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A New Class of Second-Order Response Surface Designs

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ABSTRACT Response surface methodology (RSM) refers to experimental designs for optimizing or developing processes, initially in manufacturing. In this paper, a new method is presented and an algorithm is implemented that modifies the axial part in a central composite design to achieve a good D-value and efficiency. The new designs are suitable for sequential experimentation. In comparison with known designs in the same class, the new designs are tested and found to have better D-values on a range of factors. With this new approach, efficient orthogonal designs for response surface methodology were generated for a number of parameters that were previously impossible to construct. The new generated designs and their comparison with known designs from the literature are presented in tables for practitioners' use.

INDEX TERMS Composite design, construction, D-value, Hadamard matrices, orthogonal design.

I. INTRODUCTION

The sets of techniques collectively termed response surface methodology (RSM) are used to analyse relationships between explanatory variables (factors) and one or more responses, or to maximize the response by adjusting individual variables. These sets allow for rates of change and interactions between variables, such as temperature, density, or pressure. This methodology therefore has wide applications such as design optimization in mechanical engineering [1]–[3], health engineering [4], materials engineering [5], and applied physics [6], [7]. Box and Behnken in [8] introduced a class of three-level second-order designs (SODs) for fitting second-order response surfaces over a spherical region. Additional works on Box and Behnken designs can be found in [9].

A considerably useful type of SOD is the central composite design (CCD) which was first introduced in [10] requiring five levels for each factor. Today, these designs still remain the the most popular designs for second order models in response surface methodology. [11] and [12] undertook work to reduce the points needed to construct a CCD. Small composite designs were suggested in [13] and they aimed in generating designs with small and even number of factors. The subset designs were introduced in [14]. These designs were obtained by using two-level factorial designs in subsets of factors while the other factors were held at the middle level. CCDs with a minimum number of runs for 7, 8, and 9 factors were constructed in [15]. Other small composite designs are provided in [16]. The previous mentioned designs were constructed by focusing on factorial part to reduce the number of runs and they used the classical axial part. For a comprehensive overview on response surface methodology, one is referred to [17].

Most of the known approaches that reduce the run size in the literature are focused on selecting factorial runs while keeping the axial part fixed. Composite designs were constructed in [18] by replacing the classical axial part with orthogonal designs with large number of runs resulting in large number of runs for the whole designs Georgiou *et al.* work in [19] is another research that addresses axial points, although some of their designs for odd numbers of factors are not orthogonal. In [19], the classical axial points are replaced with points from an orthogonal design (OD) for even number of factors. This method gave new results, but it was restricted to the existence of the needed ODs and it does not maintain orthogonality for designs with a minimum number of runs and odd number of factors.

All the existing composite designs in the literature, with odd number of factors, have either the classical axial part (see [10]–[16]) or an axial part that maintain only one or two of the following properties: a) minimum number of runs and b) orthogonality and c) highest D-value (see [18], [19]). This paper aims at developing a method for constructing

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designs that solve this issue and generating designs that simultaneously posses all the three desirable properties a), b) and c). The designs that succesfully posses all the three properties could exist for odd orders only (see [15], [16], and [19]). This situation strongly motivated this research and this investigation for designs that can simultaneously have all the three desirable properties and at the same time be easy to construct and use. As the used criteria have demonstrated the high efficiency of the proposed designs, these designs can be directly implemented in theoretical and practical applications with immediate benefits.

The focus of this paper is to construct second-order response surface designs and generalize the approach in [19] by replacing the axial points by a new structure of a block form that is consists of a number of different ODs. This new construction method includes all the designs with classical axial points and all the designs in [19], but the proposed approach does not need the restriction for the existence of one OD that was necessary in [19]. For this reason the method can be applied to add and even orders leading to many alternatives even in the simplest block structure. Moreover, the designs constructed from this proposed method have fewer runs, a higher D-value and have their main effect orthogonal.

II. MODEL AND DESIGN CRITERIA

Suppose that one wants to test the effects of k predictors, denoted as $x_1, x_2, \ldots, x_k$, on a response variable y, subject to random error. Generally, the first attempt is to approximate the shape of the response surface by fitting a first-order model to the response

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \varepsilon, \tag{1}$$

where β_0, β_i, i = 1,…,k are unknown parameters and ε is a random error term. When the first-order model in (1) appears inadequate to describe the true relationship between the response and the predictors due to the existence of surface curvature, it can be upgraded to a second-order model

$$\begin{aligned} y = \beta_0 &+ \sum_{i=1}^{k} \beta_i x_i \\ &+ \sum_{i=1}^{k} \beta_{ii} x_i^2 \\ &+ \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij} x_{ij} + \varepsilon, \end{aligned} \tag{2}$$

where β_0, β_1 and ε are as in (1) while β_{ii} and β_{ij} denote the unknown coefficient of the quadratic effects and the 2-factor interactions respectively. The standardization of the design matrix should be applied after the experiment has been performed and at the stage where the model matrix is being prepared for the analysis of the collected data. Standardization can follow the classic standardization method for CCD or more advance techniques such as those in [20]. This is out of the scope of this paper and is not to be explored further here.

The design which is appropriate for a given experimental situation depends on the objectives of the experimenter. Several criteria have been proposed in the literature for this purpose; see for example [21]. One of the most important criteria for the design matrix is the D-value criterion that can be used to evaluate central composite designs, where more informative design has higher D-value. The D-value criterion is calculated as $10^3|X_p'X_p|^{1/p}/n$, where X_p is the model matrix, and p is the number of coefficients in the model to be estimated, and describes the ''information per point'' for the design (see [22]). A design with all the main effects orthogonal to each other and also orthogonal to all the quadratic effects is said to satisfy the property of orthogonal quadratic effects (OQE).

Another criterion used in this paper is the average prediction variance (AVP). Given any settings of factors, the product of the error variance and a quantity that depends on the design and the factor settings is often referred to as the prediction variance. Usually, prediction variance is unknown as its value is dependent on the error variance which is also unknown prior to experimentation. More so, the error variance does not determine the ratio of the prediction variation - relative prediction variance. Thus, the value of relative prediction variance can be known before the collection of data as it solely depends on the factor settings and the design. While executing an experiment and thus fitted a least square model, the mean squared error (MSE) of the fitted model can be used to estimate the error variance. Furthermore, the multiplication of the relative prediction variance of a particular setting results in the estimated value of the actual prediction variance of that setting. Concisely, the prediction variance is small throughout the design space, the error variance reduces as sample size increase and comparatively, preferable designs are those with lower prediction variance. The designs are also evaluated in terms of the maximum prediction variance (MVP) which is part of the prediction variance where the value of MVP is the worst (least desirable from a design point of view) value of the relative prediction variance. The relative prediction variance at x_i is given by $x_i'(X_p'X_p)^{-1}x_i$ [23].

A. ORTHOGONAL DESIGNS

An orthogonal design **A**, of order n and type $(s_1, \ldots, s_u)$, which is denoted as OD $(n; s_1, \ldots, s_u)$, is a square matrix of order n with entries $\pm x_k$, where for each k, $\pm x_k$ appears exactly s_k times in each row and column of the design matrix and x_k are commuting variables. Also, all rows and columns are pairwise orthogonal.

Thus,

$$AA' = A'A = (s_1x_1^2 + \ldots + s_u x_u^2)I_n, \tag{3}$$

where I_n is the identity matrix of order n. It is known that the maximum number of variables in an orthogonal design of order n is $\rho(n)$, where $\rho(n)$ is the Radon number and $\rho(n) = 8c + 2^d$ with $n = 2^t b$, b being an odd number and $t = 4c + d$, $0 \le d < 4$ [24].

Example 1: A few examples of orthogonal designs of order 2, 4, 6, and 8 are presented in Table 1 and will be used in our construction method.

TABLE 1. Examples of orthogonal designs ODs.

$$\mathrm{OD}(2;1,1): \quad \mathrm{OD}_2(x_1,x_2)=\begin{bmatrix} x_1 & x_2 \\ -x_2 & x_1 \end{bmatrix}$$

$$\mathrm{OD}(4;1,1,1,1):$$

$$\mathrm{OD}_4(x_1,x_2,x_3,x_4)=\begin{bmatrix} x_1 & x_2 & -x_3 & x_4 \\ -x_2 & x_1 & -x_4 & -x_3 \\ x_3 & x_4 & x_1 & -x_2 \\ -x_4 & x_3 & x_2 & x_1 \end{bmatrix}$$

$$\mathrm{OD}(6;4,1):$$

$$\mathrm{OD}_6(x_1,x_2)=$$

$$\begin{bmatrix} x_1 & -x_2 & -x_1 & x_1 & 0 & x_1 \\ -x_1 & x_1 & -x_2 & x_1 & x_1 & 0 \\ -x_2 & -x_1 & x_1 & 0 & x_1 & x_1 \\ -x_1 & -x_1 & 0 & x_1 & -x_1 & -x_2 \\ 0 & -x_1 & x_1 & -x_2 & x_1 & -x_1 \\ -x_1 & 0 & -x_1 & -x_1 & -x_2 & x_1 \end{bmatrix}$$

$$\mathrm{OD}(8;1,1,1,1,1,1,1,1):$$

$$\mathrm{OD}_8(x_1,x_2,x_3,x_4,x_5,x_6,x_7,x_8)=$$

$$\begin{bmatrix} x_1 & x_2 & x_4 & x_3 & x_6 & x_5 & x_8 & x_7 \\ -x_2 & x_1 & x_3 & -x_4 & x_5 & -x_6 & x_7 & -x_8 \\ -x_4 & -x_3 & x_1 & x_2 & -x_8 & x_7 & x_6 & -x_5 \\ -x_3 & x_4 & -x_2 & x_1 & x_7 & x_8 & -x_5 & -x_6 \\ -x_6 & -x_5 & x_8 & -x_7 & x_1 & x_2 & -x_4 & x_3 \\ -x_5 & x_6 & -x_7 & -x_8 & -x_2 & x_1 & x_3 & x_4 \\ -x_8 & -x_7 & -x_6 & x_5 & x_4 & -x_3 & x_1 & x_2 \\ -x_7 & x_8 & x_5 & x_6 & -x_3 & -x_4 & -x_2 & x_1 \end{bmatrix}$$

All the designs in Example 1 maintain their orthogonality when the variables are replaced by any real value. This advantage will allow us to investigate and find the best possible replacement of the variables. By doing so, high efficiency is acheived for the designs that will be generated by the proposed method, as described in the following sections.

III. METHODOLOGY

In this section, a generalized method is presented that incorporates many known methods in the literature as special cases. The idea of this methodology is to introduce the use of orthogonal matrices in a block structure to generate the axial points. This will provide huge flexibility in the choices of matrices and will allow better coverage of the space of interest. The method is based on a block structure that is presented in this section. In the followings, $0_{n\times m}$ is used to denote an $n \times m$ matrix with all its entries equal to zero. Dimentions $n \times m$ will be ommited when they are obvious. The following Lemma is very important in our approach.

Lemma 1: If there are t orthogonal square matrices T_i of orders $n_1, n_2, \ldots, n_t$. Then, the following structure will give an orthogonal square matrix of order $n = n_1 + n_2 + \ldots + n_t$:

$$\mathbf{T}=\begin{pmatrix} 0_{n_1\times n_t} & \cdots & 0_{n_1\times n_2} & \boxed{T_1} \\ 0_{n_2\times n_t} & \cdots & \boxed{T_2} & 0_{n_2\times n_1} \\ \vdots & \iddots & \vdots & \vdots \\ \boxed{T_t} & \cdots & 0_{n_t\times n_2} & 0_{n_t\times n_1} \end{pmatrix}.$$

Proof: Since all T_i matrices are orthogonal then $\mathbf{T}'\mathbf{T}$ will be a diagonal matrix and so $\mathbf{T}$ is an orthogonal $n \times n$ matrix.

Remark: Lemma 1 is essential as it provides a useful alternative (the orthogonal square matrix $\mathbf{T}$) for the axial part of a new generalized CCD. The method is general and works for any number of blocks $t = 1, 2, \ldots.$. The special cases for $t = 1$ (see for example section II.A) and $t = 2$ will be explicitly explored in this paper.

Example 2: If $t = 2$ is used and the following matrices are selected as the needed blocks

$$\left.\begin{array}{ll} T_1 = \mathrm{OD}_4, & 4\times 4\text{matrix} \\ T_2 = b, & 1\times 1\text{matrix} \end{array}\right\} \Longrightarrow k = 4 + 1 = 5,$$

then the generated orthogonal matrix $\mathbf{T}$ is a 5×5 matrix.

In the following, the proposed construction method is described and illustrated for a modified CCD in the special cases of $k = 5, 7, 9, 11, 13,$ and 15 factors. The method builds a three-part design matrix $\mathbf{X}$ which will be suitable to fit a second-order response surface model (2) as follows:

$$X=\begin{bmatrix} F_k \\ V_k \\ C_k \\ -V_k \end{bmatrix},$$

where F_K is the factorial part, V_k the axial part and C_k the center points.

Step 1: Factorial part F_k

The k needed balanced columns are selected from an already known two-level design with suitable properties. For example, one can use columns from a 2^{k-p} fractional factorial design or select any k columns from a Hadamard matrix of order n_f. The columns chosen for the factorial part should be coming from an orthogonal two-level design so that the orthogonality of the composite designs is ensured. This part of the design is called the **F** part. So, choosing the factorial part is based on the criteria used to evaluate the design. In this paper, the columns of the factorial part are chosen in such way so that the derived composite design maximizes the D-value and has the orthogonality property.

Step 2: Axial part V_k

The selection of the axial part is crucial for the presented methodology. A few possible choices that are used in this paper will be shown, but there are a lot of other options that work as well for the new general developed method. When looking for composite designs it is desirable that these satisfy the following three properties: a) orthogonality, b) minimum number of runs and c) high D-value. In the case of designs with an odd number of factors, all three properties a), b), and c) are hard or impossible to achieve in one design. The trivial choice of axial part in the classic response surface designs, such as the central composite designs, gives only two (a and b) out of the three desirable properties. All other possible choices of axial parts require even orders to just achieve orthogonality [24]. The proposed method can be applied to generate designs with either even or odd number of factors. The designs generated with even number of factors have the same parameters and properties as the optimal designs in the literature. The interesting and new cases of of the construction methodology described in this paper, are those for designs of odd number of factors, as designs with these parameters could not exist previously. Examples of designs with $k = 5, 7, 9, 11, 13$ and 15 factors satisfying all three properties a), b) and c) are presented for the first time in this paper.

There are many possible choices of T_i for the suggested orthogonal blocked structure of the axial points, but one choice is presented that provides a higher D-value for the generated design in comparison to the known results.

To achieve finding the best D-value, there are a number of parameters that needs to be tested. For each case, a computer function using Matlab software is written to perform an exhaustive search. The best parameters were kept at each step and were used to produce the design with best D-values. All the variables on the design were replaced by integer values (−1,0,1) and the optimal case was kept. These 3 values were investigated as they perform the edges of the multidimensional hypercube and it is proofed that the optimal will occur in one of those edges. See for example [25].

In the following, the structures for generating the new axial parts of the proposed designs are developed and presented. This will be particularly helpful and will provide a direct construction when the number of factors is $k = 5, 7, 9, 11, 13$ and 15.

i. For $k = 5$ factors, the orthogonal design $\mathrm{OD}(4; 1, 1, 1, 1)$ is used to start the exhaustive search. Then, the OD_4 matrix of axial runs is extended into a 5×5 matrix of axial runs using the following structure:
$$V_5 = \begin{pmatrix} 0_{4\times 1} & \mathrm{OD}_4 \\ a & 0_{1\times 4} \end{pmatrix}.$$
The variables x_1, x_2, x_3, x_4 are suitably replaced by elements from the set $\{0, \pm a\}$. The best replacement of the variables (with respect to the D-value criterion) is selected by an exhaustive computer search.

ii. For $k = 7$ factors, the orthogonal design $\mathrm{OD}(6; 4, 1)$ is used to start the exhaustive search. Then, the OD_6 matrix of axial runs is extended into a 7×7 matrix of axial runs using the following step:
$$V_7 = \begin{pmatrix} 0_{6\times 1} & \mathrm{OD}_6 \\ a & 0_{1\times 6} \end{pmatrix}.$$
The variables x_1, x_2 are replaced by elements from the set $\{0, \pm a\}$. The best replacement of the variables (with respect to the D-value criterion) is selected by an exhaustive computer search.

iii. For $k = 9$ factors, the orthogonal design $\mathrm{OD}(8; 1, 1, 1, 1, 1, 1, 1, 1)$ is used to start the exhaustive search. Then, the OD_8 matrix of axial runs is extended into an 9×9 matrix of axial runs using the following step:
$$V_9 = \begin{pmatrix} 0_{8\times 1} & \mathrm{OD}_8 \\ a & 0_{1\times 8} \end{pmatrix}.$$
The variables $x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8$ are replaced by elements from the set $\{0, \pm a\}$. The best replacement of the variables (with respect to the D-value criterion) is selected by an exhaustive computer search.

iv. For $k = 11$ factors, the orthogonal design $\mathrm{OD}(8; 1, 1, 1, 1, 1, 1, 1, 1)$ is used to start the exhaustive search. Then, the OD_8 matrix of axial runs is extended into a 10×10 matrix by including the orthogonal design $\mathrm{OD}(2; 1, 1)$ as a second block and then the 10×10 matrix is extended into an 11×11 matrix of axial runs in the following structure:
$$V_{11} = \begin{pmatrix} 0_{8\times 1} & 0_{8\times 2} & \boxed{\mathrm{OD}_8} \\ 0_{2\times 1} & \boxed{\mathrm{OD}_2} & 0_{2\times 8} \\ a & 0_{1\times 2} & 0_{1\times 8} \end{pmatrix}.$$
The variables $x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9$ and x_{10} are replaced by elements from the set $\{0, \pm a\}$. The best replacement of the variables (with respect to the D-value criterion) is selected by an exhaustive computer search. Note that there may be up to 10 variables(elements) if different variables names in the two orthogonal designs that are used as blocks.

v. For $k = 13$ factors, the orthogonal design $\mathrm{OD}(8; 1, 1, 1, 1, 1, 1, 1, 1)$ is used to start the exhaustive search. Then, the OD_8 matrix of axial runs is extended into a 12×12 matrix by including the orthogonal design $\mathrm{OD}(4; 1, 1, 1, 1)$ as a second block and then the 12×12 matrix is extended into a 13×13 matrix of axial runs in the following structure:
$$V_{13} = \begin{pmatrix} 0_{8\times 1} & 0_{8\times 4} & \boxed{\mathrm{OD}_8} \\ 0_{4\times 1} & \boxed{\mathrm{OD}_4} & 0_{4\times 8} \\ a & 0_{1\times 4} & 0_{1\times 8} \end{pmatrix}.$$
The variables $x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8$ are replaced by elements from the set $\{0, \pm a\}$. The best replacement of the variables (with respect to the D-value criterion) is selected by an exhaustive computer search. Again, it is possible to have up to 12 variables (elements), in the axial part.

vi. For $k = 15$ factors, the orthogonal design $\mathrm{OD}(8; 1, 1, 1, 1, 1, 1, 1, 1)$ is used to start the exhaustive search. Then, the OD_8 matrix of axial runs is extended into a 12×12 matrix by including the orthogonal design $\mathrm{OD}(4; 1, 1, 1, 1)$ as a second block and then the 12×12 matrix is extended into a 14×14 matrix of axial runs by including the orthogonal design $\mathrm{OD}(2; 1, 1)$ as a third block and then the 14×14 matrix is extended into a 15×15 matrix of axial runs using the following structure:
$$V_{15} = \begin{pmatrix} 0_{8\times 1} & 0_{8\times 2} & 0_{8\times 4} & \boxed{\mathrm{OD}_8} \\ 0_{4\times 1} & 0_{4\times 2} & \boxed{\mathrm{OD}_4} & 0_{4\times 8} \\ 0_{2\times 1} & \boxed{\mathrm{OD}_2} & 0_{2\times 4} & 0_{2\times 8} \\ a & 0_{1\times 2} & 0_{1\times 4} & 0_{1\times 8} \end{pmatrix}.$$
The variables $x_1, x_2, \ldots, x_{14}$ are replaced by elements from the set $\{0, \pm a\}$. The best replacement of the variables (with respect to the D-value criterion) is selected

by an exhaustive computer search. In this case, the maximum possible number of variables(elements) in the axial part is 14.

This axial part is called the V part. A number n_c is selected as needed and the corresponding $n_c \times k$ matrix of center points is generated. This part of the design is called the center points (or C part). Note that any design which is constructed by the above process satisfies the orthogonal quadratic effects (OQE) property. Also, alternative choices of $T_i s$ such as $\mathrm{OD}_6 + \mathrm{OD}_8$ have been tested and gave designs with less D-value.

Remark: Note that the classical CCD can be considered as a special case of the presented method with axial points being of this form with $t = 1$ and T_1 being a multiple of the identity matrix.

The special case for $t = 1$ and axial parts other than the identity matrix was studied in [19]. Note that the approach with $t = 1$ is not suitable to study the case of $k \times k$ orthogonal matrices of many odd values of k. In this paper, it is illustrated how this extension can easily overcome these difficulties, even for $t = 2$, and generate orthogonal RSM designs using the proposed $k \times k$ orthogonal matrices as axial parts when k is odd. Illustrative examples of the new designs with improved properties are explicitly provided for $k = 5$ and $k = 9$. More results and more new designs that are obtained by the proposed method are tabulated and presented in section IV.

Remark: With the proposed method, all the known designs in [19] can be regenerated. Furthermore, this method was able to discover new designs in cases of odd number of factors with the orthogonality property.

The construction method is illustrated with the help of the following explicit examples.

Example 3: For the design with $k = 5$ factors and $n = 26$ runs, five columns out of a Hadamard matrix of order 16 are selected for the factorial part. To do this, all possible choices of 5 columns are searched from all 5 inequivalent Hadamard matrices of order 16. For the axial part, the orthogonal design OD_4 (x_1, x_2, x_3, x_4) of order 4 is used and the variables x_1, x_2, x_3, and x_4 are replaced by a, 0, $-a$ and a, respectively. This can be written as OD_4 $(a, 0, -a, a)$. In short, this is one of the best replacements of the variables from the set $\{0, \pm a\}$.

This result was discovered and verified by an exhaustive computer search but note that multiple alternative replacements gave the same best result, with respect to the D-value criterion. The axial part is constructed by extending the 4×4 orthogonal matrix using the method that was described in section III. The structure of the desirable composite design X is $X' = (F', V', C', -V'))$, where F and V are defined as Eq. (4) and Eq. (5), shown at the bottom of the page. If needed, one $C = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ or more central points can be added. In this illustrative example, center points are not added, but this can be done as and when needed by the practitioners.

The produced final design matrix $X_{26,5}$ as (6), shown at the bottom of the page. can be used to fit a sequential

$$F = \begin{pmatrix} 1 & 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 & -1 \\ -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 \end{pmatrix} \tag{4}$$

$$V = \left(\begin{array}{c|cccc} 0 & a & 0 & a & a \\ 0 & 0 & a & -a & a \\ 0 & -a & a & a & 0 \\ 0 & -a & -a & 0 & a \\ \hline a & 0 & 0 & 0 & 0 \end{array}\right) \tag{5}$$

$$X'_{26,5} = (F'; V'; -V') = \left(\begin{array}{c||cccc|c||cccc|c} ++++++++-------- & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & -a \\ \hline ++++----++++---- & a & 0 & -a & -a & 0 & -a & 0 & a & a & 0 \\ ++--++--++--++-- & 0 & a & a & -a & 0 & 0 & -a & -a & a & 0 \\ +-+-+--++-+-+-+- & a & -a & a & 0 & 0 & -a & a & -a & 0 & 0 \\ -++-+-+-+--+-++- & a & a & 0 & a & 0 & -a & -a & 0 & -a & 0 \end{array}\right) \tag{6}$$

TABLE 2. The generated designs.

Design parameters			Design construction		
Name	p	(n_f, n_c, n_a)	Factorial Part F (coded runs)	Axial Part V (coded runs)	D-val $a = 1$
$D_{5,22}$	21	$(12, 0, 5)$	0,6,7,9,11,12,17,18,21,26,28,31	13,61,65,75,81	311
$D_{5,26}$	21	$(16, 0, 5)$	30,29,27,24,23,20,18,17,15,12,10,9,6,5,3,0	31,16,66,73,81	457
$D_{5,30}$	21	$(20, 0, 5)$	31,30,29,26,25,22,20,19,17,16, 13,12,11,10,8,7,6,5,3,0	39,64,59,22,81	424
$D_{5,34}$	21	$(24, 0, 5)$	30,30,29,27,25,24,23,21,20,18,18,17,15,12,12, 11,10,9,7,6, 5,3,0,0	31,16,66,73,81	448
$D_{7,38}$	36	$(24, 0, 7)$	127,58,18,92,113,21,67,7,110,44,33,72,103, 10,34,13,105,68,118,31,91,52,57,80	1791,597,199,795,265,817,1001	348
$D_{9,55}$	55	$(36, 1, 9)$	17,28,34,39,41,69,74,114,125,150,154,173,174, 193,194,213,249,254,267,276,280,311,332,335, 358,371,376,403,415,417,420,424,452,459,496,511	1063,4809,5924,5622,1636,4918, 1585,4695,6561	153
$D_{11,78}$	78	$(56, 0, 11)$	2047,2047,1751,1899,949,474,1261,630,315,1181, 1614,807,403,201,100,1074,537,1292,646, 1347,1697,1872,936,1492,746,1397,1722, 861,1454,1839,919,459,1253,1650,1849,924,1486, 743,371,1209,604,302,151,75,37,1042,1545,1796, 1922,1985,992,1520,760,380,1214,1631	276,181,4404,749,4866,811, 2700,1557,32805,26244,59049	139
$D_{13,106}$	105	$(80, 0, 13)$	4096,6448,7320,7756,5926,7059,7625,5860,4978, 6585,7388,7790,7991,6043,7117,5606,4851,6521, 5308,6750,7471,7831,8011,8101,8146,6121,7156, 7674,5885,4990,4543,4319,6255,7223,5659,4877, 4486,6339,5217,6704,5400,6796,5446,6819,5457, 6824,7508,7850,5973,5034,6613,7402,7797,7994, 6045,5070,6631,5363,4729,4412,4254,4175,4135, 6163,5129,6660,7426,5761,6976,5536,4816,4456, 4276,6234,7213,5654,4875,6533,5314,4705	5417,6037,4994,1456,4281,6229,3274,4076, 419904,511758,111537,387099,531441	218
$D_{13,110}$	105	$(84, 0, 13)$	4096,6760,7476,5786,6989,7590,5843,4969,6580, 5338,6765,7478,7835,8013,6054,5075,4585,6388, 7290,5693,4894,4495,6343,5219,6705,5400,6796, 7494,7843,8017,8104,8148,8170,6133,7162,5629, 4862,6527,7359,7775,5935,7063,7627,5861,4978, 6585,5340,4718,4407,6299,7245,5670,6931,5513, 4804,4450,4273,4184,4140,4118,6155,5125,6658, 5377,6784,7488,7840,5968,5032,6612,7402,7797,5946, 5021,4558,4327,6259,5177,6684,7438,5767,4931,6561,5328	4829,2186,5665,3146,5489,3346,5793,3530,400221, 170586,275562,426465,531441	271
$D_{15,136}$	136	$(104, 2, 15)$	0,466,233,16500,24634,28701,14350,7175,3587,18177, 25472,12736,22752,11376,5688,19228,25998,29383, 14691,23729,11864,5932,19350,26059,29413,14706, 7353,3676,18222,25495,29131,30949,31858,32313, 32540,16270,8135,4067,18417,9208,20988,26878, 13439,23103,27935,30351,15175,23971,28369,30568, 15284,24026,12013,22390,11195,5597,19182,9591, 4795,2397,1198,16983,8491,4245,18506,25637,12818, 22793,11396,5698,19233,26000,13000,22884,27826, 30297,31532,15766,24267,28517,14258,23513,11756, 22262,11131,5565,2782,17775,8887,4443,2221, 17494,8747,4373,18570,9285,21026,26897,29832, 14916, 7458,3729,1864,932	2177,2797,3131,3967,4235,6191,3305,4089,170586, 209952,301806,275562,1062882,1062882,4782969	97
$D_{15,138}$	136	$(108, 0, 15)$	32735,23145,27956,30378,15205,23986,12009,22388, 27578,30189,15094,7547,3773,1902,951,491,16629, 24698,12349,6190,19495,26147,13089,6560,3296, 1648,824,428,16614,24691,28729,14380,23590,11811, 22305,27552,30176,15088,23928,28348,14190,23479, 11755,5877,19322,26045,29422,14711,7355,20077, 10038,21419,27109,13554,32704,23110,27907,30353, 15192,23948,11990,22347,27525,30162,15049,7492, 3714,1873,904,468,16586,24645,12290,6161,19480, 26140,13086,6559,3295,1615,775,403,16601,24652, 28678,14355,23577,11804,22302,27551,30175,15055, 28291,14161,23432,11732,5834,19269,9602,23879, 21201,10568,5252,19026,9481,21140,26970,13453	4829,2186,5665,3146,5489,3346,5793,3530,400221,170586, 275562,426465,3188646,1594323,4782969	162

second-order response surface model in (2) and achieves a higher D-value than any known design in the literature using minimum runs. The D-value of this design and the D-value of all the generated designs are presented in Table 2. This table shows the design parameters, design construction, and evaluation. The first column of Table 2 shows the design which is denoted by $D_{k,n}$. Here k is the number of factors and n the number of runs. The second column, p, corresponds to the number of parameters in the full second-order model having k factors. The third column shows the number of runs for the factorial part n_f, the number of centre points n_c, and the number of runs n_a for the positive axial points. Fourth column gives the factorial part F in coded form, as described by the coding scheme. Fifth column presents the axial part V in coded form as described. Finally, sixth column presents a rounded D-value of the design when $a = 1$ for comparison reasons.

Example 4: For the design with $k = 9$ factors and $n = 55$ runs, nine columns out of a Hadamard matrix of order 36 are selected for the factorial part. To do this, all possible choices of 9 columns are searched from a large number of inequivalent Hadamard matrices of order 36. Note that

Hadamard matrices of order 36 have not yet been classified so our search for the selection of the best columns from Hadamard matrices of order 36 was not exhaustive in this case. For the axial part, the orthogonal design OD_8 $(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8)$ of order 8 is used and the variables $x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8$ are replaced by the values 0, a, a, a, 0, a, 0, a. These values maximize the D-value among all the possible selections of eight values from the set $\{0, \pm a\}$. In short, this is one of the optimal replacements of the variables using elements from the set $\{0, \pm a\}$. This result was found and verified by a computer search. The axial part is constructed by extending the 8×8 orthogonal matrix using the method that was described in section III. The structure of the desirable composite design X is $X' = (F', V', C', -V'))$, where F and V are defined as Eq. (7) and Eq. (8), shown at the bottom of the page.

$$F = \begin{pmatrix}
-1 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 \\
-1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 \\
-1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 \\
-1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 \\
-1 & -1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 \\
-1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 \\
-1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 \\
-1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & -1 \\
-1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 \\
-1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\
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-1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 \\
-1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & 1 \\
-1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 \\
-1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
-1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 \\
-1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\
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1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 \\
1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}, \tag{7}$$

$$V = \begin{pmatrix}
0 & 0 & a & a & a & 0 & a & 0 & a \\
0 & -a & 0 & a & -a & a & 0 & a & 0 \\
0 & -a & -a & 0 & a & 0 & a & 0 & -a \\
0 & -a & a & -a & 0 & a & 0 & -a & 0 \\
0 & 0 & -a & 0 & -a & 0 & a & -a & a \\
0 & -a & 0 & -a & 0 & -a & 0 & a & a \\
0 & 0 & -a & 0 & a & a & -a & 0 & a \\
0 & -a & 0 & a & 0 & -a & -a & -a & 0 \\
a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} \tag{8}$$

The whole design $X_{55,9}$, is presented in coded form in Table 2.

Remark: The Coding Scheme To save space, the obtained designs are presented in a coded form. For the factorial part, -1 is replaced by zero and each run is treated as a binary number converted to the decimal system. For the axial part, a is set to 1, and every run is treated as a vector over GF(3) where -1 is replaced by 2 and written as a number over the decimal system. The inverse process is followed to get the design point i.e. converting the provided number from decimal system to binary or ternary for the factorial and axial part respectively. The number of factors k represents the length of each run, and it is necessary for both the coding and decoding scheme.

Example 5: In the design with 5 factors and 26 runs that is given in (6), the first run of the factorial part is $\begin{bmatrix}1 & 1 & 1 & 1 & -1\end{bmatrix}$. The coding scheme is illustrated by using this run. Replace -1 to zero and then convert to a decimal number: $\begin{bmatrix}1 & 1 & 1 & 1 & -1\end{bmatrix} \rightarrow \begin{bmatrix}1 & 1 & 1 & 1 & 0\end{bmatrix} \rightarrow 30$. All the factorial runs are coded following a similar process. The second run of the axial part is $\begin{bmatrix}0 & 0 & a & -a & a\end{bmatrix}$. Replace a by 1, then -1 to 2 and finally convert the resulting vector over $GF(3)$ into a decimal number: $\begin{bmatrix}0 & 0 & a & -a & a\end{bmatrix} \rightarrow \begin{bmatrix}0 & 0 & 1 & -1 & 1\end{bmatrix} \rightarrow \begin{bmatrix}0 & 0 & 1 & 2 & 1\end{bmatrix} \rightarrow 13$. All the axial runs are coded following a similar process. All coded runs of the designs are given in Table 2.

IV. RESULTS

In Table 3, AVP and MVP are generated and these results are helpful for practitioners when they are conducting an experiment as the values of AVP and MVP are presented, hence they choose designs that fit their experiments.

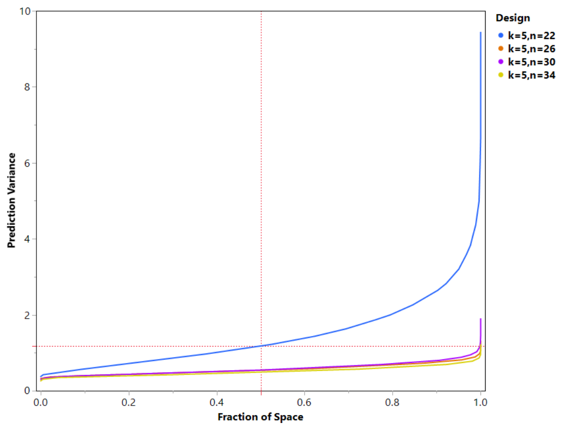

FIGURE 1. **Design space plot of $k = 5$ with a different number of runs.**

Fig. 1 is the fraction of the design space plot of four different designs of five factors and a different number of runs, with the prediction variance values ranging from 0 to 10. As depicted in the figure, the relative prediction variance for the 22-run design is uniformly higher than other three designs. Moreover, though the three other designs (26, 30, and 34 runs) are roughly the same size, it can be seen that the 26-run and 34-run designs are slightly smaller than the 30-run design. The figure also reveals that 100% of the prediction variance values of both the 26-run and 34-run designs are below 1.3, while about 90% of the prediction variance value of the 30-run design are also below 1.3. Lastly, approximately 50% of the prediction variance value of the 22-run design are above the 1.2. Fig. 2 is the fraction of the design space plot for five designs with a varying number of factors and runs, and all the designs' prediction variance values range from 0 -25. For the 38-run design of seven factors, its relative prediction variance is uniformly higher than four other designs in the plot, and also, about 55% of its prediction variance values are higher than approximately 1.25. The 55-run design of nine factors has about 90% of its prediction variance values below approximately 1.25, and its relative prediction variance is uniformly lower than the 38-run design and almost the same as the 110-run design. As for the 78-run design, the figure reveals that 100% of its prediction variance values are below 1.25 and its relative prediction variance is uniformly smaller than all the other designs in the plot. The 106-run and 110-run designs of thirteen factors have overlapping plots, revealing that both have approximately 80% of their prediction variance values below 1.25 and both have uniformly higher prediction variance than the 55-run and 78-run designs.

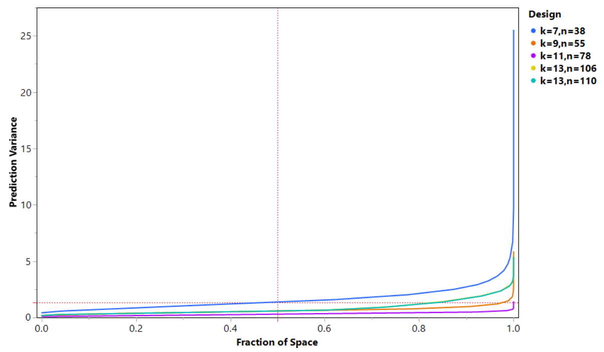

FIGURE 2. **Design space plot of $k = 7, 9, 11,$ and 13 with a different number of runs.**

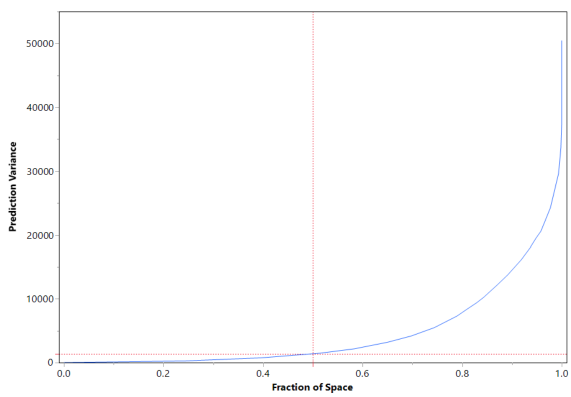

FIGURE 3. **Design space plot of $k = 15$.**

As shown in Fig. 3, this design prediction variance values ranged from 0 to 50,000. Approximately 40% of the relative prediction variance values are below 1000 and starting at 50% up to 100%, the prediction value recorded an increased value ranging from 1,000 to 50,000.

TABLE 3. Average prediction of variance and maximum prediction variance of the proposed designs.

Design	AVP	MVP	
		Value	Factors setting
K=5, n=22	1.42	9.1	(-1,-0.760,-1,-160,1)
K=5, n=26	0.56	1.3	(-1, -2.06 $\times 10^{-10}$,1,-1,-1)
K=5, n=30	0.57	1.9	(-1,0.008,-1,-1,1)
K=5, n=34	0.51	1.22	(-1,-1,1,-1,0.011)
K=7, n=38	1.88	28.71	(1,-1,-1,1,1,1,-0.8)
K=9, n=55	34.68	1471.63	(-1,1,0.131,1,-0.904,-1,-1,-0.129,-1)
K=11, n=78	11.62	715.44	(-1,-1,1,-1,-1,0.95,1,-1,1,-1,-1)
K=13, n=106	22.05	1542.78	(-1,1,-1,1,1,-0.381,1,1,1,0.304,-1,1,-1)
K=13, n=110	6.47	219.9	(-1,-1,1,-1,1,-1,-1,-0.234,-1,-1,-1,-1,0.086)
K=15, n=135	691.9	9783	(1,-1,0.091,0.013,0.009,-0.051,0.081,0.002,0.036, 0.001,1,0.006,0.017,0.042,0.012)
K=15, n=138	440.6	5044	(0.019,0.005,-1, -0.032, 0.015,-0.031, 0.003,0.055, -0.017, -0.072,0.003,- 0.044, 0.072, 0.037, -1)

TABLE 4. Composite designs comparison with respect to D-value and (run sizes).

k	p	[13]	[16]	[16]	[10]	[26]	[15]	[19]	Proposed Designs
5	21	241(21)	259(22)	355(26)	440(26)	308(36)	178(21), 259(22)	186(21), 276(22), 322(24)§, 440(26), 425(36)	311(22)§,457(26)§, 424(30)§, 484(34)§
7	36	197(36)	262(38)	226(38)	465(78)	269(36)	234(36)	291(36), 348(38)	348(38)
9	55	200(56)	246(58)	231(58)	480(146)	253(78)	222(56)	15(55), 313(56), 314(58)	153(55)§

§ states improvement of the D-value over all the designs known in the literature.

The proposed method to construct these designs is quite general and can generate designs with desirable properties. These designs are compared to the existing composite designs in the literature in Table 4. The designs which are constructed by the new method are given in Table 2.

Composite designs with the less number of runs are generated as the composite designs available in the literature and show that the method can generate the same designs as the existing composite designs and can also generate more efficient composite designs in terms of D-value with the same design parameters. These results are presented in Table 4. In the first two columns of this table, the number of factors k of the design and the number of parameters p in the full second-order model are presented. Then, the rounded D-values are given and in parentheses the total run sizes of the composite designs. Also, the proposed designs are compared with the existing composite designs in [10], [13], [15], [16], [26], and [19].

From the properties of the designs, it is anticipated that if the proposed designs are applied to any experiments that were previously conducted with the use of composite designs with lower D-values, then either (i) the cost of the experimentation will be reduced (similar power and D-value with less runs), or (ii) the power of the tests will be improved (higher power and D-value with a similar number of runs)-see Table 3. Moreover, all proposed designs are orthogonal and this was not possible in the existing literature before for this combination of factor size and run size. Therefore, in all cases, the presented designs are improvments over the existing designs except for the 7 factor case, where the same highest-known D-value was also achieved as in [19] and this is the optimal design in this class. Designs for 11, 13, and 15 factors are new and constructed in this paper for the first time with an extremely small number of runs and a high D-value. It can be seen that the suggested method generates efficient and economical response surface designs combining known designs in a new orthogonal structure. The axial points of the classical central composite design are changed to the best edge points through a computer search. The sequential experimentation, that is attained by this approach, gives orthogonal designs with higher efficiency. The newly generated designs also have a minimum number of runs and higher D-values than all the known designs in the literature.

Finally, comparing to the existing practical application in [5], the proposed design of five factors in this paper has 6 runs less and higher D-value from the design used in [5]. Thus, the results in this paper shows that the proposed designs can be useful to reduce the cost of materials used in the experiment and achieve the desired results in sufficient time.

V. CONCLUSION

New second order designs for response surface methodology are constructed and compared with the popular central composite designs and other types of response surface designs. The proposed designs are more effective in estimating the parameters in a second-order model in terms of D-value, as well as in minimizing the number of runs and in achieving orthogonality. The proposed designs are compared with other response surface designs in terms of D-value and proved to be superior. The proposed designs have a unique feature that do not exist before for the axial part. The axial part of the proposed designs maintains a minimum number of runs and orthogonality as well which result in more economical and more informative designs than current designs in the literature, in terms of D-value. Some limitations of the presented methodology include the order of designs that can be constructed. In this paper, the method is applied for finding D-optimal designs with factor size up to $k = 15$. Then next value ($k = 17$) was not feasible because it could not be completed in reasonable time. Improvements on the methodology and algorithm may allow a couple of more cases to be studied, but it really needs a breakthrough to achieve such designs in higher orders. One other issue is that the generated designs are based on second order models of the form (2) and might give poor results with respect to the D-values in higher order models. All practitioners need to be meticulous when applying the design techniques and always be aware of the risks that any modelling technique embeds.

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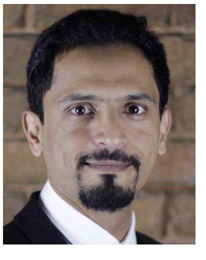

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