Preferred Robust Response Surface Design with Missing Observations Based on Integrated TOPSIS-AHP Method

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Abstract- Missing observations occur in experimental designs as a result of insufficient sampling, machine breakdown, high cost, and errors in the measurements. In nanomanufacturing, missing observations often appear in designs because the combination of factors or molecular structures selected by a designer cannot be experimented successfully. In the current paper, Box-Behnken and face-centered composite designs were studied and eight robustness criteria including D-efficiency, t_{max} , $t_{max}(1-\alpha)$, and their related sub-criteria were considered to evaluate the robustness of the aforementioned designs. Finally, the integrated TOPSIS-AHP methodology was employed to select the most suitable robust design, and a numerical example was also presented to assess the applicability of the proposed approach.

Keywords: Robustness criteria, Preferred robust response surface design, TOPSIS-AHP methodology, Nanomanufacturing

I. INTRODUCTION

In recent years, missing observation has attracted a significant attention in experimental designs [1–3]. Missing observations are frequent in experimental designs or data acquisition, arising as a result of insufficient sampling, high cost, and errors in measurements [4]. Machine breakdown, illegible recording of response, and damaged experimental resources are also the common reasons for missing observations [2]. Moreover, missing observations can appear in nanomanufacturing industries because the combination of factors selected by a designer cannot be experimented successfully, for example, the study of gas phase nanoscale lubrication is an application of missing observations in experimental designs [2]. Hence, in order to overcome the problem of missing observation, robust criteria can be employed to investigate the robustness of a design [4–7, 11–13]. Ghosh [8] examined the robustness of BIBD in the presence of missing observations. MacEachern et al. [9] studied a number of techniques to find t_{max} and then applied the

obtained value to evaluate the robustness of central composite design and factorial experiment against missing data. Whititting [10] assessed the robustness of Box-Behnken design in the presence of missing observations. Navinchandra et al. [2] proposed three new Bayesian algorithms based on predictive ability and minimization of the residual sum of squares in the presence of missing observations for factorial design. Tanco et al. [3] evaluated the robustness of some design

experiments by three robust criteria- D-efficiency, t_{\max} , and $t_{\max}(1-\alpha)$.

Multiple criteria decision-making problems can be divided into two main categories: multiple objective decision making (MODM) and multiple attribute decision making (MADM). The choice of preferred robust response design with various robustness criteria is an MADM problem, the technique for order preference by similarity to ideal solution (TOPSIS) [14], analytic hierarchy process (AHP) [15], elimination and et choice translating reality (ELECTRE) [15], grey relational analysis (GRA) [16], and VIKOR [17] are the most common methods of MADM. In order to determine the weights of each criterion in TOPSIS method, the AHP method, which works based on the decision maker judgments developed by Saaty [18], was employed in our study. Tavakkoli and Mousavi [19] proposed an integrated AHP-VIKOR

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method for plant location problem. Rao and Davim [20] applied the combined TOPSIS-AHP method for material selection [20].

In order to analyze the robustness of designs, the Box-Behnken and the face-centered composite designs were considered because these designs can precisely estimate each coefficient to achieve certain desirable properties [3]. Eight robustness criteria, such as D-efficiency, t_{max} , $t_{max}(0.99)$, t_{max}/n , $t_{max}(0.99)/n$, and $t_{max}(0.95)/n$, were estimated in the current study.

in the current study.

The present paper is divided into following sections. In Section 2, robustness criteria were introduced to investigate the designs. The combined TOPSIS-AHP methodology is explained in Section 3. A case study of the proposed methodology is presented in Section 4. The concluding remarks and some future directions are depicted in the final section.

II. ROBUSTNESS CRITERIA FOR THE EVALUATION OF EXPERIMENTAL DESIGNS

Factorial designs are common experimental designs. The most crucial aspect of these designs is k factors with two levels; the factors can be quantitative, such as temperature and pressure, or qualitative, such as machines and operators [21]. These designs cannot estimate the quadratic relationships, however, it is necessary to determine the quadratic relationships in some experimental designs. The Box-Behnken and the face-centered composite designs can estimate a full second-order polynomial model. In this paper, the robustness of the aforesaid designs in the presence of missing observations was studied for three to six factors with four center points using three robustness criteria [3], [22].

A. Box-Behnken design

Box-Behnken design consists of a set of points placed at the midpoint of each edge and the replicated center point of a multidimensional cube. The polynomial equation generated by this experimental design is presented below.

$$y_i = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + b_{12} x_1 x_2 + b_{13} x_1 x_3 + b_{23} x_2 x_3 + b_{11} x_1^2 + b_{22} x_2^2 + b_{33} x_3^2,$$
(1)

where y_i is the dependent variable, b_0 is the intercept, b_1 to b_{33} are the regression coefficients, and x_1 , x_2 and x_3 are the independent variables selected from the preliminary experiments.

B. Face-centered composite design

In many situations, the region of interest is cuboidal rather than spherical. In these cases, a useful variation of the central composite design is the face-centered composite design, which locates the stars or the axial points on the centers of the faces of a cube.

C. Explanation of robustness criteria for experimental designs

Ghosh [23] proposed the D-efficiency as the most suitable robustness criteria for experimental designs. Lal et al. [24] evaluated the robustness of experimental designs using A-efficiency, which minimizes the trace of (x^Tx) and investigates the effect of missing observation on the sum of variances of the regression coefficients. In the current research, D-efficiency was preferred instead of A-efficiency to assess the robustness of experimental designs. It is evident that in experimental designs, some observations are more important than others, hence if the most important observation is missing, the overall loss in efficiency is greater as compared to the missing of least important observation. The D-efficiency of the remaining design after missing some rows of design matrix (X_1) can be defined as

$$D - efficiency = \left(\frac{\left|X_{1}^{T}X_{1}\right|}{\left|X^{T}X\right|}\right).$$
⁽²⁾

This criterion minimizes the volume of joint confidence region on the vector of regression coefficients. In this study, two criteria were assumed: the average of D-efficiency and the minimum value (worst case) when only one arbitrary row of the design was missing. Table I presents the D-efficiency values for Box-Behnken and face-centered composite designs, and k is the number of factors and n is the number of runs.

		FCC		BI	3	
k	n	average	worst	n	average	worst
3	18	0.4440	0.2060	16	0.3750	0.2500
4	28	0.4643	0.3412	28	0.4643	0.4167
5	30	0.3000	0.0353	44	0.5227	0.5000
6	48	0.4167	0.3236	52	0.4615	0.4375

TABLE I. Average and Worst Values of D-Efficiency in FCC and BB Designs

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TABLE II.	values	IOT BB	and FUU	Designs

					/	
]	FCC	BB			
k	п	t _{max}	t _{max} /n	n	<i>t</i> _{max}	t _{max} /n
3	18	3	16.7	16	1	6.3
4	28	3	10.7	28	3	10.7
5	30	3	10.0	44	3	6.8
6	48	3	6.3	52	3	5.8

The next considered criterion in our research was t_{max} proposed by Ghosh [23]. Let assume the following linear model: $y = X \beta + \varepsilon$, (3)

where X is an $n \times p$ matrix and the *n* rows are in the form of $(1, x_{1i}, \dots, x_{ki}; x_{1i}, x_{2i}, \dots, x_{k-1,i}, x_{ki}; x_{1i}^2, \dots, x_{ki}^2)$. For the second-order polynomial model, *p* can be defined as p = (k+1)(k+2)/2, where *k* is the number of factors.

If the remaining design matrix $(n-t) \times p$ obtained after omitting *t* observations is able to estimate all parameters, it can be concluded that the design matrix *X* is robust against missing observations. In order to confirm it, the following Ghosh definition was applied.

 $t_{\max} = \max \{ t \mid 1 \le t \le n - p \text{, and each } (n - t) \times p \text{ matrix yields } | X_t^T X_t | \ne 0 \}.$ (4)

In order to further evaluate the robustness of design, two criteria t_{max} and t_{max}/n were considered (where *n* is the number of runs), and the obtained results are depicted in Table II.

The third considered criterion was t_{max} (1 – α) proposed by Tanco et al. [3], it defines the maximum number of missing observations; therefore, the parameters of the model can be estimated with a high probability. This criterion can be defined as:

 $t_{\max}(1-\alpha) = \max \{ t \mid 1 \le t \le n-p, \text{ and } p \text{ (Model is not estimable } \mid x_t \text{ }) \le \alpha \},$ (5)

where the probability of the model is computed as

$$P(Model \ is \ not \ estimable \ |x_{t}) = \frac{\sum_{l=1}^{\binom{n}{t}} I[|X_{t,l}^{T}X_{t,l}| = 0]}{\binom{n}{t}},\tag{6}$$

where $\binom{n}{t}$ is the total number of combinations for missing observations and indicator *I* counts the total number of combinations for $I\left[\left| X^{T,I} X^{T,I} \right| \right] = 0$ and the model is not estimable.

In order to compare the robustness of the designs, $t_{max}(0.95)$ and $t_{max}(0.99)$ were computed. These two criteria define the maximum number of missing observations; therefore, the models with probabilities of 95% and 99%, respectively, were estimated. The obtained results are summarized in Tables III, IV.

FCC				BB		
k	n	<i>t</i> _{max} (0.99)	$t_{max}(0.99)/n$	n	<i>t</i> _{max} (0.99)	t _{max} (0.99)/n
3	18	3	16.6	16	1	6.20
4	28	5	17.8	28	5	17.8
5	30	4	13.3	44	9	20.4
6	48	8	16.6	52	9	17.3

TABLE III. T_{MAX} (0.99) Values for BB and FCC Designs

	FCC				BB			
k	n	<i>t</i> _{max} (0.95)	$t_{max}(0.95)/n$	n	<i>t</i> _{max} (0.95)	$t_{max}(0.95)/n$		
3	18	4	22.2	16	2	12.5		
4	28	7	25.0	28	7	25.0		
5	30	5	16.6	44	12	27.2		
6	48	10	20.8	52	13	25.0		

TABLE IV. t_{max} (0.95) Values for BB and FCC Designs

III. INTEGRATED TOPSIS-AHP METHOD

In this section, the TOPSIS method was applied to select the best robust design, hence, the relative importance of different robust criteria was determined using AHP. AHP helps the decision makers to choose the best solution from several options based on the selection criteria. AHP builds a hierarchy ranking of the decision items by comparing each pair of items. The paired comparisons produce weighting scores, which measure the relative importance of the criteria.

The execution steps of the TOPSIS-AHP method are presented below.

Step1. Assume a decision matrix of n criteria and m alternatives.

where x_{ij} indicates the performance of the *i*th alternative with respect to the *j*th criterion.

Step2. Compute the normalized decision matrix. The normalized value r_{ij} can be written as

$$r_{ij} = \frac{X_{ij}}{\sqrt{\sum_{i=1}^{m} X_{ij}^{2}}}, \quad i = 1, \dots, m \quad j = 1, \dots, n$$
(8)

Step3. Determine the relative importance of the alternatives. In AHP, the values from 1 to 9 were assigned to introduce the relative importance of the alternatives. Table V indicates the comparison scale used for the weighting of two criteria [18].

The matrix for the comparison of criteria can be presented as follows:

$$A = \begin{bmatrix} 1 & a_{12} & \dots & a_{1n} \\ a_{21} & 1 & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & 1 \end{bmatrix}.$$
(9)

Every element represents the relative importance of criterion *i* with respect to criterion *j*. Therefore, it can be concluded

that $a_{ji}=1/a_{ij}$.

 W_i is the importance degree for each criterion and was calculate as

TIBLE V. Definition of Seule	values in r an wise comparsion maans
Relative importance	Description
1	Equal importance
3	Weak importance
5	Strong importance
7	Very strong importance
9	Absolute importance
2, 4, 6, 8	Intermediate values

TABLE V. Definition of Scale Values in Pair-Wise Comparsion Matrix

$$W_{j} = \frac{\left(\prod_{j=1}^{n} a_{ij}\right)^{1/n}}{\sum_{i=1}^{n} \left(\prod_{j=1}^{n} a_{ij}\right)^{1/n}}.$$
 $i, j = 1, 2, ..., n$
(10)

A consistency ratio (CR) was used to determine the inconsistency.

$$CR = \frac{CI}{RI},\tag{11}$$

where the consistency index (CI) was calculated by

$$CI = \frac{\lambda_{\max} - n}{n - 1},\tag{12}$$

where λ_{max} is the largest eigenvalue [24] and RI (obtained from Table VI) is the random index used in decision making. When the value of CR was less than 0.1, the model was validated.

TABLE VI. RANDOM CONSISTENCY INDEX

n	1	2	3	4	5	6	7	8	9	10
k	0	0	0.58	0.9		1.12	1.24	1.32	1.41	1.45

Step 4: The weighted normalized matrix V_{ij} was computed as $V_{ij} = W_j r_{ij}$

where W_i is obtained from the previous step.

Step 5. Obtain the positive ideal solutions V^+ and the negative ideal solutions V^- .

$$V^{*} = \left\{ \max v_{ij} / j \in J, \min v_{ij} / j \in J' / i = 1, 2, ..., m \right\} = \left\{ v_{1}^{*}, v_{2}^{*}, ..., v_{n}^{*} \right\},$$
(14)

 $V^{-} = \left\{ \min v_{ij} \mid j \in J, \max v_{ij} \mid j \in J' \mid i = 1, 2, \dots, m \right\} = \{v_{1}^{-}, v_{2}^{-}, \dots, v_{n}^{-}\},$

where J = (j = 1, 2, ..., n)/j is the beneficial criteria and J' = (j = 1, 2, ..., n)/j is the non-beneficial criteria.

Step 6. Calculate the separation distance between each alternative. The separation of each alternative from the positive ideal solution was defined as

$$S_i^+ = \sqrt{\sum_{J=1}^n (V_{ij} - V_j^+)^2}, \quad i = 1, 2, \dots, m$$
(16)

Similarly, calculate the separation distance of each alternative from the negative ideal solution.

(13)

(15)

$$S_i^- = \sqrt{\sum_{J=1}^n (V_{ij} - V_j^-)^2}, \quad i = 1, 2, \dots, m$$
(17)

Step 7. Calculate the relative closeness to the ideal solution.

$$C_{i} = \frac{S_{i}^{-}}{S_{i}^{-} + S_{i}^{+}},$$
(18)

Step 8. Rank the alternatives based on C_i in descending order.

TABLE VII. Decision Matrix of Robustness Criteria							
k	AVE-D	t _{max}	$t_m(0.99)$	$t_m(0.95)$			
3	0.4440	3	3	4			
4	0.4643	3	5	7			
5	0.3000	3	4	5			
6	0.4167	3	8	10			
3	0.3750	1	1	2			
4	0.4643	3	5	7			
5	0.5227	3	9	12			
6	0.4615	3	9	13			
k	W-D	$t_{\rm max}$ / n	tm(0.99)/n	tm(0.95)/n			
3	0.206	16.7	16.6	22.2			
4	0.3412	10.7	17.8	25.0			
5	0.0353	10.0	13.3	16.6			
6	0.3236	6.3	16.6	20.8			
3	0.2500	6.3	6.25	12.5			
4	0.4167	10.7	17.8	25.0			
5	0.5000	6.8	20.4	27.2			
6	0.4375	5.8	17.3	25.0			

TABLE VII. Decision Matrix of Robustness Criteria

	TABLE VIII. Normalization of Decision Matrix								
k	AVE-D	$t_{\rm max}$	$t_m(0.99)$	$t_m(0.95)$					
3	0.3602	0.2122	0.375	0.6031					
4	0.3767	0.3514	0.375	0.3864					
5	0.2434	0.0363	0.375	0.3611					
6	0.3381	0.3333	0.125	0.2275					
3	0.3043	0.2575	0.375	0.2275					
4	0.3767	0.4292	0.375	0.3864					
5	0.4241	0.5150	0.375	0.2455					
6	0.3745	0.4507	0.375	0.2094					
k	W-D	$t_{\rm max}$ / n	tm(0.99)/n	tm(0.95)/n					
3	0.1727	0.3608	0.1697	0.3522					
4	0.2878	0.3869	0.2969	0.3966					
5	0.2302	0.2891	0.2121	0.2634					
6	0.4605	0.3608	0.4242	0.3300					
3	0.0575	0.1358	0.0848	0.1983					
4	0.2878	0.3869	0.2969	0.3966					
5	0.5181	0.4434	0.5091	0.4316					
6	0.5181	0.3760	0.5515	0.3966					

	TABLE IX. Pair-wise Comparison Matrix							
1	1	1/2	1/3	5	4	3	2	
1	1	1/2	1/3	5	4	3	2	
2	2	1	2/3	10	8	6	4	
3	3	3/2	1	15	12	9	6	
1/5	1/5	1/10	1/15	1	4/5	3/5	2/5	
1/4	1/8	1/12	1/12	5/4	1	3/4	2/4	
1/3	1/6	1/6	1/9	5/3	4/3	1	2/3	
1/2	1/2	1/4	1/6	5/2	4/2	3/2	1	

TABLE IX. Pair-Wise Comparison Matrix



Fig 1. The Hierarchical Structure of Decision making

n	1	2	3	4
w	0.1207	0.1207	0.2414	0.3622
n	5	6	7	8
w	0.0241	0.0302	0.0402	0.0604

TABLE X. Weights of Robust Criterion

IV. EVALUEATION OF ROBUST DESIGN BY THE PROPOSED

The combined TOPSIS-AHP method was applied to select the most suitable robustness design for nanolubrication application. Eight efficient criteria, such as the average D-efficiency, the worst D-efficiency, t_{max} , $t_{max}(0.99)$, $t_{max}(0.95)$, $t_{max}(0.95)/n$, and $t_{max}(0.95)/n$ were considered. The hierarchical structure for the decision making is demonstrated in the following figure.

First, the decision matrix was constructed, and each element expressed the performance of considered alternative with respect to the available criterion.

The normalized decision matrix was obtained from Equation (8).

The pair-wise comparison matrix is presented in Table IX. It was assumed that the matrix was obtained based on experts' opinion.

The weights of the robust criteria were obtained using Equation (10), and the results are depicted in the Table X.

The largest eigenvalue of the pairwise comparison matrix was equal to 8 and the value of random consistency index was 1.48. The inconsistency ratio was computed near to zero. As the value of RC was less than 0.1, it can be concluded that the comparisons were consistent. The normalized weighted matrix is summarized in Table XI. The values of positive

ideal V^+ and negative ideal V^- solutions are expressed in Table XII. The separation distances between the alternatives and the ideal solutions were calculated and are illustrated in the Table XIII.

TABLE AI. NOTHIALIZED WEIghted Matrix						
k	AVE-D	t _{max}	$t_m(0.99)$	$t_m(0.95)$		
3	0.0435	0.0256	0.0905	0.2184		
4	0.0455	0.0424	0.0905	0.1399		
5	0.0294	0.0044	0.0905	0.1308		
6	0.0408	0.0402	0.0905	0.0824		
3	0.0367	0.0311	0.0302	0.0824		
4	0.0455	0.0518	0.0905	0.1399		
5	0.0512	0.0622	0.0905	0.0888		
6	0.0452	0.0544	0.0905	0.0754		
k	WORST-D	$t_{\rm max}/n$	tm(0.99)/n	tm(0.95)/n		
3	0.0042	0.0109	0.0068	0.0213		
4	0.0069	0.0117	0.0119	0.0239		
5	0.0056	0.0087	0.0085	0.0159		
6	0.0111	0.0109	0.0171	0.0199		
3	0.0014	0.0041	0.0034	0.0120		
4	0.0069	0.0117	0.0119	0.0239		
5	0.0125	0.0134	0.0205	0.0261		
6	0.0125	0.0113	0.0222	0.0239		

	TABLE XI.	Normalized	Weighted	Matrix
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TABLE	XII.	Positive	and	Negative	Ideal	Solutions

V ⁺	V ⁻
0.0512	0.0294
0.0622	0.0044
0.0905	0.0302
0.2184	0.0758
0.0125	0.0014
0.0134	0.0041
0.0222	0.0034
0.0239	0.0120

S^+	S ⁻
0.7891	0.9217
0.8534	0.9586
0.5964	0.6982
0.9019	0.9806
0.3935	0.4832
0.8829	0.9895
0.1268	1.2066
0.0689	1.440

TABLE XIII. Separation Distance

TABLE XIV. Relative Closeness to Ideal Solution

n	1	2	3	4
С	0.5387	0.5290	0.5393	0.5209
n	5	6	7	8
С	0.4488	0.4715	0.9049	0.9413



Fig 2. The relative closeness ratio for different robust experimental designs

TABLE AV. Relative closeness to Ideal Solution				
n	1	2	3	4
С	0.4954	0.5895	0.3675	0.5526
n	5	6	7	8
С	0.2806	0.6127	0.7199	0.6814

TABLE XV. Relative Closeness to Ideal Solution

Based on the relative closeness values, the robustness for the nanolubrication experiment can be prioritized as (Table XIV):

 $c_8 > c_7 > c_3 > c_1 > c_2 > c_4 > c_6 > c_5$

The model for equal weights was also evaluated in this study. The relative closeness to the ideal solution is presented in Table XV.

Based on the relative closeness values, the preferred response surface design was ranked as:

 $c_7 > c_8 > c_6 > c_2 > c_4 > c_1 > c_3 > c_5$

The results reveal that the proposed method was sensitive to the weights of criteria, hence, it is reasonable to extract them by some decision-making methods, such as AHP.

V. CONCLUSION AND FUTURE RESEARCH

Missing observations can occur in many industrial applications, such as nanomanufacturing, therefore, the selection of a preferred design with missing observations results in an effective economic decision. The integrated TPOSIS-AHP methodology was employed to select the robust design, and the Box-Behnken and the face-centered composite designs were applied. In order to evaluate the robustness of the Box-Behnken and the face-centered composite designs, eight efficient robustness criteria were considered. The face-centered composite design with the factor k = 6 was selected as the preferred robust design with missing observations. In our future research, other robust criteria will be proposed to evaluate the experimental designs in the presence of missing data. Moreover, this method will be applied to the cases of correlated observations and outliers in our future research.

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