

Comparative Study on Robust Design Optimization Models for Multiple Chemical Responses

Vo Thanh Nha, Sangmun Shin, Woo-Sik Jeong, Chul-Soo Kim, Hwa-il Kim, and Seong Hoon Jeong

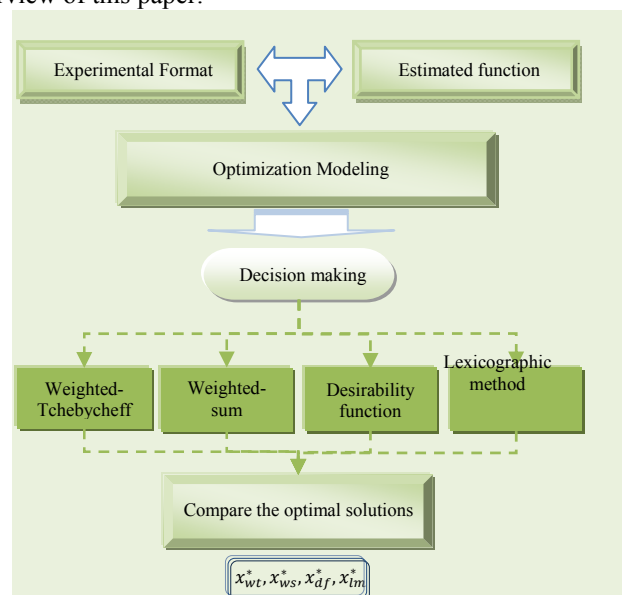
Abstract—Improving the quality of products is one of significant research issues in many industrial situations. In order to address these issues, many researchers and practitioners have considered that robust design (RD) is one of the most effective methodologies to find the optimal factor settings on many chemical formulation problems. To these problems, a robust optimization method for a number of multiple responses is often required. The primary objective of this paper is to investigate existing multi-objective RD methods and to conduct their associated comparative study. In addition, a fitted function for each response is obtained by using response surface methodology (RSM). In order to perform a comparative study in terms of optimization aspects, a number of existing multi-objective optimization models and criteria are utilized. Final, a chemical chase study is performed for verification purposes.

Index Terms—Robust design, comparative study, multi-objective optimization, Response Surface Methodology (RSM).

I. INTRODUCTION

Robust design (RD) is one of the most effective methodologies which can improve the quality of a product. A number of researches have been developed RD and its applications to many industrial problems for more than twenty years. RD was introduced by Taguchi in 1979. Based on the Taguchi's RD philology, Vining and Myers [1] introduced a dual-response approach based on response surface methodology (RSM) as an alternative for modeling process relationships by separately estimating the response functions of the process mean and variance in order to achieve the primary goal of RD by minimizing the process variance while adjusting the process mean at the target. Del Castillo and Montgomery [2] and Copeland and Nelson [3] showed that the optimization technique proposed by Vining and Myers [1] might not always guarantee the optimal RD solutions, and proposed standard non-linear programming techniques, such as the generalized reduced gradient and the Nelder–Mead simplex methods, which can provide better RD solutions. Modified dual-response approaches using fuzzy theory were further developed by Kim and Lin [4]. However, Lin and Tu [5] pointed out that the RD solutions obtained from the dual-response model may not necessarily be optimal since this model forces the process mean to be located at the

target value, and proposed the mean squares error (MSE) model, relaxing the zero-bias assumption. Because the MSE approach provide a small process bias with process variance is less than mostly equal to the variance obtained from the Vining and Myers' model. Thus, the MSE model may provide better (or equal, at least) RD solutions unless the zero-bias assumption must be met. Further modifications to the MSE model have been discussed by Kim and Cho [6], Shin and Cho [7]. However, most of those identified RD models were considered as a single response problem, even though a number of real-world problems are often related to multi-response optimization problems. In order to address these multi-response problems using the RD principle, a number of multi-objective RD models have been proposed by Kovach and Cho [8] and Shin and Cho [9]. To this end, a robust optimization method for a number of multiple responses is often required. The primary objective of this paper is to investigate existing multi-objective RD methods (i.e., weighted sum (WS), weighted-Tchebycheff (WT), lexicographic method (LM) and desirability function (DF) approach) and to conduct their associated comparative study. In addition, a fitted function for each response is obtained by using response surface methodology (RSM). In order to perform a comparative study in terms of optimization aspects, a number of existing multi-objective optimization models and criteria are utilized. Final, a chemical chase study is performed for verification purposes. Figure 1 illustrates an overview of this paper.



II. MODEL DEVELOPMENT

A. Experiment Format

Assuming that a number of responses (y_1, y_2, \dots, y_n) is

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influenced by a number of control factors (x_1, x_2, \dots, x_N). And the number of replication was observed at each response y_i which is q replications. Based on the observation value, the mean and variance for each response can be found. Table 1 represents a standard experiment format for this study.

TABLE I: THE GENERAL EXPERIMENTAL FORMAT FOR MULTIPLE CHARACTERISTICS

runs	X	y1		
		Replications	\bar{y}_1	s_1^2
1	Control factor settings	y111	\bar{y}_{11}	s_{11}^2
		y112....y11q		
...		...		
k		y1k1	\bar{y}_{1k}	s_{1k}^2
		y1k2....y1kq		
runs	X	y2		
		Replications	\bar{y}_2	s_2^2
1	Control factor settings	y211	\bar{y}_{21}	s_{21}^2
		y212....y21q		
...		...		
k		y2k1	\bar{y}_{2k}	s_{2k}^2
		y2k2....y2kq		
...				
runs	X	yn		
		Replications	\bar{y}_n	s_n^2
1	Control factor settings	yn11	\bar{y}_{n1}	s_{n1}^2
		yn12....yn1q		
...		...		
k		ynk1	\bar{y}_{nk}	s_{nk}^2
		ynk2....ynkq		

B. Response Surface Methodology (RSM)

Based on the proposed experimental framework, an estimation method must then be developed for obtaining functional relationships between input factors and their associated output responses. It is known that response surface methodology (RSM) is one of popular estimation methods. RSM is a collection of mathematical and statistical techniques that is useful for modeling and analyzing these problems when the response of interest is influenced by several factors. Its objective is to optimize (either minimize or maximize) the optimal function of output responses. RSM is typically used to optimize the optimal function by estimating input-output functional forms when the exact functional relationships are not known or very complicated [14]. As a comprehensive presentation of RSM, Myers and Montgomery [14] provided insightful comments on the current status and future direction of RSM. Using the output responses (i.e., mean responses y_i and variance responses s_i^2), the second-ordered estimated response functions of the process mean and variance are given as

$$\hat{\mu}(x) = \hat{\alpha}_0 + \mathbf{x}^T \mathbf{a} + \mathbf{x}^T \mathbf{A} \mathbf{x} \quad (1)$$

where
and

$$\hat{\sigma}^2(x) = \hat{\beta}_0 + \mathbf{x}^T \mathbf{b} + \mathbf{x}^T \mathbf{B} \mathbf{x} \quad (2)$$

where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}, \mathbf{a} = \begin{bmatrix} \hat{\alpha}_1 \\ \hat{\alpha}_2 \\ \vdots \\ \hat{\alpha}_N \end{bmatrix} \text{ and}$$

$$\mathbf{A} = \begin{bmatrix} \hat{\alpha}_{11} & \hat{\alpha}_{12}/2 & \cdots & \hat{\alpha}_{1N}/2 \\ \hat{\alpha}_{12}/2 & \hat{\alpha}_{22} & \cdots & \hat{\alpha}_{2N}/2 \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\alpha}_{1N}/2 & \hat{\alpha}_{2N}/2 & \cdots & \hat{\alpha}_{NN} \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}, \mathbf{b} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_N \end{bmatrix} \text{ and}$$

$$\mathbf{B} = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & \cdots & \hat{\beta}_{1N}/2 \\ \hat{\beta}_{12}/2 & \hat{\beta}_{22} & \cdots & \hat{\beta}_{2N}/2 \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\beta}_{1N}/2 & \hat{\beta}_{2N}/2 & \cdots & \hat{\beta}_{NN} \end{bmatrix}$$

and where vector \mathbf{a} and matrix \mathbf{A} denote the estimated regression coefficients for the process mean; and vector \mathbf{b} and matrix \mathbf{B} represent the estimated regression coefficients for the process variance, respectively.

C. Optimization Models

By using RSM as discussed in the previous section, the fitted functions of the process mean and variance (i.e., $\hat{\mu}_i(\mathbf{x})$ and $\hat{\sigma}_i^2(\mathbf{x})$) are obtained at each response y_i . After obtaining the estimated functions, the next step is to find the optimal factor settings (i.e., the optimal chemical formulation). By using the MSE concept, the objective function for each response y_i can be expressed as $\text{MSE}_i(\mathbf{x}) = \hat{\mu}_i(\mathbf{x}) + \hat{\sigma}_i^2(\mathbf{x})$. Based on this formulation, the general optimization model can be identified as follows:

$$\begin{aligned} &\text{Minimize } \{\text{MSE}_1(\mathbf{x}), \text{MSE}_2(\mathbf{x}), \dots, \text{MSE}_i(\mathbf{x}), \dots, \text{MSE}_n(\mathbf{x})\} \\ &\text{Subject to: } \mathbf{x} \in \Omega \end{aligned} \quad (3)$$

Where $\text{MSE}_i(\mathbf{x}) = \hat{\mu}_i(\mathbf{x}) + \hat{\sigma}_i^2(\mathbf{x})$

In order to address this multi-objective optimization, we use a number of methods (i.e., WS, WT, LM and DF) for handling the multi-responses as shown in Table II.

III. PILOT STUDY

In this paper, a chemical case study is conducted for multiple responses reported in the chemical engineering literature (Jauregi et al., 1997) is employed to demonstrate the use of the existing multi-response optimization approaches. When surfactant solutions are mixed at high speeds, micro bubbles (10–100 μm in diameter) are formed. It is postulated that these bubbles, called colloidal gas aphrons (CGAs), are composed of a gaseous inner core surrounded by a thin soapy film. The properties of the CGAs are measured by two responses, such as stability (y_1) and temperature (y_2). The purpose of this experiment is to determine the effects of concentration of surfactant (x_1), concentration of salt (x_2), and time of stirring (x_3) on the CGA properties. The experimental data is displayed in Table 3. By using Equations (1) and (2), the fitted response function of each response can be obtained as

$$\begin{aligned} y_{1\mu}(x) &= 4.9778 + 0.8170x_1 - 0.4480x_2 + 0.0390x_3 \\ &\quad - 0.1113x_1x_2 + 0.0688x_1x_3 - 0.0613x_2x_3 \\ &\quad - 0.1372x_1^2 + 0.2878x_2^2 - 0.0672x_3^2 \\ y_{1\sigma}(x) &= -0.0180 - 0.0208x_1 + 0.0632x_2 + 0.0476x_3 \end{aligned}$$

$$\begin{aligned}
 & -0.0146x_1x_2 - 0.0561x_1x_3 + 0.0522x_2x_3 \\
 & + 0.0495x_1^2 + 0.0379x_2^2 + 0.0489x_3^2 \\
 y_{2\mu}(x) = & 28.9202 - 1.4800x_1 - 0.0900x_2 + 2.3300x_3 \\
 & - 0.0875x_1x_2 - 0.7125x_1x_3 + 0.4000x_2x_3 \\
 & - 0.6078x_1^2 - 1.0078x_2^2 - 0.6078x_3^2 \\
 y_{2\sigma}(x) = & 34.8412 - 29.0930x_1 + 8.0802x_2 + 78.6949x_3 \\
 & - 8.9552x_1x_2 - 25.2268x_1x_3 + 0.2055x_2x_3 \\
 & + 11.6216x_1^2 + 41.3620x_2^2 + 11.0680x_3^2
 \end{aligned}$$

TABLE II: THE OPTIMIZATION MODELS FOR MULTI-RESPONSES

Weighted-sum	$ \begin{aligned} & \text{Minimize } \sum_{i=1}^n \omega_i \text{MSE}_i(\mathbf{x}) \\ & \text{Subject to} \\ & \quad \sum_{i=1}^n \omega_i = 1, i = \overline{1, n}, \\ & \quad \mathbf{x} \in \Omega, \\ & \text{where} \\ & \quad \text{MSE}_i(\mathbf{x}) = \hat{\mu}_i(\mathbf{x}) + \hat{\sigma}_i^2(\mathbf{x}) \end{aligned} $	(4)
Desirability function	$ \begin{aligned} & \text{Minimize } \prod_{i=1}^n d_i(\mathbf{x}) \\ & \text{Subject to} \\ & \quad \mathbf{x} \in \Omega \\ & \text{Where} \\ & \quad d_i(\mathbf{x}) = \begin{cases} 0 & \text{if } \text{MSE}_i(\mathbf{x}) < \text{MSE}_i^{\min} \\ \frac{\text{MSE}_i(\mathbf{x}) - \text{MSE}_i^{\min}}{\text{MSE}_i^{\max} - \text{MSE}_i^{\min}} & \text{if } \text{MSE}_i^{\min} \leq \text{MSE}_i(\mathbf{x}) \leq \text{MSE}_i^{\max} \\ 1 & \text{if } \text{MSE}_i(\mathbf{x}) > \text{MSE}_i^{\max} \end{cases} \\ & \quad \text{MSE}_i^{\min} = \text{minimize}\{\text{MSE}_i(\mathbf{x}) \mathbf{x} \in \Omega\} \\ & \quad \text{MSE}_i^{\max} = \text{maximize}\{\text{MSE}_i(\mathbf{x}) \mathbf{x} \in \Omega\} \\ & \quad \text{MSE}_i(\mathbf{x}) = \hat{\mu}_i(\mathbf{x}) + \hat{\sigma}_i^2(\mathbf{x}) \end{aligned} $	(5)
Weighted-Tchebycheff method	$ \begin{aligned} & \text{Minimize } \{\varepsilon, e^T(\mathbf{MSE} - \mathbf{U}^*)\} \\ & \text{Subject to} \\ & \quad \omega_i[\text{MSE}_i(\mathbf{x}) - U_i^*] - \varepsilon \leq 0, i = \overline{1, n}, \\ & \quad \sum_{i=1}^n \omega_i = 1, \\ & \quad \mathbf{x} \in \Omega, \\ & \text{Where} \\ & \quad \text{MSE}_i(\mathbf{x}) = \hat{\mu}_i(\mathbf{x}) + \hat{\sigma}_i^2(\mathbf{x}), \\ & \quad U_i^* = \text{min}\{\text{MSE}_i(\mathbf{x}) \mathbf{x} \in \Omega\}, \\ & \quad \mathbf{MSE} = \begin{bmatrix} \text{MSE}_1(\mathbf{x}) \\ \vdots \\ \text{MSE}_n(\mathbf{x}) \end{bmatrix}, \mathbf{U}^* = \begin{bmatrix} U_1^* \\ \vdots \\ U_n^* \end{bmatrix} \end{aligned} $	(6)
Lexicographic method	$ \begin{aligned} & \text{First step} \\ & \text{Minimize } \text{MSE}_1(\mathbf{x}) \\ & \text{Subject to} \\ & \quad \mathbf{x} \in \Omega \\ & \text{Where} \\ & \quad \text{MSE}_1(\mathbf{x}) = \hat{\mu}_1(\mathbf{x}) + \hat{\sigma}_1^2(\mathbf{x}), \\ & \text{Generalized priority optimization model for second step} \\ & \text{Minimize } \text{MSE}_j(\mathbf{x}) \\ & \text{Subject to} \\ & \quad \text{MSE}_j(\mathbf{x}) = \text{MSE}_j^*, j = \overline{1, 1-1}, \\ & \quad \mathbf{x} \in \Omega, \\ & \text{Where} \\ & \quad \text{MSE}_j^* = \text{MSE}_j(\mathbf{x}_j^*), \\ & \quad \text{MSE}_i(\mathbf{x}) = \hat{\mu}_i(\mathbf{x}) + \hat{\sigma}_i^2(\mathbf{x}) \end{aligned} $	(7)

After obtaining the estimated functions of the process mean and variance for responses y_1 and y_2 , the optimization models which are given in Table 2 is applied in order to find the optimal factor settings. By setting the target values for both responses y_1 and y_2 as 7 and 30, respectively, the optimal solutions by using four models, such as WS, WT, LG and DF, are obtained as follows: $x_{ws}^*(0.7269; 0.0842; -0.3592)$, $x_{wt}^*(-1.0000; -0.0289; -0.7890)$, $x_{lm}^*(0.1688; 0.1306; 0.2609)$, and $x_{df}^*(1.0000; -1.0000; -0.0020)$, respectively, as shown in Table IV.

TABLE III: THE CAG STUDY

runs	x1	x2	x3	rep	y1	y2	\bar{y}_1	\bar{y}_2	s_1^2	s_2^2
1	-1	-1	-1	1	4.5	29	4.5	26	0	4.24
	-1	-1	-1	2	4.5	23				
2	1	-1	-1	1	6.04	23	6.22	24.2	0.25	1.7
	1	-1	-1	2	6.39	25.4				
3	-1	1	-1	1	3.81	22	3.95	24.5	0.2	3.54
	-1	1	-1	2	4.09	27				
4	1	1	-1	1	5.67	25.5	5.43	23.25	0.34	3.18
	1	1	-1	2	5.19	21				
5	-1	-1	1	1	4.67	20	4.45	30.5	0.32	14.85
	-1	-1	1	2	4.22	41				
6	1	-1	1	1	6.73	35.5	6.65	26.75	0.11	12.37
	1	-1	1	2	6.57	18				
7	-1	1	1	1	3.4	43	3.86	31.5	0.65	16.26
	-1	1	1	2	4.32	20				
8	1	1	1	1	5.72	19	5.41	26.5	0.45	10.61
	1	1	1	2	5.09	34				
9	-1	0	0	1	4.09	36	4.24	30	0.21	8.49
	-1	0	0	2	4.38	24				
10	1	0	0	1	5.52	30	5.46	27	0.09	4.24
	1	0	0	2	5.39	24				
11	0	-1	0	1	5.92	32	5.93	27.7	0.01	6.08
	0	-1	0	2	5.93	23.4				
12	0	1	0	1	4.74	36	4.62	28.5	0.17	10.61
	0	1	0	2	4.5	21				
13	0	0	-1	1	5.01	27	4.86	25.5	0.22	2.12
	0	0	-1	2	4.7	24				
14	0	0	1	1	4.94	38	4.98	31.5	0.05	9.19
	0	0	1	2	5.01	25				
15	0	0	0	1	4.85	34	4.94	28.17	0.06	6.37
	0	0	0	2	4.94	34				
	0	0	0	3	4.98	33				
	0	0	0	4	4.89	24				
	0	0	0	5	4.94	19				
	0	0	0	6	5.01	25				

In addition, Figure 2 insulates the criterion space of y_1 and y_2 and the optimal factor settings. Based on these results, we obtained four different solutions and each set of the optimal solutions has different criteria (i.e., weight and priority).

IV. CONCLUSION

The primary goal of this paper is to make a comparison between methodologies which were used in the RD optimization step. We utilized a combination of the estimated

function of the process mean and variance at each response into one objective function. A chemical case study was conducted in order to demonstrate how the proposed methodology can provide solutions. Based on the case study results, there are two main criteria in the decision making process of the optimization model which are weight and priority. In effect, these criteria depend on the purpose of each problem associated with importance of quality characteristics. This comparative study can provide a guide line to select a suitable optimization model for a given situation. In this paper, a comparative study was performed based on only RD optimization methodologies while considering the estimation method by using RSM. For further study, a number of different estimation methodologies can be considered and compared.

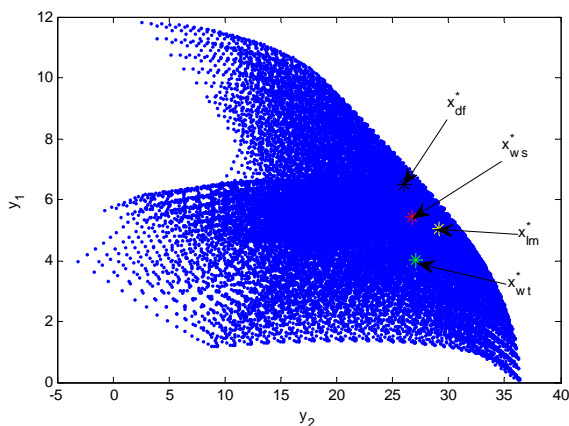


Fig. 2. The criterion space of y_1 and y_2 .

TABLE IV: THE OPTIMAL SETTINGS FOR MULTI-RESPONSES BASED ON THE FOUR MODELS: WEIGHTED-SUM, WEIGHTED-TCHEBYCHEFF, LEXICOGRAPHICAL METHOD AND DESIRABILITY FUNCTION

Models	Optimal value(x^*)			\bar{y}_1	s_1^2	T1	\bar{y}_2	s_2^2	T2
	x1	x2	x3						
WS	0.73	0.08	-0.36	5.42	0.00		26.76	0.00	
WT	-1.00	-0.03	-0.79	4.01	0.00		27.02	0.00	
LM	0.17	0.13	0.26	5.06	0.00	7	29.17	52.00	
DF	1.00	-1.00	0.00	6.50	0.00		26.00	59.50	30

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