncertainty. The key idea of the proposed methodology is to integrate the probability-based approach with the desirability approach in order to push the search process to highly desirable and highly reliable operating conditions. This strategy would also provide efficient DM involvement particularly when a feasible solution does not exist, while still meeting the statistical requirements.

In a multiresponse problem, when the number of factors or responses grows moderately high and the responses are strictly constrained, in most cases, a common set of input variables satisfying all the responses may not be possible. Hence, a penalized desirability metric providing information for the degree of infeasibility to differentiate between several partially infeasible points might help the DM articulate his/her preferences in an informative way. From that point on, a progressive articulation of the DM's preferences can be embedded to relax the constraints on infeasible responses with a minimum number of adjustments. In this Chapter, details of the proposed methodology are presented to show necessary formulations and calculations when a penalized desirability metric is used as an optimization criteria in accordance with the probability-

based approach. The proposed methodology will be illustrated using an example from the literature.

4.2 PROPOSED MATHEMATICAL APPROACH

Following Peterson (2004)'s notation, we let $\boldsymbol{Y} = (Y_1, Y_2 ... Y_m)^T$ be the multivariate $(m \times 1)$ response vector and let $\boldsymbol{x} = (x_1, x_2, ..., x_k)^T$ be the $(k \times 1)$ vector of factor variables. Suppose we have unreplicated experimental data for $\boldsymbol{Y}$ and we are simply interested in $\boldsymbol{Y}$ being in some desirable subset of the response space S, then we can consider the discrete desirability function, $I(\boldsymbol{Y} \in S)$, where $I(\cdot)$ is the 0-1 indicator function. (If $\boldsymbol{Y} \in S$, $I(\boldsymbol{Y} \in S) = 1$, else 0).

Bayesian predictive density for $\boldsymbol{Y}$ can be obtained in closed form and is given by a multivariate t- distribution with v degrees of freedom (Press, 1989)

$$f(\boldsymbol{Y}|\boldsymbol{x}) = \frac{\Gamma\left(\frac{v+m}{2}\right)}{(\pi v)^{m/2}} \sqrt{|\mathbf{H}|} \left[1 + \frac{1}{v}(\boldsymbol{Y} - \hat{\boldsymbol{\beta}}^T \boldsymbol{x})^T \mathbf{H} (\boldsymbol{Y} - \hat{\boldsymbol{\beta}}^T \boldsymbol{x})\right]^{-(v+m)/2} \tag{4.1}$$

where $v = \mathrm{N} - p - m + 1$, $\hat{\boldsymbol{\beta}}$ is the Ordinary Least Squares (OLS) estimator of $\boldsymbol{\beta}$, $\Gamma(.)$ denotes the gamma function and $\mathbf{H}$ is the estimate of the variance-covariance matrix of $\hat{\boldsymbol{y}}(\boldsymbol{x})$, the predicted mean response at $\boldsymbol{x}$ and given by:

$$\mathbf{H} = \left(\frac{v}{n-p}\right) \frac{\hat{\Sigma}_\varepsilon^{-1}}{1 + \boldsymbol{x}^T (\mathbf{X}^T \mathbf{X})^{-1} \boldsymbol{x}} \tag{4.2}$$

and

$$\hat{\Sigma}_\varepsilon = \frac{1}{n-p} (\boldsymbol{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T (\boldsymbol{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \tag{4.3}$$

The covariance matrix of $\boldsymbol{Y}|(\boldsymbol{x},\text{data})$ exists if $v > 2$ and is given by:

$$Var(\boldsymbol{Y}|\boldsymbol{x}, data) = \frac{v}{v-2}\mathbf{H}^{-1}$$

Therefore, we have that:

$$\boldsymbol{Y}|\boldsymbol{x}, data \sim T_m^v\left(\hat{\boldsymbol{\beta}}^T\boldsymbol{x}, \frac{v}{v-2}\mathbf{H}^{-1}\right) \tag{4.4}$$

To obtain $p(x)$ we need to integrate (4.1) over the specification region S:

$$p(x) = \int_S f(\boldsymbol{y}|\boldsymbol{x}, data)dy \tag{4.5}$$

One way of performing this integration numerically is by Monte Carlo simulation. Given that $\boldsymbol{Y}|\boldsymbol{x}, data$ is distributed as multivariate t, the following equation can be used to generate random $\boldsymbol{Y}$ values from multivariate t-distributions for different settings of input variables:

$$\boldsymbol{Y} = \mathbf{H}^{-1/2}\mathbf{z}\sqrt{v/s} + \hat{\boldsymbol{\beta}}^T\boldsymbol{x} \tag{4.6}$$

Where $\mathbf{z}$ is sampled from a $N_m(\mathbf{0}, \mathbf{I}_m)$ and s is sampled from a chi-square distribution with v degrees of freedom. It follows that $\boldsymbol{Y}$ has a multivariate t-distribution with v degrees of freedom. Since we are simply interested in $\boldsymbol{Y}$ being in some desirable subset of the response space S, integral in (4.5) can be approximated as:

$$p(x) \cong \frac{1}{N}\sum_{i=1}^{N} I(\boldsymbol{Y} \in S) \tag{4.7}$$

where N is the number of simulations performed for each design setting x. The dispersion of probability distribution depends on both the natural variability of data and model parameter uncertainty, which of course is intimately related to the sample size and experimental design used in the study. As we notice from (4.2) and (4.6), the $\mathbf{H}$ matrix used in simulating response data considers the scaled prediction

variance, $1+\boldsymbol{x}^T(\mathbf{X}^T\mathbf{X})^{-1}\boldsymbol{x}$, which reflects the parameter uncertainty of the regression models therefore avoiding poor prediction properties.

Here, all we need to do is sample from the posterior predictive distribution of $\boldsymbol{Y}$ for a given $\boldsymbol{x}$ value, then construct the posterior predictive distribution of $I(\boldsymbol{Y} \in S)$ conditional on $\boldsymbol{x}$. From a quality perspective, this gives us a measure of the reliability of $\boldsymbol{Y}$ being in S for a given $\boldsymbol{x}$. As can be seen from the formulations, this measure takes into account the variance-covariance structure of the data and the uncertainty of the model parameters through the posterior predictive distribution of $\boldsymbol{Y}$. A search of the x-space then provides the experimenter with information on conditions for optimizing the reliability of $\boldsymbol{Y}$ being in S.

Peterson (2004) used a conformance probability metric both in the optimization of multiresponses and also in the calculation of the reliability of optimum solutions found by different optimization methods such as desirability and squared error loss methods. For example, $\boldsymbol{x}$ is the optimum operating condition found by desirability approach and D^* represents a certain proportion of the optimum value expected by DM. Then $P(D(\boldsymbol{Y}) \geq D^* | x)$ gives a reliability measure in probability units showing how future responses are likely to satisfy DM expectations. Peterson (2004) also studied the effect of how reducing process variability and increasing sample size can improve the conformance probability by simulating artificial data from posterior predictive distribution with an intent to evaluate the value of information from additional replication runs. Later Colosimo and Castillo (2006) mathematically showed that augmenting the initial design in such an artificial way would not provide any valuable information. Miro

Quesada et al (2004) extended the approach for a robust case by simulating noise factors from normal distribution and averaging $p(\boldsymbol{x})$ over noise variables.

However, conformance probability assumes all responses are equally good as long as they are within the specification limits and do not provide any information on the overall degree of satisfaction. It is very likely that for one design setting most of the simulated responses will conform to the specifications but will perform poorly on the desirability scale. To avoid that type of bias, as an optimization criterion, here, Ortiz et al's (2004) penalized desirability function should be used, which was explained in the literature search section:

$$PD(\boldsymbol{x}) = \left[d(\hat{y}_1)d(\hat{y}_2)...d(\hat{y}_m)\right]^{1/m} - \left[\left(p(\hat{y}_1)...p(\hat{y}_m)\right)^{1/m} - c\right]^2.$$

The $PD(\boldsymbol{x})$ metric can be simulated and averaged for different design settings as:

$$\overline{PD}(x_i) \cong \frac{1}{N}\sum_{j=1}^{N} PD(x_i) \tag{4.8}$$

and the optimum operating conditions can be found by the same approaches such as in conformance probability that will be detailed in the next section.

4.3 RESPONSE MODELING AND OPTIMIZATION

In the modeling of response functions $\hat{y}_i$, instead of the ordinary least square (OLS) approach, a prediction error sum of squares (PRESS) is used to prevent over-fitting. Insignificant model parameters are also dropped from further calculations for same reasons.

For the optimization of conformance probability, Miro-Quesada et al. (2004) propose applying a fine grid over the experimental region and generating $\boldsymbol{Y}$ values using Equation (4.6). After a Monte Carlo simulation, the $\hat{p}(x)$ value for each setting in the grid can be estimated. The design setting giving maximum $\hat{p}(x^*)$ is the optimum solution for the multiresponse problem. If the number of input factors is more than three, a moderate grid can be applied and a logistic regression model can be fitted to the $\hat{p}(x)$ values. The optimum setting can be found by maximizing this regression function. However, fitting a regression function to the averaged simulated responses is not an easy task due to large number of design points having zero conformance probability. Miro-Quesada et al. (2004) used a 4th order logistic regressions function which they called a "meta-model", for two controllable factors where a 11^2 full factorial design is used in the simulation. Moreover, optimizing highly nonlinear functions depending on several factors is not guaranteed and requires multiple starting points to converge to best local optima.

As an alternative, Peterson (2004) proposes applying a finer grid over the sub-regions of the experimental region after performing a screening simulation. This process continues until a standard quadratic model for the constrained region of interest is reached. Similar arguments can be applied to the simulation and optimization of the $PD(\boldsymbol{x})$ metric. In this research, validation runs have shown that a constrained simulation approach with a possibly finer grid produces better results than those obtained by optimizing a meta-model fitted to both simulated metrics. When available computer power is considered, even for controllable factor numbers larger than three, simulation times are reasonable, and constrained volume filling designs can be used. Another disadvantage of using a meta-model approach is during the DM articulation process;

when the constraints on responses are modified a new meta-model should be estimated at each iteration. Therefore, it has been experimentally shown that, with respect to both metrics, the best design setting obtained with this approach is always better than the optimum design setting obtained by maximizing meta-models.

Specifically, first a grid of moderate number of (150) design points according to alphabetical optimality criteria (A, D, V-optimality, etc.) is generated. After performing an initial simulation, by sorting according to $PD(x)$ metric, some of the factor levels which have negative or too small $PD(x)$ value are constrained. Then a finer volume filling design grid is applied to constrained factor intervals. The design setting given the maximum $PD(\boldsymbol{x})$ value is assumed to be the optimal. This approach can save reasonable simulation time for most of the cases.

Montgomery (2002) proposes several computer-generated design alternatives with different optimality criteria for constrained factors and factor level combinations. There are several readily available software programs like Design Expert™ or MATLAB™ that can create optimal designs according to different optimality criteria for constrained factor levels. A simulation can be stopped when the different design points in the grid have very close $PD(\boldsymbol{x})$ values revealing that a plateau has been reached within close proximity of the optimum point. This research used MATLAB™'s "Model Based Calibration Tool" in order to estimate the quadratic PRESS response functions and to create optimal and space-filling designs in the simulations.

The results of both optimization strategies with an example are shown in the following sections.

4.4 ARTICULATION OF DM'S PREFERENCE

One of the most important advantages of desirability transformations is the ability of the DM to revisit his/her utility when trade-offs are required among responses. A DM can change his/her initial considerations by easily adjusting bound, shape, or target of the responses. Figure 4.1 shows how a DM can articulate his/her preference information by adjusting three types of response parameters for a NTB-type response (Jeong and Kim, 2009).

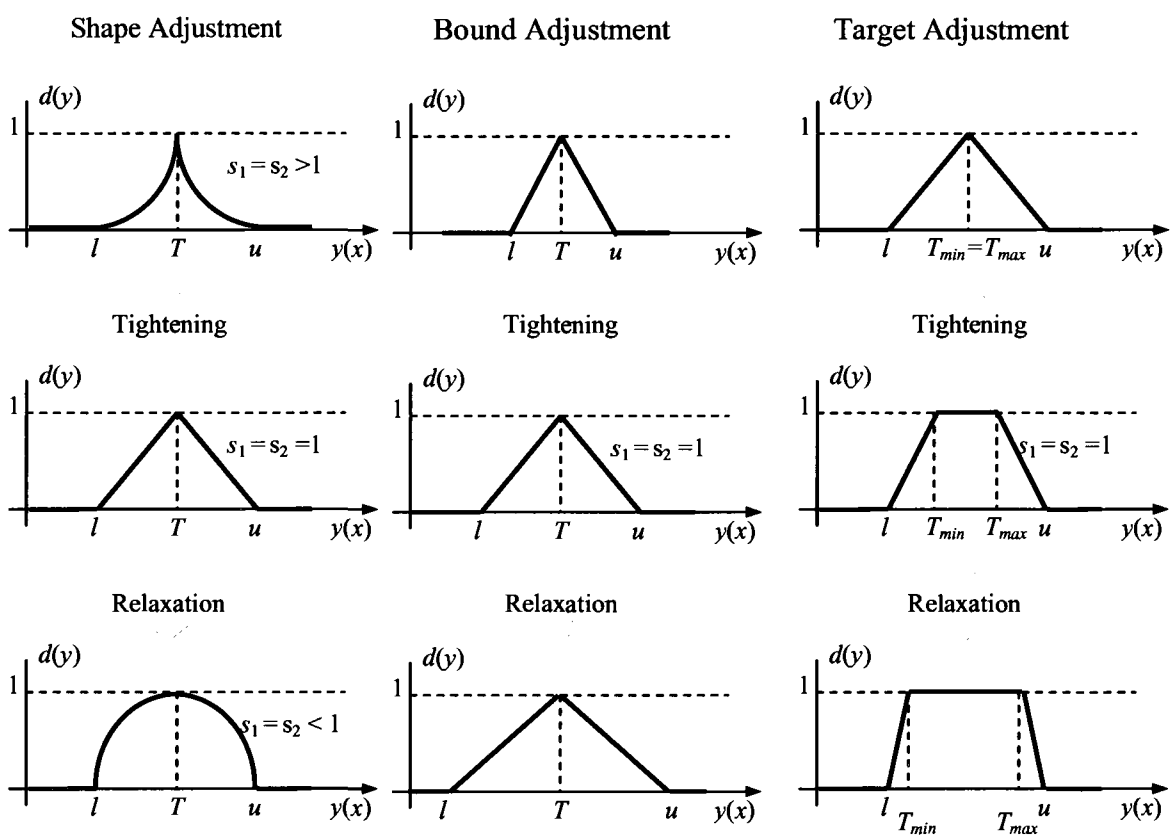


Figure 4.1 Examples of Parameter Adjustment for NTB-Type Response (adapted from Jeong and Kim, 2009)

It turns out that, as a natural byproduct of proposed approach, the marginal probabilities and individual $d(\hat{y}_i)$ values corresponding to marginal events of some of the y_i values can also be easily computed. Hence by adjusting the bound, shape, and target parameters of those responses having small values of $d(\hat{y}_i)$, the optimization can be rerun so as to achieve a compromise among responses. In the following example, progressive tightening and relaxing is defined to show how it can work for parameter adjustment as two possible strategies. For all of the examples in this study, multiple responses are assumed to be equally important. For the cases where the DM has different priorities on responses, this proposed PD metric can be modifying as in Derringer (1994):

$$D(\boldsymbol{x}) = \left[d(\hat{y}_1)^{w_1} d(\hat{y}_2)^{w_2} \ldots d(\hat{y}_m)^{w_m} \right]^{\frac{1}{\sum w_i}}.$$

This allows different importance levels to be assigned to different quality characteristics. In the same fashion, it is possible to assign different weights for penalty components. However, since the relative evaluation of quality characteristics is required with the weighting approach, when the number of responses grows high this can complicate the articulation process. Therefore, an individual shape-based and bound-based progressive articulation process is suggested as they fit well with the proposed methodology.

4.5 AN ILLUSTRATIVE EXAMPLE

The following example was taken from Miro-Quesada et al. (2004) and also used by Peterson (2004) and Miro-Quesada and Castillo (2004). It involves the optimization of a high performance liquid chromatography (HPLC) system to detect mixtures of impurities. The performance of the assay was based upon four quantitative response variables: the critical resolution (Rs), total run time, signal-to-noise ratio of the last peak,

and the tailing factor of the major peak. Three controllable factors affecting the HPLC assay were included: IPA%, temperature and pH. To extend this method for the robust design case, the controllable factor IPA% was assumed to be the noise variable, which was further assumed to be normally distributed with a mean of zero and a standard deviation of 0.1, as in Miro-Quesada et al. (2004) and Miro-Quesada and Castillo (2004). A Box-Behnken design with three center points was used.

4.5.1 RESPONSE MODELING

The response data on the coded factor levels ($-1 \le \mathbf{x} \le 1$) are presented in APPENDIX A:. Complete second order response surface models were fitted to all three responses using coded versions of the controllable factors. The resulting adjusted R^2 statistics were higher than 98% and very close to $R^2_{prediction}$ statistics for all of the responses. This indicates that the models fit the data very well.

The conformance region for responses specified as:

$$S = \{\boldsymbol{y} = [y_{Rs}\ y_{Time}\ y_{S/N}\ y_{Tail}] : y_{Rs} \ge 1.8,\ y_{Time} \le 15,\ y_{S/N} \ge 300,\ 0.75 \le y_{Tail} \le 0.85\}$$

Estimated second order response functions are:

$$\begin{aligned}
\hat{y}_1 &= 2.19 + 0.23x_1 - 0.21x_2 - 0.015x_1^2 - 0.02x_2^2 \\
\hat{y}_2 &= 13.92 - 1.75x_1 - 4x_2 + 0.25x_3 + 0.385x_1^2 + 0.75x_1x_2 + 0.25x_1x_3 + 0.885x_2^2 \\
\hat{y}_3 &= 279.29 + 37x_1 + 82.375x_2 - 5.125x_3 + 12x_1x_2 + 3.09x_3^2 \\
\hat{y}_4 &= 0.786 - 0.013x_1 + 0.06x_2 + 0.004x_1^2 + 0.014x_2^2
\end{aligned}$$

The same second order regression model was assumed for each response, although some of the parameters were found insignificant and zeroed. Individual inspection of the residuals did not indicate deviations from normality. Small discrepancies observed between RMSE and PRESS RMSE values indicate that models

can be used for prediction. Interested readers may refer to Raghunathan (2000) for an extensive discussion on model checking for multivariate normality of simulated responses in a Bayesian fashion. Chiao and Hamada (2001) used Mahalonobis distance to check for the multivariate normality for the replicated experiments case. Mecklin and Mundform (2005) compared performance of several multivariate normality tests using a Monte Carlo simulation.

For desirability function transformations, initial bounds on responses can be determined based on the physical range of the response or by subjective judgments. In this example STB type responses were individually minimized to determine the lower limits, and LTB type response functions were maximized to determine the upper limits subject to experimental region constraint ($-1 \leq \mathbf{x} \leq 1$). MATLAB's "fmincon" routine is used as an optimization tool. Shape parameter is assumed equal to 1 for all responses. The resulting desirability functions are depicted in Figure 4.2. Wurl and Albin (1999) give an excellent discussion for parameter selection for different multiresponse optimization techniques. Their results showed that different parameters may result different optimum solutions also depending on the optimization technique used.

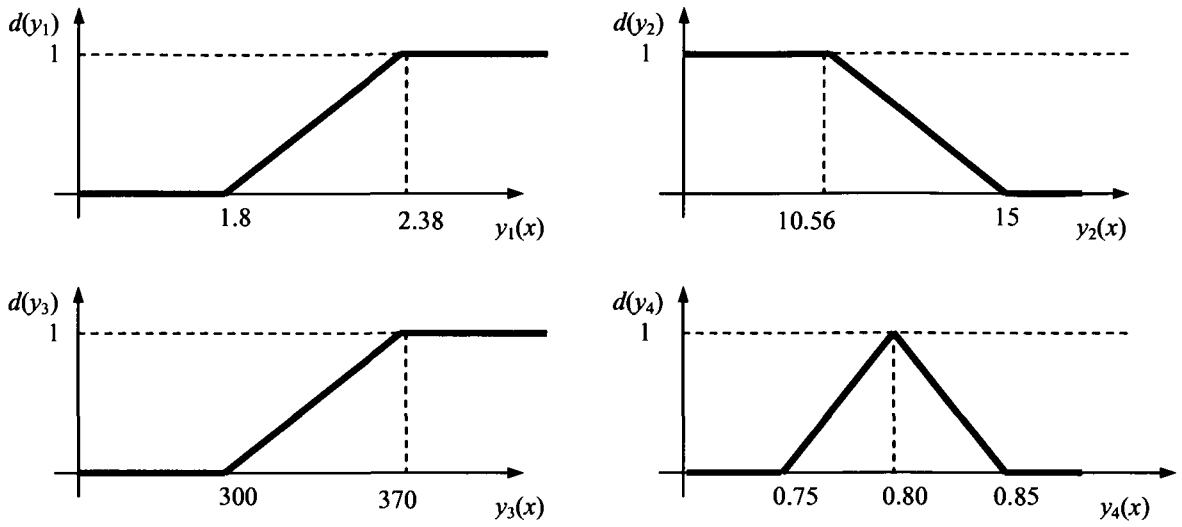


Figure 4.2 Desirability Function Graphs for the Responses for HPLC Example

4.5.2 SIMULATION AND OPTIMIZATION

It is now possible to generate response data for the design settings that were not included in the original design. First we need to estimate the residual covariance matrix in (4.3):

$$\hat{\Sigma}_{\varepsilon} = \frac{1}{n-p}(\boldsymbol{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^{T}(\boldsymbol{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})$$

$$= \begin{bmatrix} .0006 & .0029 & .0132 & 0 \\ & .1346 & .3370 & .0001 \\ & & 2.3423 & -.0022 \\ & & & 0 \end{bmatrix}.$$

Then, using (4.4) it is possible to generate response data conditional on the design settings. Note that these estimations are only valid within the experimental region of interest. Response functions nor the meta-model would not work outside the initial input factors' boundaries ($-\mathbf{1} \le \mathbf{x} \le \mathbf{1}$).

In order to get an estimate for conformance probability $p(x)$ conditional on design settings, a moderate size grid should first be built for controllable factors. Each controllable factor is represented at 11 levels {−1, −.8, −.6, −.4, −.2, 0, .2, .4, .6, .8, 1} totaling $11^2 = 121$ design settings. 5000 simulations were performed for each setting in the design grid and MATLAB code used in the simulation as can be seen in Appendix B.

In order to interpolate between grid points, a fourth order polynomial logistic regression model was fit to the simulated $p(x)$ values using MATLAB's "regress" multiple linear regression command. Since probability value changes between 0-1, a logistic regression transformation is applied to $p(x)$ values:

$$\log\left(\frac{p(x)}{1-p(x)}\right) = f(x) \tag{4.9}$$

where $f(x)$ consist of regression coefficients. The fitted model is given by the following equation:

$$\begin{aligned} f(x) = &-11.45 + 53.61x_2 - 1.91x_3 - 1.62x_2x_3 + 2.73x_2^2 + 2.84x_3^2 + 12.21x_2^2x_3 \\ &-8.75x_2x_3^2 + 6.02x_2^2x_3^2 - 125.3x_2^3 - 0.35x_3^3 - 8.88x_2^3x_3 + 0.59x_2x_3^3 \\ &+78.58x_2^4 - 0.08x_3^4 \end{aligned} \tag{4.10}$$

with $R^2 = 0.9925$ and $p < 0.00005$. In order to use above model for predicting conformance probability for different settings, Equation (4.10) must be transformed as:

$$\hat{p}(x) = \frac{1}{1-e^{-f(x)}}. \tag{4.11}$$

Our problem now reduces to:

$$\begin{aligned} &\max \hat{p}(x) \\ &s.t. \quad -1 \le x \le 1 \end{aligned}. \tag{4.12}$$

Since there are only two dependent variables, conformance probability can be depicted graphically. Figure 4.3 and Figure 4.4 show the surface and contour plots of

$\hat{p}(x)$ dependent on x_2 (pH) and x_3 (temperature) respectively. It can also be seen from the graph that conformance probability is insensitive to the changes in x_3, and the optimum is located around $x_2 = [0.4, 0.6]$. Therefore, $x_2 = [-1, 0]$ points were excluded from the grid and the remaining points were used while fitting regression functions.

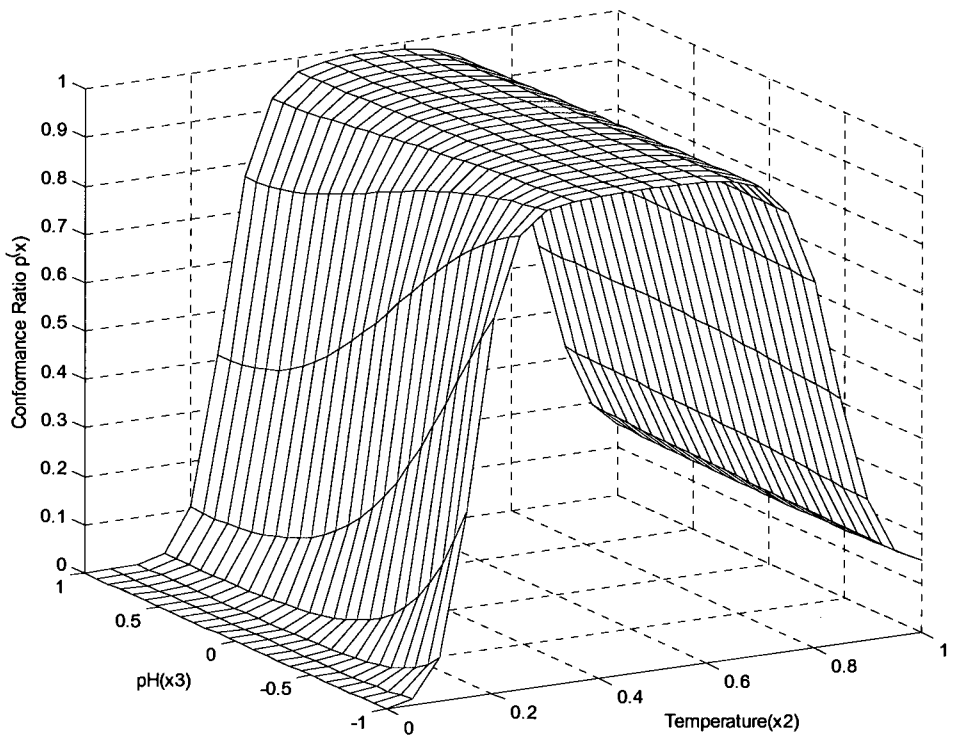


Figure 4.3 Surface Plot of $\hat{p}(x)$ Found by Logistic Regression Function

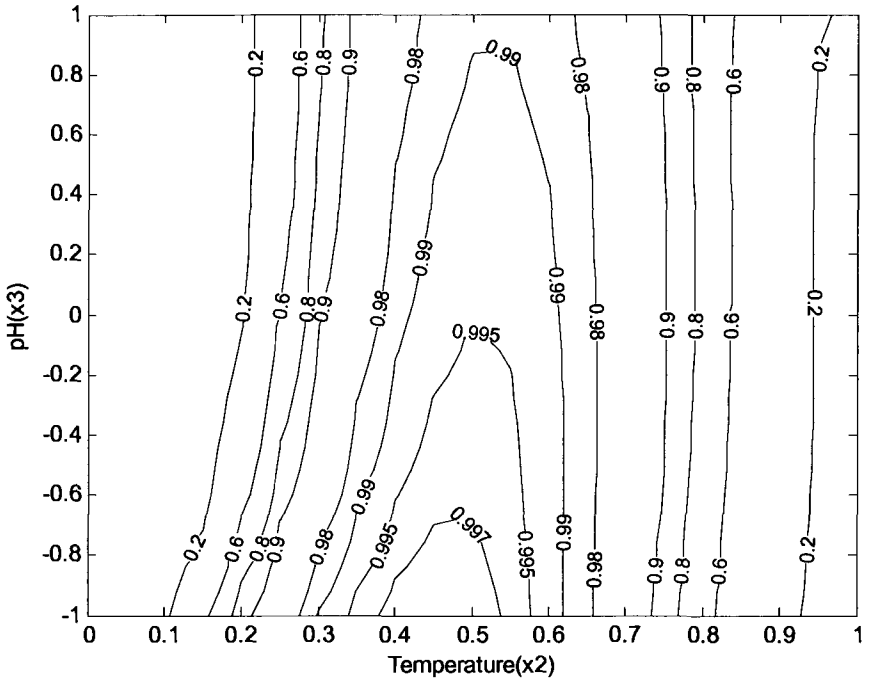


Figure 4.4 Contour Plot of $\hat{p}(x)$ Found by Logistic Regression Function

An important point worth mentioning here is that conformance probability is "bathtub U-shaped" and is too high as one can assume that the product will be of superior quality with the optimum settings. However, conformance probability does not carry any information on the degree of satisfaction and assumes highly desirable points will be included in the solution obtained. Therefore, the search for highly desirable points will stop when the maximum conformance probability achieved and it lacks the incentive to move towards the more highly desirable points.

In order to check the assumption that high conformance provide high desirability the penalized desirability metric $PD(\boldsymbol{x})$ must be calculated as in (4.8), for the same simulated responses and fit another regression model for it. As the meta-model for

conformance probability, the meta-model for $PD(\boldsymbol{x})$ metric is of the fourth order and is obtained via the ordinary least square approach:

$$\begin{aligned}\widehat{PD}(x) = &-0.33 + 1.62x_2 - 0.246x_3 + 0.754x_2x_3 + 3.5x_2^2 + 0.156x_3^2 - 0.895x_2^2x_3 \\ &- 0.329x_2x_3^2 + 0.198x_2^2x_3^2 - 9.266x_2^3 - 0.016x_3^3 + 0.39x_2^3x_3 - 0.02x_2x_3^3 \\ &+ 4.52x_2^4 - 0.02x_3^4\end{aligned}$$

with $R^2 = 0.994$ and $p < 0.00005$. Figure 4.5 and Figure 4.6 show the surface plot of the $\widehat{PD}(\boldsymbol{x})$ dependent on x_2 (pH) and x_3 (temperature) respectively. Although it may seem similar to graph of $\hat{p}(x)$ in Figure 4.5, the saddle shape can be distinguished, more specifically tilted, towards two extremes of the x_3 variable. The plot of $\hat{p}(x)$ has a larger flat surface or is "bathtub U-shaped" at the peak revealing that specifications are attainable for several design points. On the other hand, the plot of $\widehat{PD}(x)$ has a ridge type peak which is indicative of a narrow optimal region. This relationship is depicted more eloquently in Figure 4.7. For small values of $P(x)$, an almost absolute linear relationship exists between two simulated metrics. For large values of $P(x)$ however, dispersion of the $PD(x)$ metric increases and it is possible to obtain different $PD(x)$ values for different design points which have the same $P(x)$ values, and vice versa. Therefore it is important to differentiate among these points to move towards highly desirable and highly reliable points at the same time.

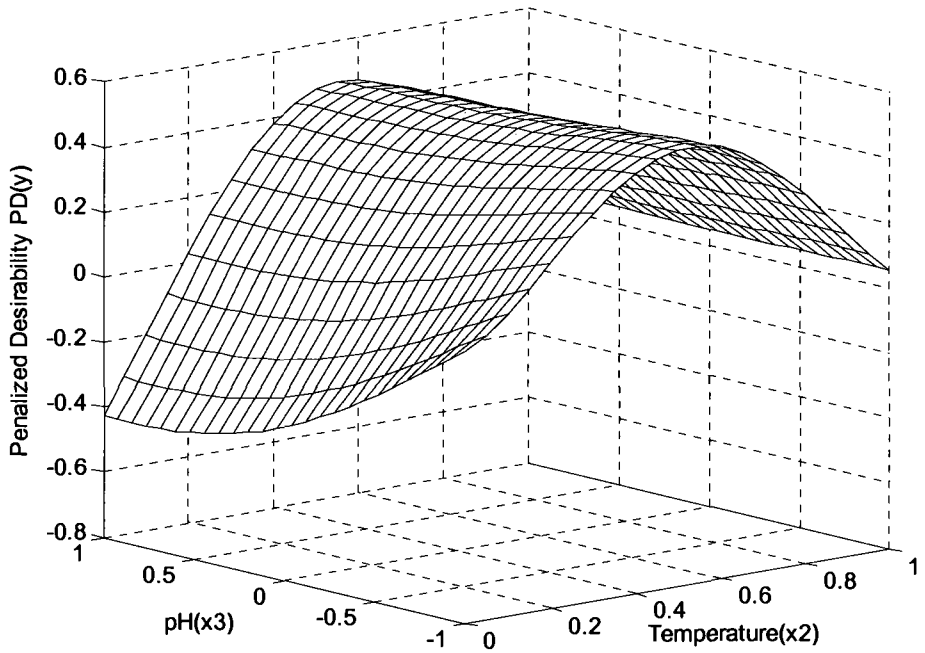


Figure 4.5 Surface Plot of $\widehat{PD}(x)$ Found by a Fourth Order Regression Function

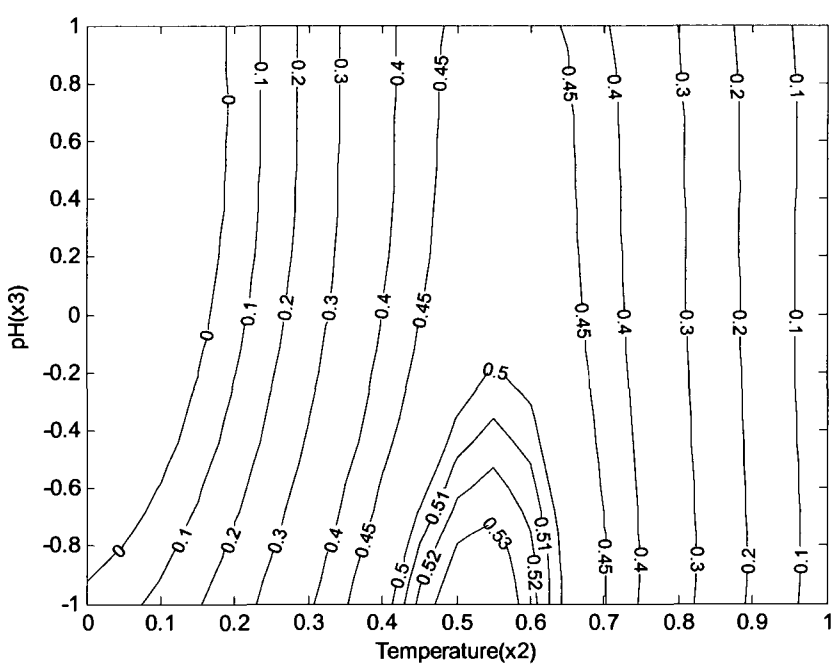


Figure 4.6 Contour Plot of $\widehat{PD}(x)$ Found by a Fourth Order Regression Function

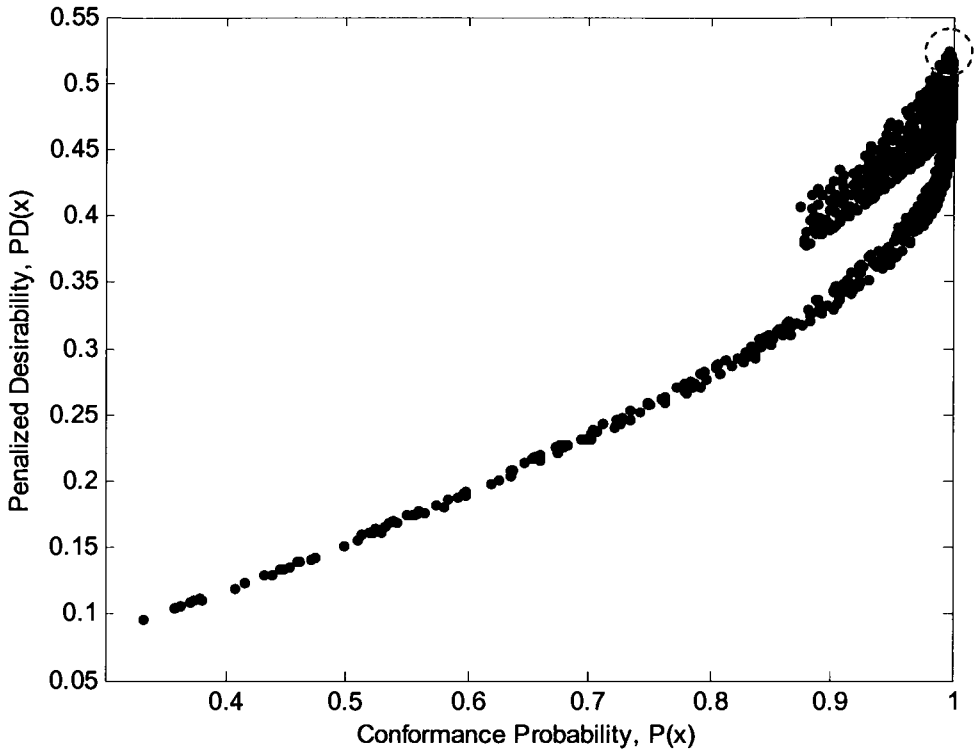


Figure 4.7 Scatter Diagram of Simulated *P*(*x*) and *PD*(*x*) values

The fitted responses are highly nonlinear and MATLAB's "fmincon" routine was used for the optimization with different starting points. Table 4.1 shows the optimization results obtained by two different meta-models. In the first column of Table 4.1, we see two optimum operating conditions, x_1* found by the conformance probability $\hat{p}(x)$ metric, and x_2* found by the integrated approach, the $\widehat{PD}(x)$ metric. Column 2 shows the conformance probability and Column 3 shows the penalized desirability value at each optimum point. As a validation, the third and fourth columns give the estimates of each metric obtained from 100,000 Monte Carlo samples (denoted by $\bar{p}(x)$ and $\overline{PD}(x)$). The

standard error, which is given in the last column and estimated by $\hat{\sigma}_{\hat{p}(x)} = \sqrt{\overline{p}(1-\overline{p})/100,000}$, indicates that the differences are significant.

Table 4.1 Optimal Solutions Found by Meta-models

x^*	$\hat{p}(y \in S \mid x)$	$\widehat{PD}(x)$	$\overline{p}(y \in S \mid x)$	$\overline{PD}(x)$	$\hat{\sigma}_{\hat{p}(x)}$
x_1^* =[0.4549, –1]	0.9981	0.5252	0.9803	0.5068	0.0004
x_2^* =[0.5275, –1]	0.9974	0.5416	0.9762	0.5130	0.0005

As expected, each meta-model produced different but very close optimal operating conditions and the function evaluations at the optima are very close. Each method favors its own metric in the optimization process. However, while x_1* gives slightly better ($(0.9803-0.9762)/0.9762 \cong 0.42\%$) conformance probability, x_2* gives a lot better ($(0.5130-0.5068)/0.5068 \cong 1.21\%$) desirability. This result showed that when both metrics are considered only Pareto optimums are possible and relying solely on the $p(x)$ metric in the optimization can give biased solutions with respect to response means.

As mentioned in Section 4.3, using a meta-model in the optimization has several disadvantages and as another alternative exploring a solution space using direct simulation is desirable. First x_2 was constrained to the [0.25, 0.75] interval and created a finer grid. MATLAB's "mbcmodel" tool with "Halton Sequence" is used as a space filling design type in order to sample from the remaining constrained region. 1,000 design points were generated and 5,000 screening simulations were performed at each setting. The best solutions were selected with respect to both metrics and performed 100,000 validation runs. Results are shown in Table 4.2.

Table 4.2 Optimal Solutions Found by Direct Simulation

x^*	$\hat{p}(y \in S \mid x)$	$\widehat{PD}(x)$	$\overline{p}(y \in S \mid x)$	$\overline{PD}(x)$	$\hat{\sigma}_{\hat{p}(x)}$
x_3^* =[0.4351, –0.8128]	0.9973	0.5025	0.9816	0.4899	0.0004
x_4^* =[0.5195, –0.9918]	0.9975	0.5406	0.9769	0.5127	0.0005

In the first column of Table 4.2, we see the best operating conditions obtained according to both metrics with direct simulation. x_3* and x_4* represents the best operating conditions according to conformance probability and the penalized desirability metric, respectively. The results are parallel and similar to those obtained via the meta-model approach. When the validation runs were checked, the average conformance probability achieved was slightly greater than that obtained via the meta-model approach ((0.9816-0.9803)/0.9803 = 0.013%), and the average $PD(x)$ value was slightly less than that obtained via the meta-model approach ((0.5127 – 0.5130) / 0.5130 = 0.05%), a formal hypothesis on the equality of proportions obtained by either methods could not be rejected at α = 0.01 level. Here, the results are dependent on the grid size used in the simulation. Considering available computer power, it is believed that even for controllable factors larger than two using a constrained and possibly finer grid in the simulation is the simpler optimization strategy. Therefore a direct simulation strategy is recommended with the proposed approach and will be applied as an optimization method for the examples in the rest of the study.

There is supportive evidence to reject the hypothesis in (3.9). However, for a multiresponse problem, optimal operating condition is the function of experimental design, number of controllable factors, number of responses, and number of experimental

runs used in the study. Therefore in order to generalize these results, in the next section the methodology is applied to several examples from published literature.

As a byproduct of this simulation, it is possible to estimate the individual response values and associated desirability values. The vectors of expected responses at optimality given by each method are:

$$\hat{Y}(x_1^*) = \begin{bmatrix} 2.09 \\ 12.04 \\ 324.97 \\ 0.82 \end{bmatrix}, \quad \hat{Y}(x_2^*) = \begin{bmatrix} 2.07 \\ 11.81 \\ 330.95 \\ 0.82 \end{bmatrix},$$

in desirability units:

$$d(\hat{Y}(x_1^*)) = \begin{bmatrix} 0.51 \\ 0.67 \\ 0.36 \\ 0.67 \end{bmatrix}, \quad d(\hat{Y}(x_2^*)) = \begin{bmatrix} 0.48 \\ 0.72 \\ 0.44 \\ 0.56 \end{bmatrix}.$$

Note that x_2* gives a better balance among responses in the sense that relatively smaller differences are observed among mean response values. In general, the difference between maximum and minimum desirability values is expected to be smaller in the $PD(x)$ metric. Assuming each response has the same importance from the DM perspective, x_2* would be preferable. Therefore, the first example showed that the methodology is very promising while satisfying statistical properties such as correlation, robustness, and parameter uncertainty but also giving higher desirability for mean responses overall.

4.5.3 PROGRESSIVE ARTICULATION OF DM'S PREFERENCE INFORMATION

As an example of progressive articulation of DM preferences; a third response may be found unsatisfactory and may need further improvement. Tightening and relaxing are the two basic strategies that can be considered. Specifically, either of the following options can be applied as the tightening strategy:

- Because it is an LTB type response, its lower bound can be increased by an amount of Δ in order to push it to higher expected response values, as depicted in Figure 4.8.

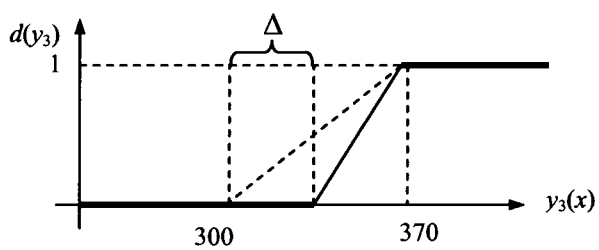


Figure 4.8 Bound Adjustment for Tightening Strategy for HPLC Example

For example, lets assume a DM is convinced that $\Delta = 20$ and a new lower limit for y_3 is 320. When the optimization problem was resolved by using the direct simulation approach, the new best solution according to the $PD(x)$ metric and respective performance metric values are shown in Table 4.3. Note that these values are calculated according to initial lower bound of y_3.

Table 4.3 New Best Solution After Bound Adjustment

x^*	$\hat{p}(y \in S \mid x)$	$\widehat{PD}(x)$	$\overline{p}(y \in S \mid x)$	$\overline{PD}(x)$
x^* =[0.6329, – 0.9924]	0.9886	0.5072	0.9570	0.4561

The vector of expected responses at new optimum point is:

$$\hat{Y}(x^*) = \begin{bmatrix} 2.05 \\ 11.50 \\ 339.55 \\ 0.83 \end{bmatrix},$$

in desirability units:

$$d(\hat{Y}(x^*)) = \begin{bmatrix} 0.43 \\ 0.79 \\ 0.57 \\ 0.40 \end{bmatrix},$$

As you notice, a significant improvement is obtained in y_3.

- Shape parameter can be chosen as $s_3>1$ in order to reward higher desirability values respectively (Figure 4.9).

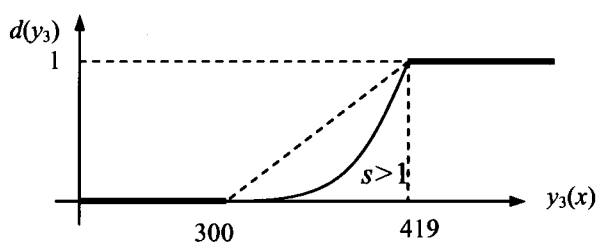


Figure 4.9 Shape Adjustment for Tightening Strategy for HPLC Example

Relaxing strategy might be more costly since the other three responses other than y_3 should be considered simultaneously in the articulation process. Note that either strategy requires sacrifices from other responses, which may result smaller $d(\hat{y}_i)$ values in the new optimum solution for the rest of the responses.

4.6 PROPOSED APPROACH SUMMARY

In this section, a proposed integrated probability-based approach has been formalized to apply unreplicated multiresponse experiments. Two different optimization strategies are also discussed, namely meta-model and direct simulation using a finer grid, which can be used with the proposed method. A constrained direct simulation strategy is empirically shown to have an easier applicability over the meta-model approach. The applicability of the proposed method is shown with an example and the initial results showed that the proposed approach produces satisfactory points with respect to conformance ratio and better results with respect to response targets. In Figure 4.10, a flowchart summarizing the basic steps of the proposed approach is presented.

The improvements obtained by using the proposed method are dependent on the size of the grid used in the simulation, the experimental design, the number of controllable factors, and the number and type of the responses used in the study. Therefore, in order to generalize results obtained by the proposed methodology, in the next chapter, several examples from published literature will be studied regarding these dependencies.

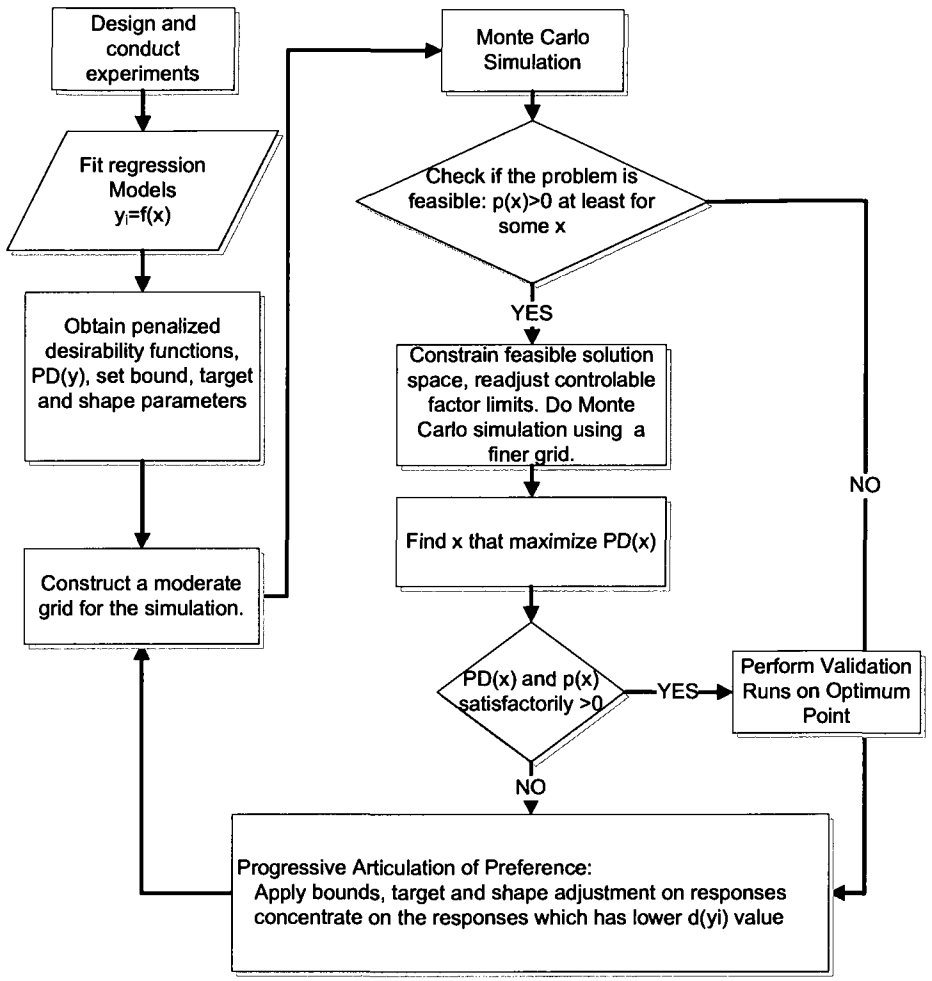


Figure 4.10 Basic Steps of the Proposed Approach

5 EVALUATION OF THE INTEGRATED PROBABILITY-BASED APPROACH

5.1 TEST CASES

In order to compare our methodology, five different test data sets were selected from published literature on MRSM, varying according to number of controllable factors, response types and number of runs. All the designs allow standard second order models which can model pure quadratic effects and two-way interactions. Table 5.1 summarizes the data sets sorted according to number of runs which is also a function of number of controllable factors. While the first and second cases have only LTB type responses, the rest of the cases have mixed type responses. The second and fourth cases have noise variables to show the applicability in a robust case.

Table 5.1 Summary of the Test Data Sets Used in the Study

Test Data	Type of Design	Number of Cont. Factors (+Noise Var.)	Number of Responses	Response Types	Number of Runs
1. Schmidt (1979)	CCD with 5 center points	2	4	LTB(4)	13
2. Quesada (2004)	Box–Behnken with 3 center points	2+1	4	STB(1), LTB(2), NTB(1)	15
3. Derringer and Suich (1980)	CCD with 6 center points	3	4	LTB(2), NTB(2)	20
4. Romano (2004)	CCD with 3 center points	3+2	2	NTB(1), STB(1)	25
5. Khuri and Conlon (1981)	CCD with 6 center points	5	4	LTB(4)	32

For all of the cases, controllable factors are coded between [-1, 1] and the response function parameters are estimated according to PRESS residuals provided in APPENDIX A. $R^2_{\text{Adj.}}$, $R^2_{\text{Prediction}}$ and PRESS RMSE values are also reported. Except the second responses in the third and fifth cases, the second order models are adequate for prediction. Since there is not any justification behind these poor fits, for the sake of illustration the data was retained and used the same quadratic models. In practice, however, poor prediction properties need to be resolved before further analysis is done.

For those cases where specification limits are not provided, STB type responses were individually minimized to determine the lower limits and maximized LTB type response functions to determine the upper limits, subject to experimental region constraint ($-\mathbf{1} \leq \mathbf{x} \leq \mathbf{1}$). These limits are used in conformance probability and penalized desirability calculations. Shape parameter is assumed equal to 1 for all responses.

For each data set in Table 5.1, after performing 5,000 screening simulations at 150 design points, some of the controllable factors are constrained and a finer grid is applied with the same number of simulations. A Latin Hypercube sampling is used as a space filling design in order to equally sample among the remaining constrained regions. Table 5.2 shows constrained factor limits in coded units and the number of design points used in the simulation.

Table 5.2 Constrained Factor Limits

Test Data	Constrained Factor Intervals	Number of Design Points
1. Schmidt (1979)	x1=[-0.7072, 0.7072], x2=[-1,1]	1000
2. Quesada (2004)	x2=[0.25 0.75], x3=[-1, 1]	1000
3. Derringer and Suich (1980)	x1=[-0.63, 0.63], x2=[-0.63, 0.7], x3=[-0.7, 0.7]	1500
4. Romano (2004)	x1=[0.25 1], x2=[-0.6 1], x3=[-1 1]	1000
5. Khuri and Conlon (1981)	x1=[-1,0.5], x2[-1,1], x3=[-0.5,1], x4=[-1,1], x5=[-1,1]	1500

The maximum conformance probability and penalized desirability settings are reported in Table 5.3. In the column, denoted by x^*, $x^*_{p(x)}$ is the best setting attained with the conformance ratio and $x^*_{PD(x)}$ is the best setting attained with the penalized desirability function. As a validation, the third and fourth columns give the estimates of each metric obtained from 100,000 Monte Carlo samples (denoted by $\overline{p}(x)$ and $\overline{PD}(x)$). Relative comparisons of each validation run with respect to $\overline{PD}(x)$ are also provided. For example for the first data set, the best setting obtained by $PD(x)$ metric produces 0.346% worse conformance probability but 2.061% better overall desirability than those obtained by $p(x)$ metric on the average. The standard error of simulation for the $\overline{p}(x)$ calculated using $\sqrt{(\overline{p}(x)(1-\overline{p}(x)))/100,000}$ formula and averaged $\overline{PD}(x)$ values have very similar standard errors for 100,000 samples.

Table 5.3 Comparison of Proposed Method at the Best Solution Obtained for Different Data Sets

Test Data	x^*	$\bar{p}(x)$	$\overline{PD}(x)$	$\bar{p}(x)\%$	$\overline{PD}(x)\%$	$\hat{\sigma}_{\bar{p}(x)}$
1. Schmidt (1979)	$x^*_{p(x)} = [0.0786, -0.4575]$	**0.9867**	0.6129	-0.346	2.061	0.0004
	$x^*_{PD(x)} = [-0.1635, -0.0831]$	0.9833	**0.6258**			0.0004
2. Quesada (2004)	$x^*_{p(x)} = [0.4351, -0.8128]$	**0.9816**	0.4899	-0.482	4.434	0.0004
	$x^*_{PD(x)} = [0.5195, -0.9918]$	0.9769	**0.5127**			0.0005
3. Derringer and Suich (1980)	$x^*_{p(x)} = [-0.3350, 0.3211, -0.5879]$	0.2944	0.1366	0.490	2.706	0.0014
	$x^*_{PD(x)} = [-0.1685, 0.3966, -0.6346]$	**0.2959**	**0.1404**			0.0014
4. Romano (2004)	$x^*_{p(x)} = [0.5345, 0.4074, -0.8919]$	**0.9877**	0.4491	-0.091	1.427	0.0003
	$x^*_{PD(x)} = [0.3686, 0.7021, -0.9499]$	0.9868	**0.4556**			0.0004
5. Khuri and Conlon (1981)	$x^*_{p(x)} = [0.0607, 0.3983, 0.1815, 0.2515, -0.9239]$	**0.9917**	0.4617	-1.734	17.495	0.0003
	$x^*_{PD(x)} = [-0.8069, -0.3169, 0.4837, 0.6891, 0.984]$	0.9748	**0,5596**			0.0005

As can be seen from Table 5.3, due to the small standard error in the validation runs, difference between estimated means for the $PD(\boldsymbol{x})$ metric is always significant. For the $p(\boldsymbol{x})$ metric however, for some data the $PD(\boldsymbol{x})$ metric provides very close conformance ratio and for the third data set it has even better conformance. A general observation, on the other hand, when the proposed approach is used in the optimization, relative improvement obtained in the overall desirability is always bigger than the relative reduction in conformance probability. This is because while calculating the *PD(x)* metric both the spread and the desirability of responses are considered. This conclusion can be

generalized to the robust case where noise variables are included (second and fourth data sets).

In order to visually inspect the relationship between the two metrics, histograms and scatter plots of simulated $p(\boldsymbol{x})$ and $PD(x)$ values of five test cases are depicted in Figure 5.1 through Figure 5.5. Except the 3rd test case in Figure 5.3 where low conformance and low desirability achieved, similar behavior is observed between simulated $p(\boldsymbol{x})$ and $PD(x)$ values. When the problem is tightly constrained however, a linear relationship is observed between the two metrics.

The fifth data set has a very unique characteristic which benefits and also highlights the advantages of the proposed method. For this particular data set, the conformance ratio achieved with the $p(\boldsymbol{x})$ metric is very high and all the responses are the LTB type. Note that the relative improvement achieved for the overall desirability with the $PD(\boldsymbol{x})$ metric is so large (17.495%) with respect to the relative degradation against the $p(\boldsymbol{x})$ metric (–1.734%). This result supports the idea that was explained in Section 3.7: when high conformance ratio is achieved, particularly for the problems where only single type and one-sided responses are included, optimization through the $p(\boldsymbol{x})$ metric prematurely stops the search procedure, and this can cause a bias in mean responses. On the other hand, the $PD(\boldsymbol{x})$ metric searches through more desirable and also low variance regions of the solution space, hence provide a better balance between these two performance measures.

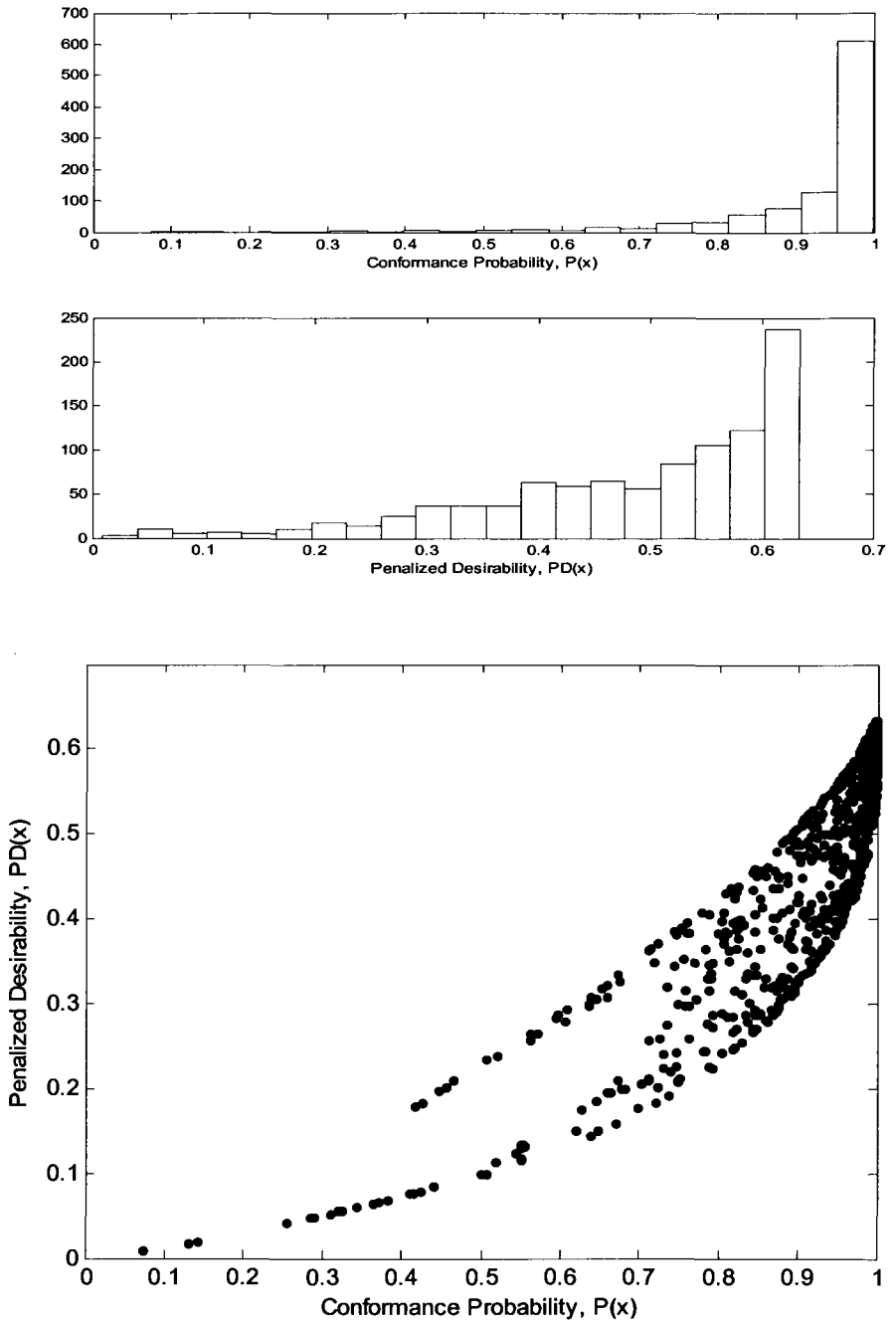


Figure 5.1 Histogram and Scatter Diagram of Simulated *P*(*x*) and *PD*(*x*) Values for Scmidt (1979) Data

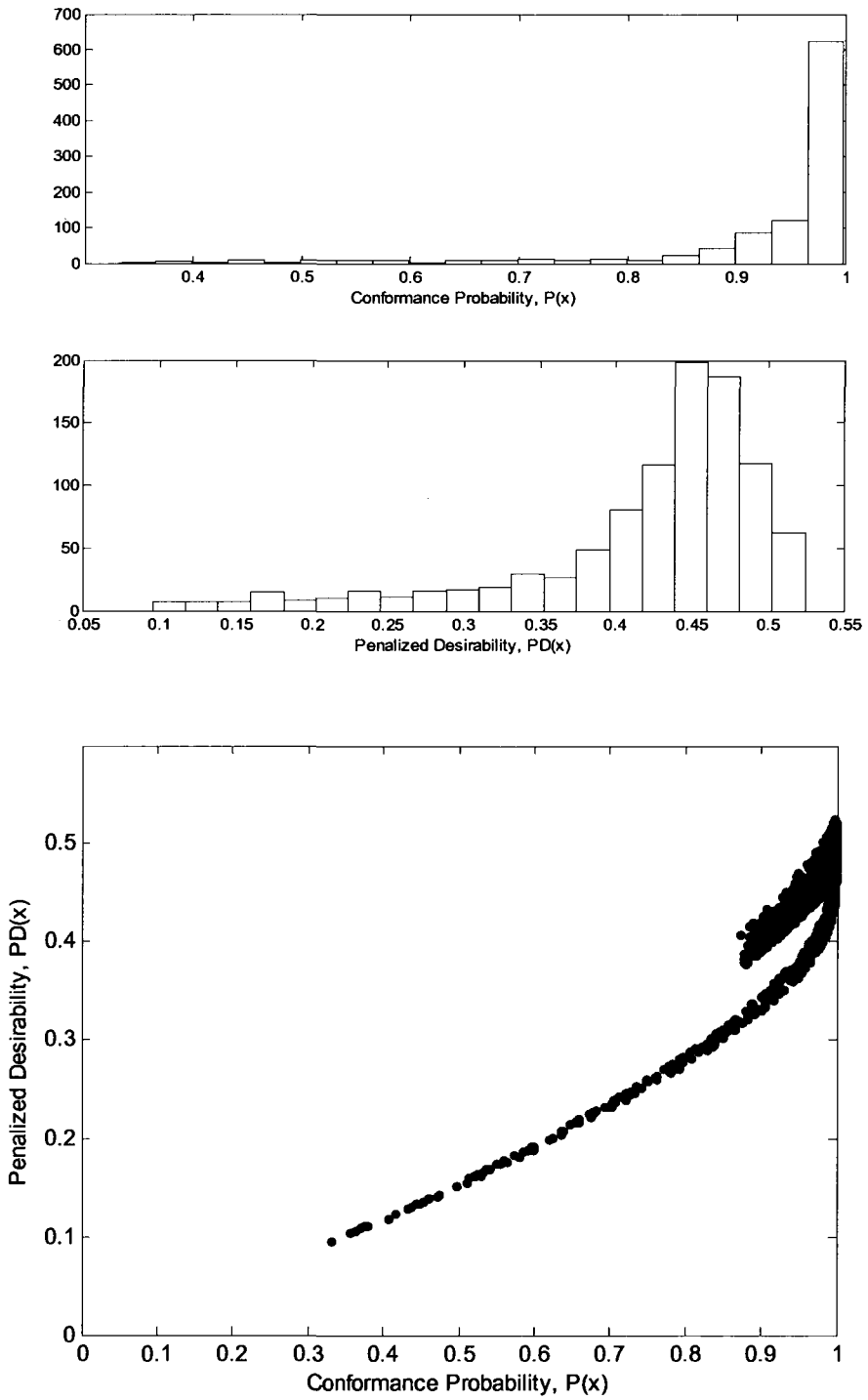


Figure 5.2 Histogram and Scatter Diagram of Simulated *P*(*x*) and *PD*(*x*) Values for Quesada (2004) Data

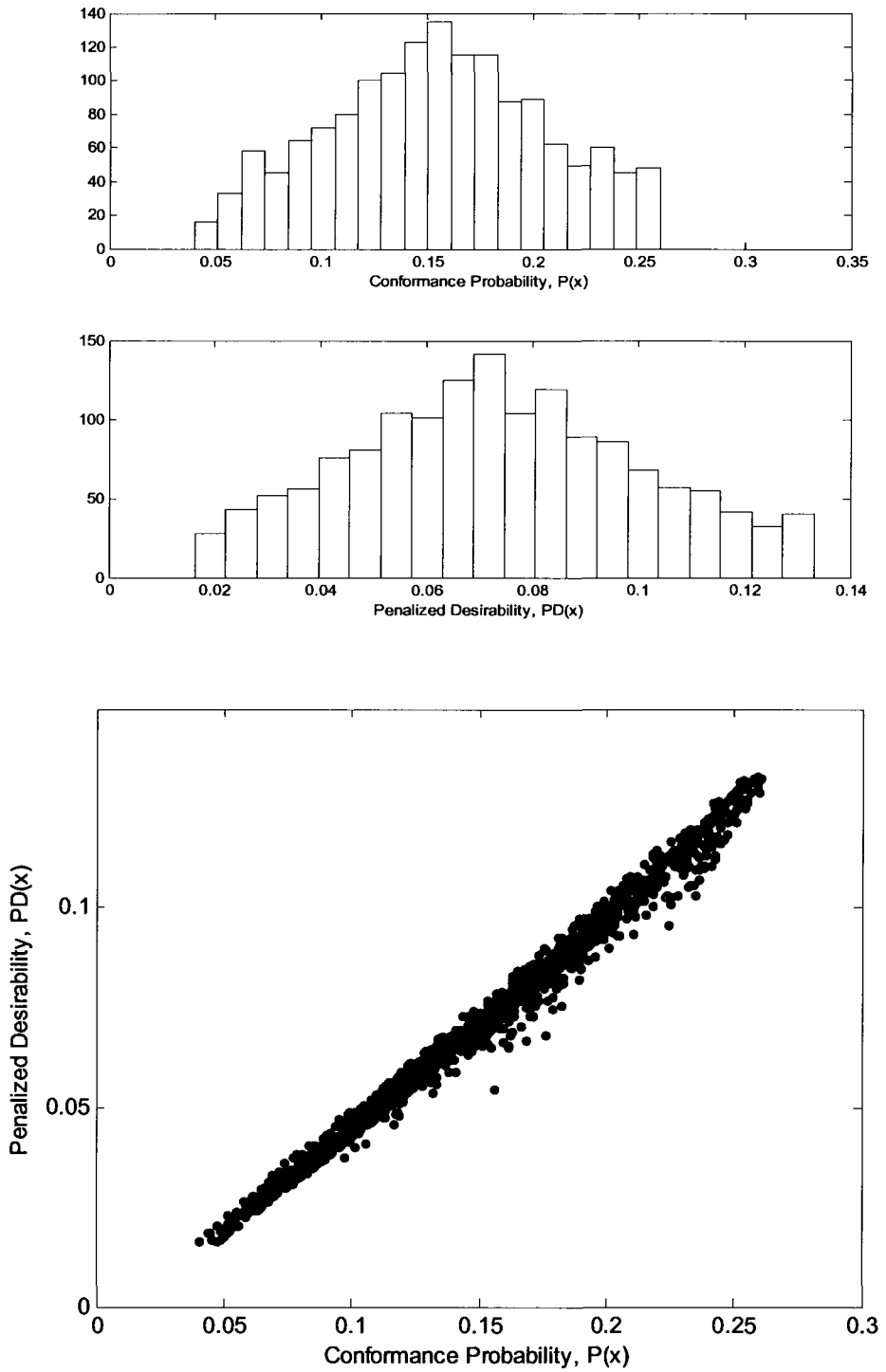


Figure 5.3 Histogram and Scatter Diagram of Simulated *P*(*x*) and *PD*(*x*) Values for Derringer and Suich (1980) Data

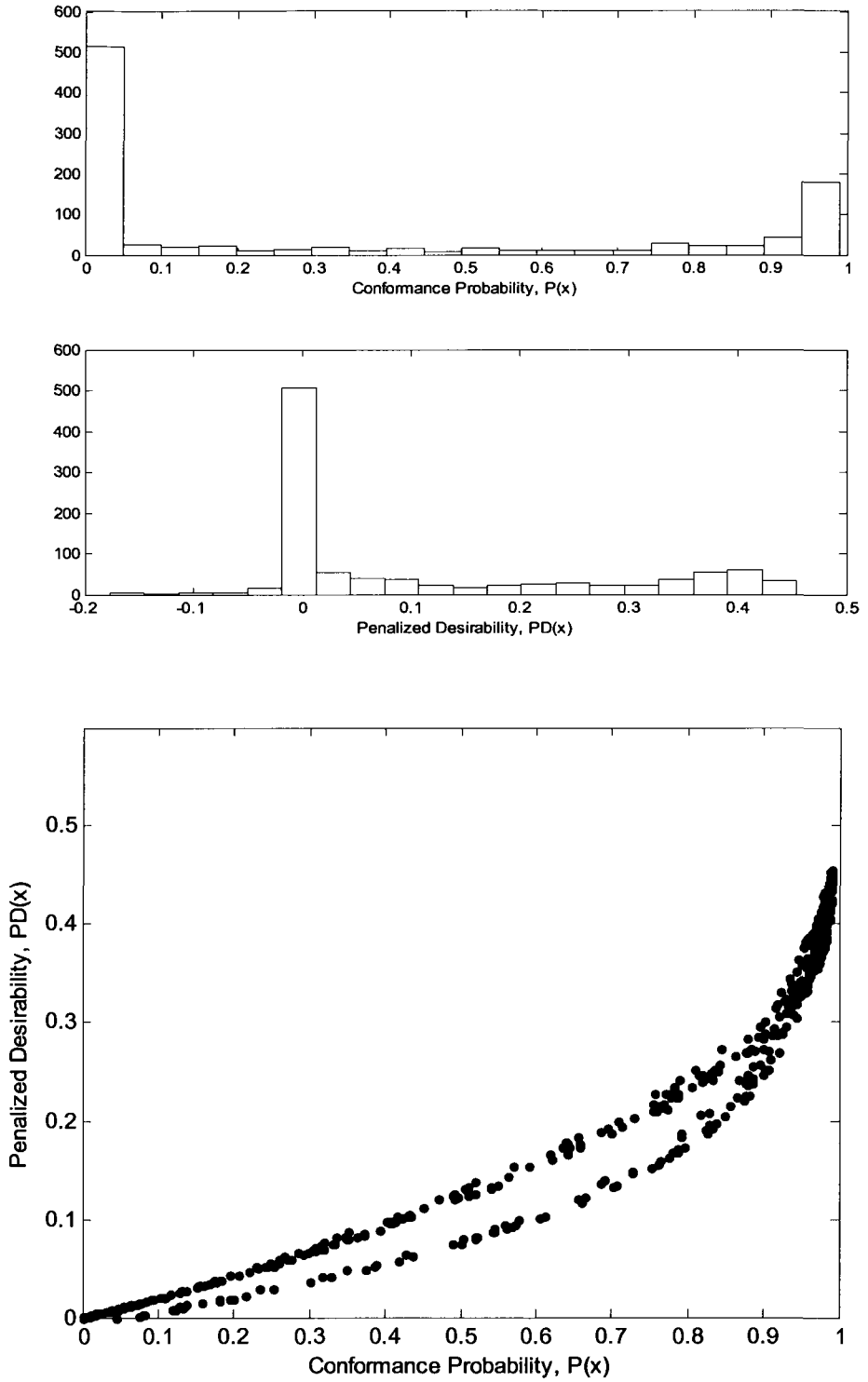


Figure 5.4 Histogram and Scatter Diagram of Simulated *P*(*x*) and *PD*(*x*) Values for Romano (2004) Data

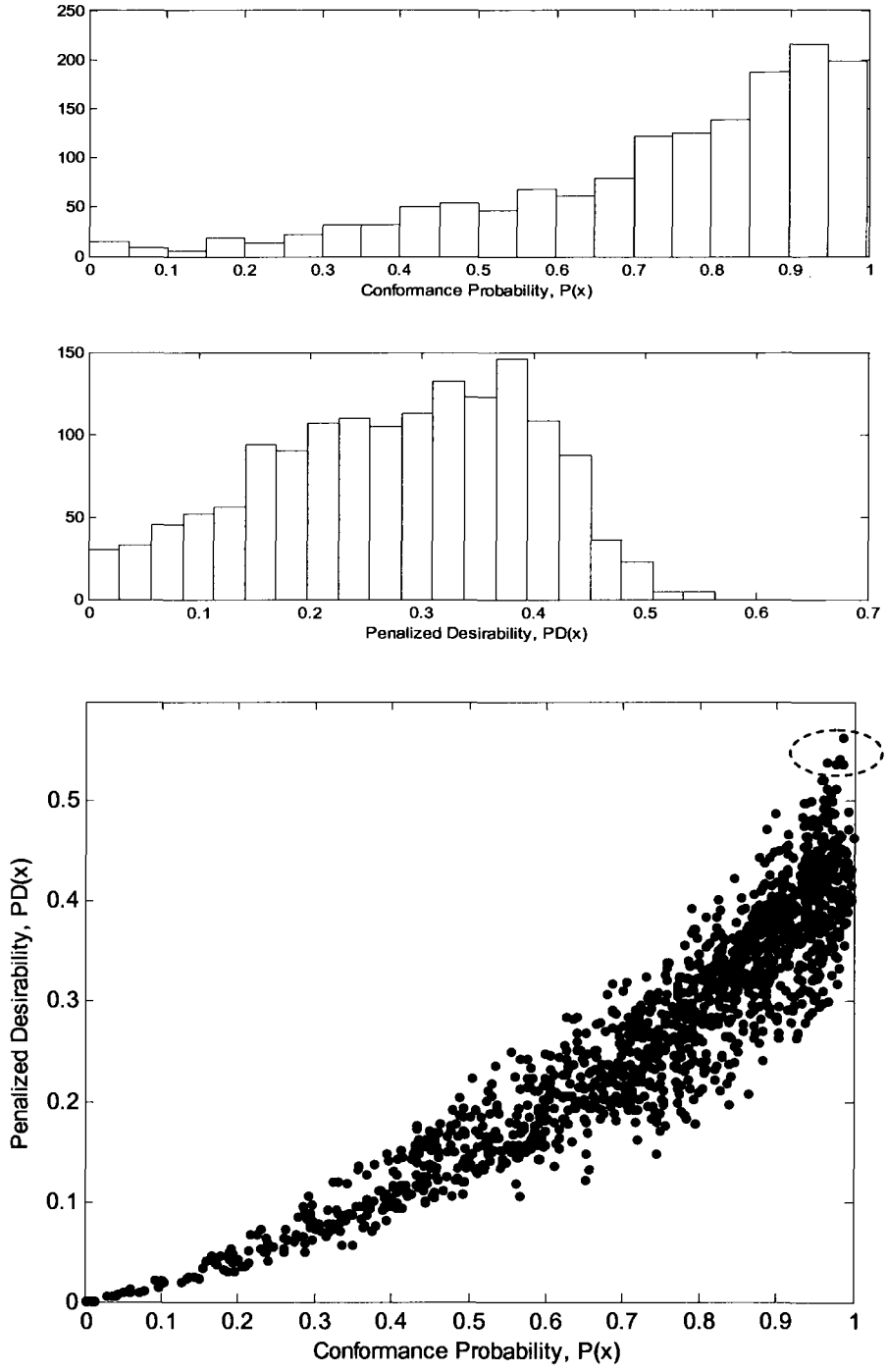


Figure 5.5 Histogram and Scatter Diagram of Simulated *P*(*x*) and *PD*(*x*) Values for Khuri and Conlon (1981) Data

For this example, because there are 5 input factors, it is not possible to visualize conformance probability or penalized desirability values dependent on all of the input factors at the same time. In Figure 5.5, histograms of simulated metrics for a 1500-point design grid shows that, while the maximum $P(x)$ value can be achieved by several design points, only a few points can give maximum the $PD\,(x)$ value. Again in Figure 5.5, the scatter diagram of two metrics shows that, although best design points with respect to $PD(x)$ metric provide almost maximum conformance ratio, the best design points with respect to $P(x)$ metric provide a vide range of the $PD(x)$ metric. Moreover, the two metrics are correlated and the relation is very similar to that in Figure 4.7.

This situation can be further exploited dependent on input factors. In Figure 5.6 through Figure 5.10, we see the distribution of simulated metrics for a 1500-point design grid, dependent on controllable factors. Because the other factors are not fixed at some point, the simulated values look disperse, however it gives an idea about the influence of controllable factors on both metrics. For example, while the $P(x)$ metric is slightly increasing towards $x_1 = 0$, the $PD(x)$ metric has distinctive maximum around $x_1 = -0.8$. These points are marked with an ellipsoid in the figures. Although the dispersion of the two metrics seem correlated, the locations of the best point changes for all of the input variables.

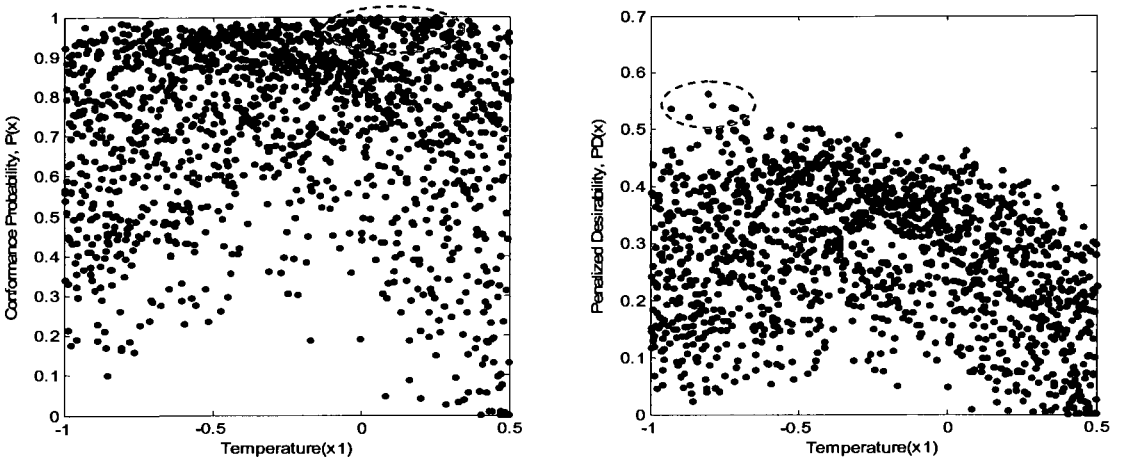


Figure 5.6 Distribution of $P(x)$ and $PD(x)$ Metrics with Respect to x_1

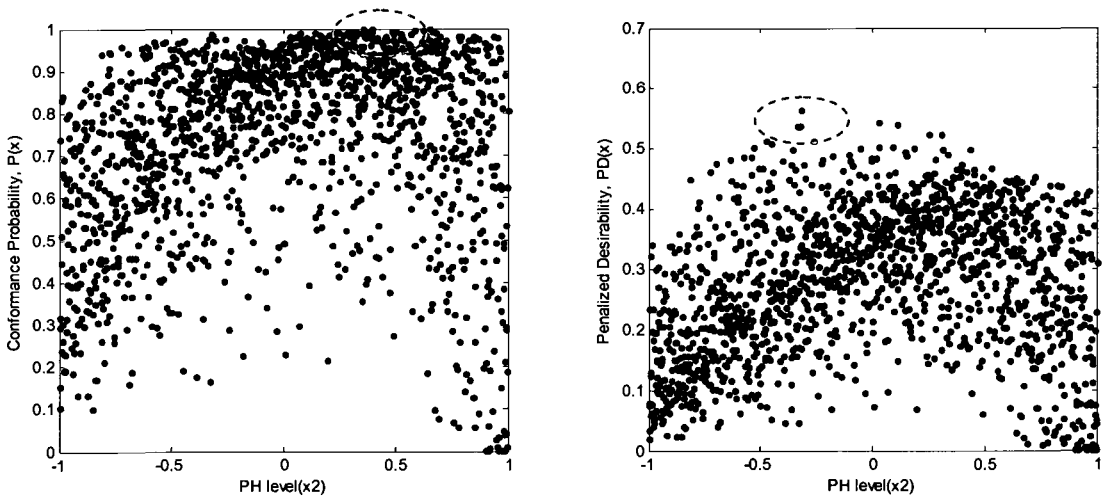


Figure 5.7 Distribution of $P(x)$ and $PD(x)$ Metrics with Respect to x_2

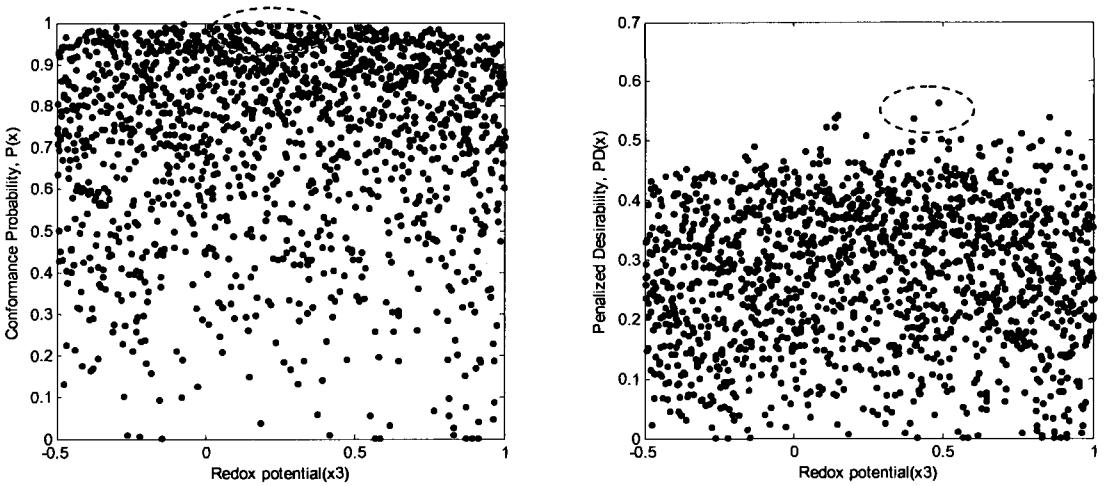


Figure 5.8 Distribution of $P(x)$ and $PD(x)$ Metrics with Respect to x_3

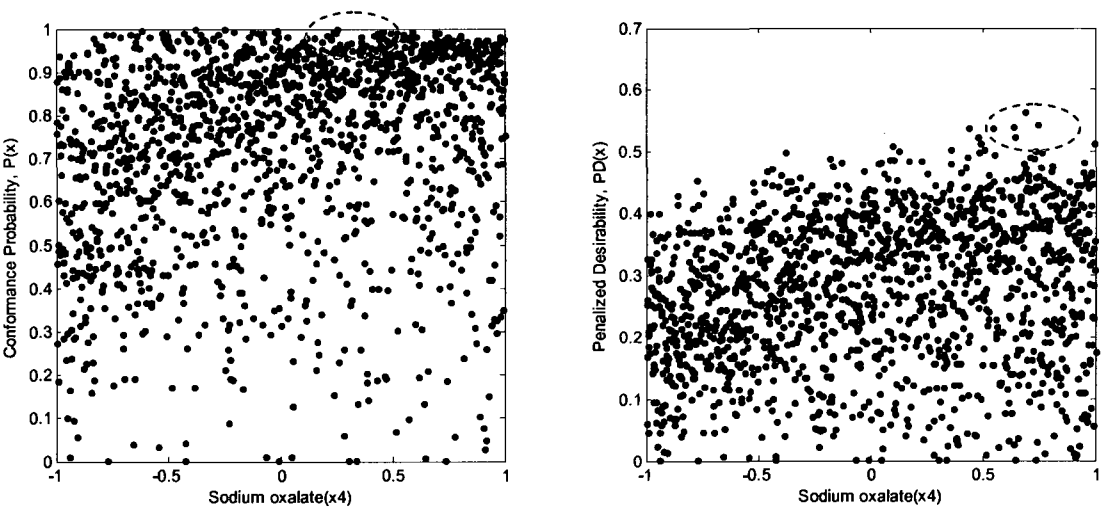


Figure 5.9 Distribution of $P(x)$ and $PD(x)$ Metrics with Respect to x_4

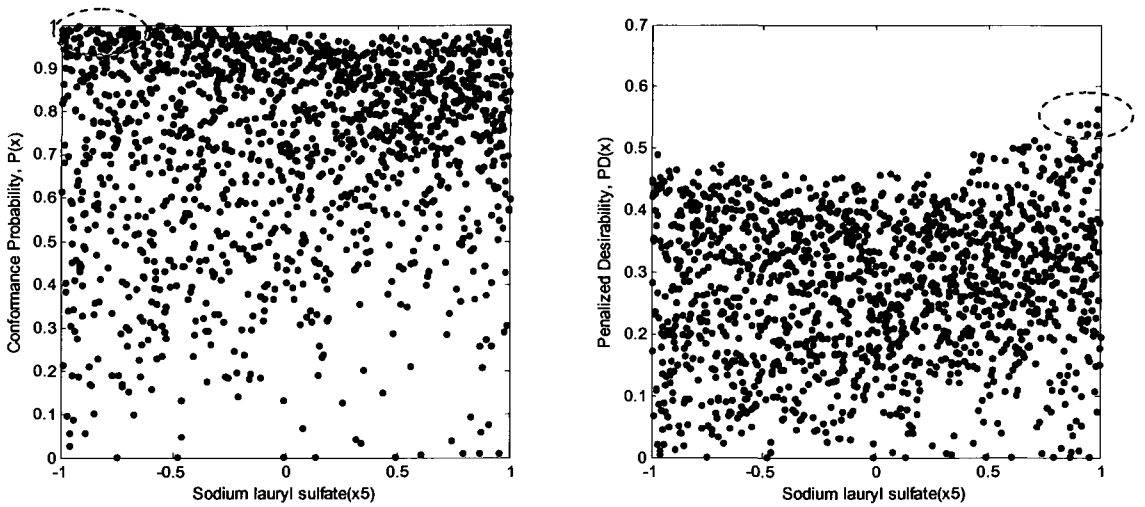


Figure 5.10 Distribution of $P(x)$ and $PD(x)$ Metrics with Respect to x_5

Notice that the first data set also has single type and one sided responses but the conformance probability is little farther than the conformance achieved with the fifth data set; this may be caused because relative differences between two metrics are not as far apart as the fifth data set.

Contrary to Quesada (2004), these results specifically show that the conformance ratio is not the ultimate methodology that ends the explicit trade-offs between mean and variance, therefore only Pareto optimums can be possible, and the proposed integrated approach maintains the balance between highly reliable and highly desirable points more efficiently. Since the second and fourth data sets include noise variables and have similar results in terms of relative performance values, the results can be generalized to the RPD problem, too. For the studied data sets, despite the fact that the $PD(x)$ metric provided relatively poor but reasonably good solution points in terms of conformance probability, it is recommended that $p(x)$ metric should be maintained and the DM must be informed about the reliability of the solutions obtained. Moreover, with the proposed approach,

reliability of each point in the grid can be estimated and for the problems where DMs like to behave risk aversely or where low variance solutions are preferred, a comprehensive set of nondominated solutions can help DMs find the best compromise solution.

As a byproduct of the simulation runs, individual desirability averages are also estimated and reported in Table 5.4. Since the overall desirability is the geometric mean of individual desirabilities, it always tries to maintain the balance among responses, in the sense that relatively smaller differences are observed when they are equally important to DM. For this particular data set, the best setting obtained by the $PD(\boldsymbol{x})$ gives greater desirability for the first three responses and only the fourth response's desirability is smaller. This explains why the overall desirability is a lot bigger than that obtained by the $p(\boldsymbol{x})$ metric.

Table 5.4 Individual Desirability Estimates at the Best Solution Obtained (Khuri and Conlon (1981)

Model Terms	$\bar{d}(y_1)$	$\bar{d}(y_2)$	$\bar{d}(y_3)$	$\bar{d}(y_4)$
$\boldsymbol{x}^*_{p(x)}$	0.4530	0.4123	0.4366	0.6778
$\boldsymbol{x}^*_{PD(x)}$	0.7852	0.4654	0.5856	0.6173

6 RESEARCH CONTRIBUTION AND FUTURE WORK

This chapter concludes the dissertation work. Section 6.1 summarizes the main contributions of the proposed methodology in the optimization of multiple responses. Section 6.2 defines some additional research directions for further study.

6.1 RESEARCH CONTRIBUTION

A procedure initially proposed by Peterson (2000) was extended to employ a penalized desirability metric in order to take full advantage of both probability-based and desirability approaches. A probability-based paradigm provides statistically sound approaches for MRSM that can handle correlation structure between responses and also incorporate parameter uncertainty of the response models. Peterson (2004) estimated the reliability of solutions found according to several MRSM methods and also showed that conformance ratio produces very reliable solutions. On the other hand, conformance probability does not consider mean response values and particularly for problems where only single type and one-sided responses included can converge to biased solutions.

Having utilized the advantages of probability-based and desirability approaches, the proposed approach provided better solutions in terms of response targets but also provided reliable solutions close to those obtained with conformance probability metric. Moreover, the proposed approach is superior not only in maintaining the balance between variation and desirability of responses but also meeting statistical requirements. It was shown that in addition to statistical considerations, like correlation and parameter

uncertainty, the proposed approach can handle different types of responses properly and allows progressive articulation of DMs to achieve compromising solutions efficiently.

An optimization process was proposed not necessarily giving the optimum solution but the best solution depending on the grid structure used in the simulation of multiple responses. There are two approaches that can be used in the optimization of penalized desirability metric, the first is meta-model approach and the other is a direct simulation approach. For controllable factor numbers greater than three, considering modeling and optimization issues, the direct simulation approach has easier applicability than the meta-model approach. With the available computer power it is not difficult to exploit design space with a possibly fine grid composed of different levels of controllable factors. Moreover these cases showed that the direct simulation process provides better solutions with respect to overall desirability and also conformance probability metrics.

6.2 FUTURE WORK

An integrated probability-based approach was proposed for the optimization of multiple responses and showed that this methodology works satisfactorily with five different data sets. However there is still room for further improvement to use this methodology efficiently.

It was assumed that users have advanced modeling capabilities, particularly for the simulation of multiple responses. The computer code provided in Appendix B is problem specific and needs modifications when the number of responses and input variables changes. This may pose problems regarding efficient use of this methodology. Therefore, a user friendly code should be developed both for the desirability transformations and also for simulations.

As another limitation to proposed approach, standard Monte Carlo methods that were used in the simulations produced a set of independent simulated values according to some prespecified distribution and these values may be too disperse, not allowing posterior analysis of the responses. MCMC methods on the other hand, produce chains in which each of the simulated values is mildly dependent on the preceding value (Gill, 2002). These are the sample values that can be used to describe the posterior distribution of interest and may well fit the multiresponse optimization problem. There are several MCMC methods developed so far like Gibbs sampler and Metropolis-Hasting (M-H) algorithm. WinBUGS (Bayesian inference using Gibbs sampling) software is open source and can be used to implement Gibbs sampling method. These techniques can be incorporated with the proposed approach to work within a user friendly computer code.

It is assumed that the noise variables are distributed normally with a zero mean and with a known constant variance. Therefore in the presence of noise variables, the assumption of normality and distribution parameters should be checked carefully before using the proposed methodology. That type of problem can be solved by prior experimentation to see the behavior of noise variables in effect.

The test cases exhibited here can be characterized as typical applications in manufacturing industries. However, the applicability of proposed approach is not limited to the manufacturing industry where a unique discipline is involved, such as biochemistry or food production with a relatively small number of responses. The significance of the proposed approach will be best understood when it is applied to decision making problems where interdisciplinary engineering approaches are required.

For example, in military air operations it is essential to have a high level of accessibility of aircraft and aircrew during battle conditions. Success of the operation can be

decomposed into several conflicting and correlated responses such as the number of missions accomplished, the number of maintenance actions performed, the cost of operation (fuel, ammunition, spares) and aircraft availability. These responses are related to several resources in the system like the number of repairmen, different repair schedules or sortie durations, and the type and the amount of ammunition being used. There are also noise variables like logistic delays and conflict duration, etc. Although it is hard or impossible to experiment with this type of problem, a simulation might be an alternative and the proposed approach can help DMs spend less time with the simulations and can help different stakeholders articulate their preferences with less compromise and can help them achieve robust operating conditions.

NOMENCLATURE

β	=	regression coefficients
c	=	penalization constant
k	=	number of input variables
l	=	lower specification limit of a response
m	=	number of responses
N	=	number of experimental runs
p	=	number of regression coefficients in the model
q	=	number of linearly dependent responses
r	=	number of linearly independent responses
s	=	shape parameter of a response
S	=	feasible region of multiple responses
T	=	target specification for a response
u	=	upper specification limit of a response
y	=	response function
$\hat{y}$	=	estimate of a response function
ε	=	unexplained variation in the response model
μ	=	response mean
$\mathbf{\Sigma}$	=	variance covariance matrix of multiple responses
$\mathbf{H}$	=	estimate of variance covariance matrix of $\hat{y}$
$\boldsymbol{\theta}$	=	response targets
STB	=	smaller the better type response
LTB	=	larger the better type response
NTB	=	nominal the best type response
$p(\hat{y}_i)$	=	desirability value of ith response
$p(\hat{y}_i)$	=	penalty component of ith response in case of infeasibility
$P(\boldsymbol{x}_i)$	=	overall penalty for the ith design setting
$p(\boldsymbol{x}_i)$	=	conformance probability of ith design setting

$\overline{p}(\boldsymbol{x}_i)$	=	conformance probability of ith design setting in the validation runs
$PD(\boldsymbol{x}_i)$	=	penalized desirability value of ith design setting
$\overline{PD}(\boldsymbol{x}_i)$	=	penalized desirability value of ith design setting in the validation runs

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APPENDIX A: TEST CASES

In this appendix, the details of the experimental data used in the dissertation are presented.

A.1 SCHMIDT (1979)

Schmidt (1979) studied the effects of cysteine (x_1) and calcium chloride (x_2) combinations on the textural and water-holding characteristics of dialyzed whey protein concentrates (WPC) gel systems. The texture characteristics are measured by hardness (y_1), cohesiveness (y_2), springiness (y_3), and compressible water (y_4). The first table gives the experimental design with coded input levels and response values and the second table gives estimated regression coefficients for the data.

x_1	x_2	y_1	y_2	y_3	y_4
-1	-1	2.48	0.55	1.95	0.22
1	-1	0.91	0.52	1.37	0.67
-1	1	0.71	0.67	1.74	0.57
1	1	0.41	0.36	1.20	0.69
-1.414	0	2.28	0.59	1.75	0.33
1.414	0	0.35	0.31	1.13	0.67
0	-1.414	2.14	0.54	1.68	0.42
0	1.414	0.78	0.51	1.51	0.57
0	0	1.50	0.66	1.80	0.44
0	0	1.66	0.66	1.79	0.50
0	0	1.48	0.66	1.79	0.50
0	0	1.41	0.66	1.77	0.43
0	0	1.58	0.66	1.73	0.47

Model Terms	y_1 (LTB)	y_2 (LTB)	y_3 (LTB)	y_4 (LTB)
Specifications	(.35, 3.178)	(.31, .685)	(1.13, 1.895)	(.22, .691)
Intercept	1.526	.66	1.776	.468
x_1	-.813	-.1301	-.353	.1858
x_2	-.7412	0	-.1097	.1029
x_1^2	-.341	-.1912	-.3122	.052
x_2^2	-.196	-.14	-.1572	.047
$x_1 x_2$	.635	-.116	0	-.165
RMSE	.20	.023	.047	.041
PRESS RMSE	.37	.037	0	0
R^2 Adj.	.9169	.9642	.9644	.9094
$R^2_{\text{Prediction}}$	.691	.898	.901	.741

A.2 QUESADA (2004)

Quesada (2004) studied the optimization of a high performance liquid chromatography (HPLC) system to detect mixtures of impurities. The performance of the assay was based upon four quantitative response variables: the critical resolution (y_1), total run time (y_2), signal-to-noise ratio of the last peak (y_3), and the tailing factor of the major peak (y_4). Three controllable factors affecting the HPLC assay were included: %IPA (x_1), temperature (x_2) and pH (x_3). The first table gives the experimental design with coded input levels and response values and second table gives estimated regression coefficients for the data.

x_1	x_2	x_3	y_1	y_2	y_3	y_4
-1	-1	0	2.14	22	172	0.76
-1	1	0	1.73	12	311	0.88
-1	0	-1	1.93	16	251	0.8
-1	0	1	1.95	16	241	0.8
0	0	0	2.17	14	278	0.79
0	1	-1	1.97	11	371	0.86
0	-1	1	2.38	19	194	0.74
0	1	1	1.98	11	360	0.86
0	-1	-1	2.37	18	204	0.74
0	0	0	2.2	14	280	0.78
1	0	1	2.42	13	314	0.78
1	-1	0	2.61	17	223	0.73
1	1	0	2.14	10	410	0.85
1	0	-1	2.42	12	324	0.78
0	0	0	2.2	14	281	0.79

Model Terms	y_1 (LTB)	y_2 (STB)	y_3 (LTB)	y_4 (NTB)
Specifications	(1.8, 2.38)	(10.56, 15)	(300, 370)	(.75, .8, .85)
Intercept	2.193	13.923	279.286	.786
x_1(*noise*)	.23	-1.75	37	-.013
x_2	-.21	-4	82.375	.06
x_3	0	.25	-5.125	0
x_1^2	-.0154	.385	0	.004
x_2^2	-.0204	.885	0	.014
x_3^2	0	0	3.089	0
$x_1 x_2$	0	.75	12	0
$x_1 x_3$	0	.25	0	0
RMSE	.019	.34	1.25	.0034
PRESS RMSE	.025	.554	1.88	.0041
R^2 Adj.	.9937	.9899	.9997	.9946
$R^2_{\text{Prediction}}$	.988	.971	.999	.992

A.3 DERRINGER AND SUICH (1980)

Derringer and Suich (1980) studied the effect of hydrated silica level (x_1), silane coupling agent level (x_2) and sulfur level (x_3) to improve the quality of tire tread compounds which are characterized by four properties. The properties to be optimized and constraint levels were as follows:

PICO Abrasion Index, y_1 $120 < y_1$

200% Modulus, y_2 $1000 < y_2$

Elongation at Break, y_3 $400 < y_3 < 600$

Hardness, y_4 $60 < y_4 < 75$

x_1	x_2	x_3	y_1	y_2	y_3	y_4
-1	-1	1	102	900	470	67.5
1	-1	-1	120	860	410	65
-1	1	-1	117	800	570	77.5
1	1	1	198	2294	240	74.5
-1	-1	-1	103	490	640	62.5
1	-1	1	132	1289	270	67
-1	1	1	132	1270	410	78
1	1	-1	139	1090	380	70
-1.633	0	0	102	770	590	76
1.633	0	0	154	1690	260	70
0	-1.633	0	96	700	520	63
0	1.633	0	163	1540	380	75
0	0	-1.633	116	2184	520	65
0	0	1.633	153	1784	290	71
0	0	0	133	1300	380	70
0	0	0	133	1300	380	68.5
0	0	0	140	1145	430	68
0	0	0	142	1090	430	68
0	0	0	145	1260	390	69
0	0	0	142	1344	390	70

Model Terms	y_1 (LTB)	y_2 (LTB)	y_3 (NTB)	y_4 (NTB)
Specifications	(120, 170)	(1000, 1300)	(400, 500,600)	(60, 67.5, 75)
Intercept	137.921	1412.89	400.7143	68.725
x_1	16.494	268.151	-99.6664	-1.410
x_2	17.881	246.503	-31.3964	4.320
x_3	10.907	0	-73.919	1.635
x_1^2	-3.897	-97.794	7.9018	1.575
x_2^2	-3.335	-139.044	0	0
x_3^2	0	0	0	0
$x_1 x_2$	5.125	0	8.75	-1.625
$x_1 x_3$	7.125	0	0	0
$x_2 x_3$	7.875	0	0	0
RMSE	5.621	370.611	18.709	1.137
PRESS RMSE	9.436	396.241	23.00	1.467
R^2 Adj.	.9467	.3772	.9709	.9359
$R^2_{\text{Prediction}}$	.842	.251	.954	.888

A.4 ROMANO (2004)

Romano (2004) studied material behavior of a force transducer. The design of the element is intended to minimize the transducer's inaccuracy, which originates from two major sources, namely non-linearity (y_1) and hysteresis (y_2). Control factors are the three parameters defining the element configuration, lozenge angle (x_1), bore diameter (x_2) and half-length of the vertical segment (x_3). On a force transducer noise factors are the deviation of the lozenge angle from its nominal value (x_4) and the deviation of the bore diameter from its nominal value (x_5)

x_1	x_2	x_3	x_4	x_5	y_1	y_2
-1	-1	-1	-1	1	1.81	1.10
-1	-1	-1	1	-1	1.69	1.11
-1	-1	1	-1	-1	1.90	1.07
-1	-1	1	1	1	1.78	1.07
-1	1	-1	-1	-1	1.80	1.47
-1	1	-1	1	1	1.63	1.18
-1	1	1	-1	1	1.92	1.41
-1	1	1	1	-1	1.78	1.58
1	-1	-1	-1	-1	1.36	1.57
1	-1	-1	1	1	1.22	2.03
1	-1	1	-1	1	1.48	1.38
1	-1	1	1	-1	1.44	1.68
1	1	-1	-1	1	0.693	3.37
1	1	-1	1	-1	0.616	3.75
1	1	1	-1	-1	0.95	2.81
1	1	1	1	1	0.817	2.83
-1	0	0	0	0	1.79	1.24
1	0	0	0	0	1.03	2.46
0	-1	0	0	0	1.53	1.23
0	1	0	0	0	1.22	1.73
0	0	-1	0	0	1.30	1.63
0	0	1	0	0	1.44	1.67
0	0	0	0	0	1.38	1.73
0	0	0	0	0	1.39	1.74
0	0	0	0	0	1.40	1.74

Model Terms	y_1 (NTB)	y_2 (STB)
Specifications	(.9, 1, 1.1)	(1, 3)
Intercept	1.38	1.6386
x_1	-.361	.5917
x_2	-.1547	.4383
x_3	.0771	-.095
x_4(*noise*)	-.0588	0
x_5(*noise*)	-.0116	0
x_1^2	.0481	.2009
$x_1 x_2$	-.1484	.3006
$x_1 x_3$	.0218	-.1431
$x_2 x_3$	.013	0
RMSE	.02	.183
PRESS RMSE	.029	.225
R^2 Adj.	.9970	.9359
$R^2_{\text{Prediction}}$	.994	.899

A.5 KHURI AND CONLON (1981)

Khuri and Conlon (1981) studied the effects of heating temperature (x_1), PH level (x_2), Redox potential (x_3), sodium oxalate (x_4), and sodium lauryl sulfate (x_5) on foaming properties of whey protein concentrates (WPC). Four dependent responses to be maximized are maximum overrun (y_1), time at first drop (y_2,), undenatured protein (y_3), and soluble protein (y_4).

x_1	x_2	x_3	x_4	x_5	y_1	y_2	y_3	y_4
-1	-1	-1	-1	1	1082	4.5	80.6	81.4
1	-1	-1	-1	-1	824	7.5	67.9	69.6
-1	1	-1	-1	-1	953	8.3	83.1	105
1	1	-1	-1	1	759	17	38.1	81.2
-1	-1	1	-1	-1	1163	6.7	79.7	80.8
1	-1	1	-1	1	839	9.5	74.7	76.3
-1	1	1	-1	1	1343	12	71.2	103
1	1	1	-1	-1	736	36	36.8	76.9
-1	-1	-1	1	-1	1027	4	81.7	87.2
1	-1	-1	1	1	836	5	66.8	74
-1	1	-1	1	1	1272	12.5	73	98.5
1	1	-1	1	-1	825	20	40.5	94.1
-1	-1	1	1	1	1363	15	74.9	95.9
1	-1	1	1	-1	855	7.5	74.2	76.8
-1	1	1	1	-1	1284	18.5	63.5	100
1	1	1	1	1	851	12	42.8	104
-2	0	0	0	0	1283	12	80.9	100
2	0	0	0	0	651	8.5	42.4	50.5
0	-2	0	0	0	1217	4.5	73.4	71.2
0	2	0	0	0	982	10.5	45	101
0	0	-2	0	0	884	9	66	85.8
0	0	2	0	0	1147	9	71.7	103
0	0	0	-2	0	1081	9	77.5	104
0	0	0	2	0	1036	10	76.3	89.4
0	0	0	0	-2	1213	16	67.4	105
0	0	0	0	2	1103	8.5	86.5	113
0	0	0	0	0	1171	11	77.4	102
0	0	0	0	0	1179	9	74.6	104
0	0	0	0	0	1183	9	79.8	107
0	0	0	0	0	1120	10	78.3	104
0	0	0	0	0	1180	9.5	74.8	101
0	0	0	0	0	1195	11	80.9	103

Model Terms	y_1 (LTB)	y_2 (LTB)	y_3 (LTB)	y_4 (LTB)
Specifications	(651, 1363)	(4, 36)	(36.8, 86.5)	(50.5, 113)
Intercept	1146.9	10.275	77.170	102.939
x_1	-352.17	2.1667	-20.242	-16.492
x_2	0	7.383	-17.4	15.03
x_3	115.2	3.2	0	4.758
x_4	0	0	-1.43	0
x_5	38.2	-3	0	0
x_1^2	-216.9	0	-16.42	-29.19
x_2^2	0	0	-18.87	-18.34
x_3^2	-168.4	0	-9.219	-10.04
x_4^2	-125.4	0	0	0
x_5^2	0	3.95	0	0
$x_1 x_2$	-100	8.6	-24.83	0
$x_1 x_3$	-195.5	0	11.08	0
$x_1 x_4$	0	-11	7.075	0
$x_1 x_5$	-147	-8.5	0	0
$x_2 x_3$	0	0	-6.725	0
$x_2 x_5$	0	-9.4	0	0
$x_3 x_5$	0	0	6.025	16.38
RMSE	73.193	3.358	3.892	6.285
PRESS RMSE	88.966	4.466	4.351	8.133
R^2 Adj.	.8580	.6833	.9291	.8117
$R^2_{\text{Prediction}}$	.783	.422	.909	.675

APPENDIX B: MATLAB CODE FOR SIMULATING MULTIPLE RESPONSES

This computer algorithm is written in MATLAB to simulate multiple responses for HPLC test case. The code, which is specific to this example, can generate multiple responses either for 121 design points or 1,000 design points, and calculates conformance probability as well as the penalized desirability value for each setting in the grid. The same code can be modified for other cases by providing individual response parameters as well as experimental data such as *x* and *y* vectors.

```
clear all; clc;
%Initial design for independent variables
x1=[-1 -1 -1 -1 0 0 0 0 0 0 1 1 1 1 0]';%noise variable
x2=[-1 1 0 0 0 1 -1 1 -1 0 0 -1 1 0 0]';
x3=[0 0 -1 1 0 -1 1 1 -1 0 1 0 0 -1 0]';
x=[x1 x2 x3];

%Response data
y1=[2.14 1.73 1.93 1.95 2.17 1.97 2.38 1.98 2.37 2.2 2.42 2.61 2.14
2.42 2.2]';
y2=[22  12  16  16  14  11  19  11  18  14  13  17  10  12  14]';
y3=[172 311 251 241 278 371 194 360 204 280 314 223 410 324 281]';
y4=[0.76 0.88 0.8 0.8 0.79 0.86 0.74 0.86 0.74 0.78 0.78 0.73 0.85 0.78
0.79]';

n=length(x1); %number of experimental runs
%second order terms and 2 way interactions included in the model
xm=[ones(n,1) x1 x2 x3 x1.^2 x1.*x2 x1.*x3 x2.^2 x3.^2];
y=[y1 y2 y3 y4];

q=length(y(1,:));%number of responses
m=length(x(1,:));%# of factors
%Regression coefficients for individual responses obtained by mbcmodel
tool (Model Terms in Appendix A.2)
B=[2.1931 0.23 -0.21 0 -0.015385 0 0 -0.020385 0;
    13.9231 -1.75 -4 0.25 0.384615 0.75 0.25 0.884615 0;
    279.2857 37 82.375 -5.125 0 12 0 0 3.089286;
    0.78615 -0.0125 0.06 0 0.0042308 0 0 0.014231 0]';
```

```
p=length(B(:,1));%number of regression parameters
v=n-p-q+1;%degrees of fredom
U=y-xm*B;%residuals
V=U'*U;%variance covariance of Y

xminv=inv(xm'*xm);
mvnmu=zeros(1,q);%mean for random variable z
mvnsigma=eye(q);% var-covar for random variable z

DDquesada_1000; %use to create 1000x3 design grid
model = [1 0 0;0 1 0;0 0 1;2 0 0;1 1 0;1 0 1;0 2 0;0 0 2];
D = x2fx(DD, model);
D=[ones(length(D),1) D];

ly1=1.8;uy1=2.38;%LTB
ly2=10.56;uy2=15;%STB
ly3=300;uy3=369.88;%LTB
ly4=.75;uy4=.85;ty4=.8;%NTB

lowerspec=[ly1 ly2 ly3 ly4];
upperspec=[uy1 uy2 uy3 uy4];

xnstd=.1; %standard deviation of noise variable
d=[];%desirability vector for responses
cp=.0001;%penalization constant
yrand=[];%vector for randomly generated responses
N=5000; %# of simulation runs for each setting
tic;

for i=1:length(D);
    c=0;
    for j=1:N;
    randn('state',j); rand('state',j);
        s(j,1)=chi2rnd(v);%chi-square random variable
        z(j,:)=mvnrnd(mvnmu,mvnsigma);%multivariate normal random
variable z
        xn=xnstd*randn;
        Yest=[1 xn D(i,3:4) xn^2 xn*D(i,3) xn*D(i,4) D(i,8:9)]*B;
        sca_predvar=1+[1 xn D(i,3:4) xn^2 xn*D(i,3) xn*D(i,4)
D(i,8:9)]*xminv*[1 xn D(i,3:4) xn^2 xn*D(i,3) xn*D(i,4)
D(i,8:9)]';%scaled prediction variance %
        yrand(j,:)=((sca_predvar/s(j,:))^.5)*z(j,:)*(V^.5)+Yest;

       if
((yrand(j,1)>=ly1)&(yrand(j,2)<=uy2)&(yrand(j,3)>=ly3)&(yrand(j,4)>=ly4
)&(yrand(j,4)<=uy4));
       c=c+1;
       else c=c;
       end

      %Penalized desirability calculations
        if yrand(j,1)<=ly1;%y1:LTB, desirability and penalty function
evaluations
           dy1=0;py1=cp+abs((yrand(j,1)-ly1)/(uy1-ly1));
       elseif yrand(j,1)<=uy1;
```

```
            dy1=(yrand(j,1)-ly1)/(uy1-ly1);py1=cp;
            else dy1=1;py1=cp;
        end

         if yrand(j,2)<=ly2;%y2:STB,
            dy2=1;py2=cp;
         elseif yrand(j,2)<=uy2;
            dy2=(uy2-yrand(j,2))/(uy2-ly2);py2=cp;
            else dy2=0;py2=cp+abs((yrand(j,2)-uy2)/(uy2-ly2));
         end

         if yrand(j,3)<=ly3;%y3:LTB,
            dy3=0;py3=cp+abs((yrand(j,3)-ly3)/(uy3-ly3));
        elseif yrand(j,3)<=uy3;
            dy3=(yrand(j,3)-ly3)/(uy3-ly3);py3=cp;
            else dy3=1;py3=cp;
         end

        if yrand(j,4)<=ly4;%y4:NTB,
            dy4=0;py4=cp+abs((yrand(j,4)-ly4)/(ty4-ly4));
         elseif yrand(j,4)<=ty4;
            dy4=(yrand(j,4)-ly4)/(ty4-ly4);py4=cp;
            elseif yrand(j,4)<=uy4;
            dy4=(uy4-yrand(j,4))/(uy4-ty4);py4=cp;
         else dy4=0;py4=cp+abs((yrand(j,4)-uy4)/(uy4-ty4));
        end
        d(j)=(dy1*dy2*dy3*dy4)^(1/q);%desirability component
        pp(j)=((py1*py2*py3*py4)^(1/q)-cp)^2;%penalty component
        PD(j)=d(j)-pp(j); %overal penalized desirability function

    end

%Vector of Probability of conformance
Prob_c(i,:)=c/N;
%Vector of average Penalized desirability
PDmean(i)=mean(PD);
end
PDmean=PDmean';
toc;
time=toc;
```

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