Efficiency of Custom A-, D-, and I- Optimal Designs Relative to CCD, BBD, and MCCD

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The efficiencies of custom A-, D-, and I-optimal designs are compared with the CCDs, BBDs, and MCCDs on standard and non-standard second-order models using the D-, G-, and A-efficiency metrics. Custom A-, D-, and I-optimal designs are constructed for the standard models but for the non-standard model, custom A-, D-, and I-designs with sample sizes 13, 15, 21, and 25 respectively are adapted from Iwundu and Israel (2024). The results of the evaluation of the designs are presented. The results show that for standard models, custom A-, D-, and I-optimal designs performed as well as the CCD but outperformed the BBD. Specifically, the D-optimal designs are more D-efficient. The A-, and I-optimal have the same result as the CCD for the three variables. For non-standard models, custom A-, D-, and I-optimal designs have larger efficiency values than the CCDs, BBDs, and MCCDs for specified design sizes. The D-optimal designs have larger D- and G-efficiency values. A-optimal designs have larger A-efficiency values and in most cases have the same efficiency value as the I-optimal design. Thus, custom designs can be adopted in the design of experiments for reliable and consistent results that meet experimental objectives.

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1.0 Introduction

Over the years, standard designs have gained wide applications in many scientific and industrial studies due to their flexibility. They have served as a building block of many experimentally based research and development studies (Johnson *et al*., 2011). Some of the standard designs include the 2^k or 3^k full factorial Designs and their associated fractions; Plackett-Burman designs, which bear some relationship with the 2^k series of fractional factorial designs; the Central Composite Design (CCD) and the Box-Behnken design (BBD). According to Nguyen and Piepel (2005), they have served as preferred response surface designs where the experimental regions of interest are either a sphere or a cube. Akinlana (2022) added that they are often associated with regular design regions and specific run sizes.

Standard or classical designs are proven to perform well under good experimental conditions that satisfy the research problem and the design specification. For example, consider the modelling approach described by Myers *et al*. (2016), where a second-order response surface model can explain

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the relationship between a response and multiple continuous factors. A common response surface design to determine the best factor settings is the Central Composite Design (CCD). The CCD is the most popular class of standard designs introduced by Box and Wilson (1951) for fitting quadratic models. The CCD is a second-order design that obtains information from a correctly planned factorial experiment, and it is made up of three components, namely, the factorial points, the axial points, and the centre points. The factorial points, also known as the cube points, are the vertices of the n-dimensional cube which are coming from a 2^k factorial design (or fractional factorial of resolution V) of the first-order model. They contribute substantially to the estimation of linear terms and two-factor interactions. The $2k$ axial points located on the axes of the coordinate system symmetrical to the centre point contribute to the estimation of the quadratic terms. The centre point, n_c is the point at the centre of the design space that provides an estimate for pure error. The total number of experimental runs associated with a CCD is $2^k + 2(k) + n_c$. Since the introduction of CCD by Box and Wilson (1951), the CCD has been used and studied by many researchers. Oyejola and Nwanya (2015) used optimality criteria to compare five different types of CCD when the star points are replicated. Bhattacharya (2021), explored three different types of CCD and their significance in various experimental designs. Iwundu and Oko (2021) examined the efficiency and optimality properties of four varieties of the CCD.

Another efficient second-order design introduced by Box and Behnken (1960) is the Box-Behnken Design (BBD). The BBDs are a class of rotatable or nearly rotatable three-level incomplete factorial designs developed as an alternative to the extensive full factorial design (Box and Behnken, 1960; Ferreira *et al*, 2007). The total number of experiments (N) required for the development of BBD is defined as $N = 2k(k - 1) + n_c$, (where k is the number of factors and n_c is the number of centre points) and the number of factors must be greater than 2. The designs are created to minimise the number of experiments, specifically in quadratic model fitting. According to Witek-Krowiak *et al*, (2014), the BBD is slightly more labour-efficient than the CCD but much more labour-efficient than the Full Factorial Design (FFD).

In constructing the BBD, two factors or treatments are paired together one at a time, in a 2^2 factorial design scaled ± 1 while the remaining factors are fixed at the mid-point, this implies that the BBD does not contain combinations for which all factors are simultaneously at their highest or lowest levels, unlike the CCD. Hence, the BBDs are useful in avoiding experiments performed under extreme conditions, for which unsatisfactory results might occur. Many studies have shown the application and efficiency of the BBD (Ye *et al*, 2017; Viana *et al*, 2020; Iwundu and Cosmos, 2022; Zambare *et al*, 2023).

Despite the usefulness of standard designs, a non-standard experimental situation may arise that could lead to the need for an alternative design. One such alternative design introduced by Iwundu (2018) is the Modified Central Composite Design (MCCD). Iwundu (2018) stated that the MCCD is a second-order design for non-standard models when knowledge of the non-standard model can be ascertained before experimentation or from a past experiment. The design is similar in structure to the CCD but constructed based on the principles of the loss function related to the hat matrix, H. As Iwundu and Otaru (2019) described, where there are multiple losses associated with the specified CCD portions, the less influential design points may be removed from the full CCD, resulting in a design that is similar in structure to the CCD known as the MCCD. Jaja *et al*, (2021), investigated the robustness of the CCD and MCCD in the presence of missing design points for non-standard models. It was observed from the result that the MCCD based on the available statistics is more A-optimal, but the CCD is more robust to missing observations. Again, Iwundu and Nwoshopo (2022) studied the efficiency of the Standard CCD and the MCCD with a five-variable non-standard model. The result showed that the D- and G-efficiencies of the design reduce for the CCD as the number of missing quadratic terms increases, but they increase for the MCCD as the number of missing quadratic terms increases.

Again, certain experimental situations such as non-standard models, irregular design regions, mixture experiments, etc, may lead to the need to create optimal designs using a computer algorithm (Kiefer and Wolfowitz 1959; Montgomery 2001). According to Smucker *et* al., (2018), optimal designs (designs created to satisfy certain optimality criteria) have become an alternative designs to classical designs, especially in non-standard situations, and are also as efficient as classical designs in some standard or unconstrained situations. When handling large factors, levels, or complex experimental spaces, it may be difficult for experimenters to manually search or evaluate all possible combinations of factor levels in a high-dimensional design space. Hence, computer algorithms are employed as viable tools to construct optimal designs based on mathematical optimisation techniques and statistical properties given the available resources and constraints (Akinlana 2022; Fela *et al,*2023; Ginocchi *et al*, 2024)

Among other computer programs, the JMP statistical software has shown wide applications in the construction of designs in certain experimental conditions, such as mixture experiments, mixed factor experiments, and non-standard models (Mei-Fen *et al.*, 2010). The JMP software includes a platform for custom design to provide users with the flexibility and capability to create experimental designs that are tailored to their specific research objectives and constraints. According to Johnson *et al.* (2011), rather than force a standard design into the space of the research problem, custom designs can be readily tailored to the problem and resource limitations.

In most second-order experiments, it may be difficult to combine all the factors, especially when the factors are large or a non-standard model is involved. This study is concerned with examining the quality of custom A-, D-, I-optimal designs and some other second-order designs, and with guidelines for choosing the appropriate design. Custom A-, D-, and I-optimal designs, CCD, BBD, and MCCD are constructed for second-order standard and non-standard models. For non-standard models, custom A-, D-, and I-optimal designs with sample sizes 13, 15, 21, and 25 with efficiency values are adapted from Iwundu and Israel (2024). Our interest in this work is to compare the efficiency and robustness of custom A-, D-, and I-optimal designs with the CCDs, BBDs, and MCCDs using standard and non-standard second-order models for specified design sizes, thereby deemphasising the use of standard designs in most inappropriate experimental situations. From the result, it is observed that custom A-D-, and I-optimal designs are efficient designs, especially in non-standard second-order models.

2. Methodology

2.1 Research Models

In Response Surface Methodology (RSM), standard designs are majorly constructed for fitting standard second-order models given as

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} {x_{ii}}^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + \varepsilon \qquad (1)$$

and written in matrix form as

$$y = X\beta + \varepsilon \qquad (2)$$

The vector y is a vector of observations with dimension $(N \times 1)$;
X is the model or design matrix, and it is a function of the model in use, with dimension $(N \times p)$;
β is the vector of unknown parameters of dimension $(p \times 1)$;
ε is the vector of random errors of dimension $(N \times 1)$ assumed to be independent and normally distributed with a mean 0 and variance σ^2; and
p is the total number of parameters in the specified model, and N is the sample size or number of experimental runs. The number of parameters, p, of a standard second-order model is determined by

$$p = \frac{(k+1)(k+2)}{2}$$

For a standard second-order model with three variables, the model with 10 parameters is given as

$$y\,(x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} {x_1}^2 + \beta_{22} {x_2}^2 + \beta_{33} {x_3}^2 + \varepsilon \qquad (3)$$

A four-variable standard second-order model containing 15 parameters is given as

$$y\ (x_1, x_2, x_3, x_4) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{14} x_1 x_4 + \beta_{23} x_2 x_3 + \beta_{24} x_2 x_4 + \beta_{34} x_3 x_4 + \beta_{11} {x_1}^2 + \beta_{22} {x_2}^2 + \beta_{33} {x_3}^2 + \beta_{44} {x_4}^2 + \varepsilon \qquad (4)$$

When some terms in the standard second-order models are adjudged insignificant and have been removed from the standard model given in Equation 1, the resulting model is known as a reduced or non-standard model. For this research, the non-standard models considered are;

i. $\hat{y}\ (x_1, x_2, x_3) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_{11} {x_1}^2$ (5)
(Source: Myers *et al*., 2009).

ii. $\hat{y}\ (x_1, x_2, x_3) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_{23} x_2 x_3 + \hat{\beta}_{33} {x_3}^2$ (6)
(Source: Ossia and Big-Alabo, 2022).

iii. $\hat{y}\ (x_1, x_2, x_3) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_{12} x_1 x_2 + \hat{\beta}_{13} x_1 x_3 + \hat{\beta}_{11} {x_1}^2$ (7)
(Source: Iwundu, 2018).

iv. $\hat{y}\ (x_1, x_2, x_3, x_4) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_4 x_4 + \hat{\beta}_{12} x_1 x_2 + \hat{\beta}_{23} x_2 x_3 + \hat{\beta}_{11} {x_1}^2 + \hat{\beta}_{44} {x_4}^2$ (Source: Iwundu and Otaru, 2019) (8)

2.2 Construction of Second-Order Designs

For a standard second-order model, the design measure, ξ_N supported by the vector of design points is formed as

$$\xi_N = \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \vdots \\ \underline{x}_N \end{bmatrix}$$

where $\underline{x}_i$ is the i^{th} discrete points in the design region χ, associated with the k controllable or independent variables.

An $N \times p$ model matrix is formed using the design measure and the specified model. For example, the CCD for a full parameter (p) model in k variables, N number of design points, and an axial distance α and n_c= 1 centre point is represented algebraically as;

$$X_{N\times p} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} & x_{11}x_{12} & x_{11}x_{13} & \cdots & x_{11}x_{1k} & {x_{11}}^2 & {x_{12}}^2 & \cdots & {x_{1k}}^2 \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} & x_{21}x_{22} & x_{21}x_{23} & \cdots & x_{21}x_{2k} & {x_{21}}^2 & {x_{22}}^2 & \cdots & {x_{2k}}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} & x_{n1}x_{n2} & x_{n1}x_{n3} & \cdots & x_{n1}x_{nk} & {x_{n1}}^2 & {x_{n2}}^2 & \cdots & {x_{nk}}^2 \\ 1 & -\propto & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \propto^2 & 0 & \cdots & 0 \\ 1 & \propto & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \propto^2 & 0 & \cdots & 0 \\ 1 & 0 & -\propto & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \propto^2 & \cdots & 0 \\ 1 & 0 & \propto & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \propto^2 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & -\propto & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & \propto^2 \\ \vdots & \vdots & \vdots & \vdots & \propto & \vdots & \vdots & \vdots & 0 & \vdots & \vdots & \vdots & \propto^2 \\ 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

For non-standard models, the columns of the model matrix X are reduced to the number of model parameters. Specifically, for the 5-parameter non-standard model in Equation 5 with one centre point, the model matrix for a CCD is represented as

$$X_{15\times 5} = \begin{bmatrix} 1 & x_{11} & x_{12} & x_{13} & {x_{11}}^2 \\ 1 & x_{21} & x_{22} & x_{23} & {x_{21}}^2 \\ 1 & x_{31} & x_{32} & x_{33} & {x_{31}}^2 \\ 1 & x_{41} & x_{42} & x_{43} & {x_{41}}^2 \\ 1 & x_{51} & x_{52} & x_{53} & {x_{51}}^2 \\ 1 & x_{61} & x_{62} & x_{63} & {x_{61}}^2 \\ 1 & x_{71} & x_{72} & x_{73} & {x_{71}}^2 \\ 1 & x_{81} & x_{82} & x_{83} & {x_{81}}^2 \\ 1 & -\propto & 0 & 0 & \propto^2 \\ 1 & \propto & 0 & 0 & \propto^2 \\ 1 & 0 & -\propto & 0 & 0 \\ 1 & 0 & \propto & 0 & 0 \\ 1 & 0 & 0 & -\propto & 0 \\ 1 & 0 & 0 & \propto & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The information matrix $X'X$ describes the amount of information the data provides about the unknown parameters. For this research, the information matrix is denoted as

$$J = X'X$$

The inverse of the information matrix is called the dispersion or variance-covariance matrix, and it is written as

$$W = (X'X)^{-1}$$

The dispersion matrix contains the variances (main diagonal elements) and the covariances (off-diagonal elements) of the model coefficients.

The moment matrix is also known as the Normalised Information Matrix (NIM) and is denoted as

$$M = \frac{X'X}{N}$$

where N is the total number of design points used.
NIM takes away the changes in the design size and makes the designs comparable.

Both CCDs and BBDs are frequently utilised designs and can be found in several literature on optimal design of experiments, including Anslan and Cebeci (2006); Myer *et al*. (2009); Maran *et al.* (2013); Iwundu and Oko (2021), etc.

MCCDs are second-order designs that are similar in structure to the CCD but created for non-standard models based on the principles of the loss function related to the hat matrix, H (Iwundu, 2018). The construction of an MCCD follows five basic steps;

Step 1: Use an available CCD on a given non-standard model.

Step 2: Form an $N \times N$ hat matrix given as, $H = X(X'X)^{-1}X'$, which is a function of the model matrix of the CCD. The hat matrix is a square symmetric idempotent matrix expressed as,

$$H = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1N} \\ h_{21} & h_{22} & \cdots & h_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ h_{N1} & h_{N2} & \cdots & h_{NN} \end{bmatrix}$$

p represents the number of model parameters, h_{ii} called the hat-values are the elements along the main diagonal, and h_{ij} are the off-diagonal elements.

Step 3: Examine the main diagonal elements of the hat matrix to identify the elements with less influential points.

Step 4: Eliminate the less influential points from the CCD.

Step 5: The remaining design points form the MCCD.

Custom designs are created using a computer program depending on the experiment's goal and experimental conditions. The approach requires specifying a model, the expected number of runs, the region of interest, and an optimality criterion (Montgomery, 2001). This work adapted some custom A-. D-, and I-optimal designs from Iwundu and Israel (2024). Each custom design is created based on its respective optimality criteria. That is, a custom A-optimal design is constructed based on the A-optimality criterion; a custom D-optimal design is constructed based on the D-optimality criterion; and a custom I-optimal design is constructed based on the I-optimality criterion. For more on these optimality criteria and associated efficiency functions, see Rady *et al*. (2009), Goos *et al*. (2016), and Mwangi *et al*. (2019).

2.3 Design Efficiencies

The goal in most experiments is to find designs that are optimal for regression parameter estimation as well as designs optimal for prediction precision. Thus, an efficient design can greatly improve the analysis of an experiment (Alzahrani, 2024). Design efficiencies are efficiency metrics used in the optimal design of experiments to evaluate and compare the quality of different experimental designs. Each efficiency measure offers specific insight into the performance of the design, aiding in the selection of the most appropriate design for a given experimental objective. The efficiency of a design can be quantified in an interpretable form using one or more efficiency metrics (Iwundu and Nwoshopo, 2022). Wayonyi *et al.* (2021) explored and examined the D-, A-, I-, and G-optimality criteria and efficiencies in choosing a good split-plot design in mixture modelling. Akinlana (2022) utilised the D, A, G, and I efficiency metrics in comparing a D-optimal design with a Resolution IV Unique Factor Central Composite Design. Oladugba and Yankam (2022) employed the D-, A-, and G-criterion to evaluate third-order Orthogonal Uniform Composite Designs ($OUCD_4$) and Orthogonal Array Composite Designs ($OACD_4$) for a spherical region ($\alpha = \sqrt{k}$) with 5 centre points and factors ranging from 2 to 7. Iwundu and Cosmos (2022) used the D and G efficiency metrics to evaluate the efficiency of seven seven-variable Box-Behnken Design with varying centre points for full and reduced models.

This work employed the D, G, and A efficiency metrics in assessing the qualities of various second-order designs. In optimal design where parameter estimation is paramount, D-efficiency is very crucial. It measures the overall amount of information provided by the design about the model parameters. It is measured in percent and a high D-efficiency implies that the parameter estimates will have lower variances, leading to more precise estimates. D-efficiency is written symbolically as

$$D - efficiency = 100 * \frac{|X'X|^{\frac{1}{p}}}{N} \qquad (9)$$

where p denotes the number of parameters in the model, N is the sample size, and $|X'X|$ is the determinant of the information matrix.

The G-efficiency which is expressed in percent handles the worst-case prediction variance. The worst-case prediction variance is important because it highlights the most extreme scenarios where the models' prediction might be highly unreliable. Hence, the G-efficiency ensures that no point in the design space has an excessively high prediction variance thus, making the model suitable for prediction. It is represented as

$$G - efficiency = 100 \left(\frac{p}{\text{N} * \text{SPV}_{max}}\right) \quad (10)$$

where N represent the design size, p denote the parameters in the model, and SPV_{max} is the maximum scaled prediction variance at any point given as;

$$\text{SPV} = N\underline{x}'(X'X)^{-1}\underline{x}$$

where $\underline{x}$ is the design region.

The A-efficiency is concerned with the trace of the inverse of the information matrix. It measures the average variance of the parameter estimates. High A-efficiency indicates lower variance of the parameter estimates enhancing the reliability of the results. It is written symbolically as;

$$A - efficiency = \frac{100 * p}{trace\,[N(X'X)^{-1}]} \quad (11)$$

Where N is the sample size, p denotes the parameters in the model, and $(X'X)^{-1}$ is the dispersion matrix

3. Numerical Illustrations

3.1 Case 1: Standard second-order model with 10 parameters

The illustration considers the standard second-order model in three variables given in Equation (3)

The CCD with $\alpha = 1$ and one center point (n_c) is

$$\xi_{15} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

The BBD with 13 design points and $n_c = 1$ is given as

$$\xi_{13} = \begin{pmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

A 15-point Custom A-optimal design with one center point for the three variables is given as

$$\xi_{15} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & 0 & 0 \\ -1 & -1 & -1 \\ 0 & 1 & 0 \\ -1 & -1 & 1 \\ -1 & 0 & 0 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \\ 0 & 0 & 0 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & -1 & -1 \\ 0 & 0 & 1 \end{pmatrix}$$

A 15-point Custom D-optimal design with one center point is given as

$$\xi_{15} = \begin{pmatrix} 1 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & 0 & 1 \\ 1 & -1 & -1 \\ -1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 0 \\ -1 & -1 & -1 \\ 1 & -1 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \\ -1 & 1 & 1 \\ 0.08 & -1 & 0.07 \end{pmatrix}$$

A Custom I-optimal design with one center point is given as

$$\xi_{15} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ 1 & -1 & -1 \\ 0 & -1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \end{pmatrix}$$

Table 1: Efficiency Values of the Second-order Designs for the Standard Model in Three Variables

Design Size (N)	Design Type	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)
15	CCD ($\alpha = 1$)	44.72	83.62	31.29
13	BBD ($n_c = 1$)	37.88	76.92	22.38
15	Custom A-optimal Design	44.71631	83.62369	31.29074
15	Custom D-optimal Design	45.51884	79.56446	28.79352
15	Custom I-optimal Design	44.71631	83.62369	31.29074

3.2 Case 2: Standard second-order model with 15 parameters

considering the four-variable standard model in Equation (4) with 15 parameters,

The Central Composite design (CCD) with 25 design points, $\alpha = 1.0$, and $n_c = 1$ is given as;

$$\xi_{25} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The Box-Behnken Design (BBD) with 25 design points and $n_c = 1$ for the four variables is given as;

$$\xi_{25} = \begin{pmatrix} -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ -1 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & -1 & 0 \\ 1 & 0 & -1 & 0 \\ -1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & -1 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & -1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

For the four variables, a Custom A-optimal design with one center point is given as

$$\xi_{25} = \begin{pmatrix} 1 & -1 & -1 & -1 \\ 0 & -1 & 1 & -1 \\ 1 & 1 & -1 & 0 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 0 & -1 & 1 \\ 0 & 1 & 1 & 1 \\ -1 & -1 & 0 & -1 \\ 1 & -1 & 1 & 0 \\ -1 & 1 & -1 & 1 \\ -1 & 0 & -1 & -1 \\ 1 & 0 & 1 & 1 \\ -1 & 1 & 0 & -1 \\ 1 & 1 & 1 & -1 \\ 0 & 1 & -1 & 0 \\ -1 & 1 & 1 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ -1 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & 1 \\ -1 & 0 & 0 & 1 \\ -1 & -1 & -1 & 0 \end{pmatrix}$$

A Custom D-optimal design with one center point is

$$\xi_{25} = \begin{pmatrix} -1 & 1 & 0 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -0.25 & 1 & 1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & -1 \\ 0 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & 0 & 1 \\ -1 & 1 & 1 & 0 \\ -1 & 1 & -1 & -1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ -1 & -1 & -1 & 0 \\ -1 & 0 & -1 & 1 \\ 0 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & 0 \\ 0 & -1 & -1 & 1 \end{pmatrix}$$

A Custom I-optimal design with one center point for the four variables is given as

$$\xi_{25} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 0 \\ -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ 0 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 0 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ 0 & -1 & 1 & 0 \\ -0.17 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 0 & -1 & 1 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

Table 2: Efficiency Values of the Second-order Designs for the Standard Model in Four Variables

Design Size (N)	Design Type	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)
25	Full CCD ($\alpha = 1$)	44.52	91.00	25.49
	BBD	25.31	60.00	14.12
	Custom A-optimal Design	44.42933	74.25987	32.82217
	Custom D-optimal Design	47.16184	64.9343	25.85874
	Custom I-optimal Design	42.48126	59.89303	32.2389

3.3 Case 3: Non-standard model with 5 parameters

Consider the 5-parameter non-standard model in three variables given in Equation (5)

The Central Composite design (CCD) with a 15-point design, $\alpha = 1.0$, and $n_c = 1$ is given as;

$$\xi_{15} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

After careful evaluation of the hat matrix $H = X(X'X)^{-1}X'$ associated with the design's model matrix (See Appendix A), the design points (1, 0, 0) and (-1, 0, 0) are deleted from the complete design. This results in a decrease in the sample size, thus, a 13-point design called the Modified Central Composite Design (MCCD) is given below as;

$$\xi_{13} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

The 13-point BBD with $n_c = 1$ and the 15-point BBD with $n_c = 3$ shall be investigated and are respectively;

$$\xi_{13} = \begin{pmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \text{ and } \quad \xi_{15} = \begin{pmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The constructed Custom A-optimal designs for the 5-parameter non-standard model in three variables with 13 and 15 design points are respectively;

$$\xi_{13} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ -1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ 0.03 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ 0 & -1 & -1 \\ -1 & -1 & 1 \\ 0 & 1 & -1 \\ -0.04 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix}; \text{ and } \quad \xi_{15} = \begin{pmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ -1 & -1 & -1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 1 & 1 \end{pmatrix}$$

Custom D-optimal designs with 13 and 15 design points are given as

$$\xi_{13} = \begin{pmatrix} 1 & -1 & -1 \\ 0 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & -1 \\ 0 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 0 & -1 & 1 \\ -1 & -1 & 1 \\ 0 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix}; \text{ and } \quad \xi_{15} = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & -1 \\ 0 & -1 & -1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ -0.04 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 0.05 & 1 & -1 \end{pmatrix}$$

The Custom I-optimal designs for the three variables with 13 and 15 design points are given as

$$\xi_{13} = \begin{pmatrix} 0.48 & -1 & -1 \\ 0 & -1 & -1 \\ -0.3 & 1 & 1 \\ 1 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 1 \\ -1 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}; \text{ and } \xi_{15} = \begin{pmatrix} 0 & 1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 1 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 0 & -1 & -1 \\ -1 & -1 & -1 \\ 1 & 1 & -1 \\ 0 & -1 & 1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix}$$

Table 3: Efficiency Measures of Second-order Designs for the 5-parameter Non-standard Model in Three Variables

Design Size (N)	Design Type	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)
13	BBD ($n_c = 1$)	56.02	85.47	42.74
	MCCD ($\alpha = 1$)	53.08	74.07	39.22
	Custom A-optimal Design	63.43927	92.31354	47.5631
	Custom D-optimal Design	65.88084	92.30769	47.09576
	Custom I-optimal Design	61.96404	69.21453	46.55971
15	CCD ($\alpha = 1$)	58.0367	83.3333	41.66667
	BBD ($n_c = 3$)	51.93	84.85	42.42
	Custom A-optimal Design	64.68813	80	48.9083
	Custom D-optimal Design	65.64985	93.83373	44.2516
	Custom I-optimal Design	64.68813	80	48.9083

3.4 Case 4: Non-standard model with 6 parameters

Considering the 6-parameter non-standard model given in Equation (6);
The full Central Composite design (CCD) having a 15-point design with $\alpha = 1.0$ and $n_c = 1$ is given as;

$$\xi_{15} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

From the associated hat matrix in Appendix B, the design points (0, 0, 1) and (0, 0, -1) are eliminated from the complete design. This leads to an MCCD with 13-points given below;

$$\xi_{13} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The 13-point and 15-point Box-Behnken Design (BBD) with $n_c = 3\ and\ 1$ respectively is shown below.

$$\xi_{13} = \begin{pmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix}; \quad \xi_{15} = \begin{pmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The Custom A optimal design with 13 and 15 design points is given as

$$\xi_{13}=\begin{pmatrix}1&1&-1\\0&0&0\\-1&1&0\\1&-1&0\\1&-1&1\\1&1&0\\-1&1&-1\\1&-1&-1\\-1&-1&0\\-1&-1&1\\-1&1&1\\1&1&1\\-1&-1&-1\end{pmatrix};\ \xi_{15}=\begin{pmatrix}1&1&1\\1&1&0\\-1&-1&0\\1&1&0\\-1&1&0\\-1&-1&-1\\1&-1&-1\\0&0&0\\1&1&-1\\1&-1&1\\-1&-1&1\\-1&-1&0\\-1&1&-1\\-1&1&1\\1&-1&0\end{pmatrix}$$

The 13- and 15-point design of Custom D-optimal design is given as

$$\xi_{13}=\begin{pmatrix}-1&1&0\\1&-1&0\\-1&-1&1\\-1&1&1\\-1&-1&1\\-1&-1&-1\\-1&1&-1\\0&0&0\\1&-1&-1\\1&-1&1\\-1&-1&-1\\1&1&1\\1&1&-1\end{pmatrix};\ \xi_{15}=\begin{pmatrix}-1&1&-1\\-1&-1&0\\0&0&0\\-1&1&-1\\1&-1&-1\\1&-1&-1\\-1&1&1\\1&1&0\\1&-1&1\\1&1&-1\\-1&1&1\\-1&-1&1\\1&1&1\\1&-1&1\\-1&-1&-1\end{pmatrix}$$

The 13 and 15-point Custom I-optimal design is given as

$$\xi_{13}=\begin{pmatrix}-1&-1&1\\1&-1&0\\-1&1&1\\-1&1&-1\\1&-1&1\\1&-1&-1\\1&1&-1\\-1&1&0\\1&1&1\\1&1&0\\-1&-1&0\\-1&-1&-1\\0&0&0\end{pmatrix};\ \xi_{15}=\begin{pmatrix}-1&-1&1\\1&1&0\\-1&-1&0\\-1&-1&0\\-1&1&-1\\1&1&-1\\-1&1&1\\-1&-1&-1\\1&-1&-1\\1&-1&0\\-1&1&0\\1&1&0\\0&0&0\\1&1&1\\1&-1&1\end{pmatrix}$$

Table 4: Efficiency Values of Second-order Designs for the 6-parameter Non-standard Model in Three Variables

Design Size (N)	Design Type	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)
15	Full CCD ($\alpha = 1$)	57.22	76.19	43.24
	BBD ($n_c = 3$)	36.6429	47.76119	29.3578
	Custom A-optimal Design	62.64027	73.84615	49.5941
	Custom D-optimal Design	66.61465	80	37.64706
	Custom I-optimal Design	62.64027	73.84615	49.5941
13	BBD ($n_c = 1$)	50.69	73.85	40.13
	MCCD ($\alpha = 1$)	61.30	80.27	47.34
	Custom A-optimal Design	65.1364	85.2071	49.01293
	Custom D-optimal Design	65.66822	76.0181	39.96828
	Custom I-optimal Design	65.1364	85.2071	49.01293

3.5 Case 5: Non-standard model with 7 parameters

This illustration considers a 7-parameter non-standard model in three variables given in Equation (7)

The Central Composite design (CCD) having a 15-point design with $\alpha = 1.0$ and $n_c = 1$ is given as;

$$\xi_{15} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

From the associated hat-matrix of the model in Appendix C, (1, 0, 0) and (-1, 0, 0) design points are removed from the full design. This leads to an MCCD with 13 points.

$$\xi_{13} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

The 13-point and 15-point Box-Behnken Design (BBD) with $n_c = 1\ and\ 3$ respectively is shown below.

$$\xi_{13} = \begin{pmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix};\ \xi_{15} = \begin{pmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Custom A-optimal design with 13 and 15 design points for the three variable non-standard model is

$$\xi_{13} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & -1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ 0 & -1 & -1 \end{pmatrix};\ \xi_{15} = \begin{pmatrix} 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 0 & 1 & -1 \\ 1 & -1 & -1 \\ 0 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & -1 & -1 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

Custom D-optimal design with 13 and 15 design points is given as

$$\xi_{13} = \begin{pmatrix} -1 & -1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 1 & -1 \\ -1 & -1 & 1 \\ 0 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \end{pmatrix}; \; \xi_{15} = \begin{pmatrix} 0 & -1 & 1 \\ 0 & 1 & -1 \\ -1 & -1 & -1 \\ 1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \end{pmatrix}$$

The Custom I-optimal design with 13 and 15 design points is

$$\xi_{13} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & 1 & -1 \\ 0 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ 0 & 1 & 1 \\ -1 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \\ 0 & -1 & 1 \\ 1 & -1 & 1 \end{pmatrix}; \; \xi_{15} = \begin{pmatrix} 0 & -1 & 1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & -1 \\ 0 & -1 & 1 \\ 0 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

Table 5: Efficiency Values of Second-order Designs for the 7-parameter Non-standard Model in Three Variables

Design Size (N)	Design Type	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)
15	CCD ($\alpha = 1$)	56.65	71.79	44.44
	BBD ($n_c = 3$)	42.92	74.67	36.30
	Custom A-optimal Design	61.21732	74.66667	50.09585
	Custom D-optimal Design	67.23916	80	40
13	Custom I-optimal Design	61.21732	70	50.09585
	BBD ($n_c = 1$)	47.20	86.15	38.46
	MCCD ($\alpha = 1$)	61.33	76.92	48.95

	Custom A-optimal Design	64.6098	80.76923	50.48077
	Custom D-optimal Design	66.51036	85.34107	42.47021
	Custom I-optimal Design	64.6098	80.76923	50.48077

3.6 Case 6: Non-standard model with 9 parameters

Considering the 9-parameter non-standard model given in Equation (8),
The Central Composite design (CCD) with 25 design points, $\alpha = 1.0$, and $n_c = 1$ is given as;

$$\xi_{25} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The matrix result in Appendix D showed that (0, 1, 0, 0), (0, -1, 0, 0), (0, 0, 1, 0), and (0, 0, -1, 0) design points were less influential, so they were removed from the full design. This resulted in a 21-point MCCD, as shown below.

$$\xi_{21} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix};$$

For the 9-parameter non-standard model, the 25-point Box-Behnken Design (BBD) with $n_c = 1$ is given as;

$$\xi_{25} = \begin{pmatrix} -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ -1 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & -1 & 0 \\ 1 & 0 & -1 & 0 \\ -1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & -1 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & -1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The Custom A-optimal design for the four variables with 21 and 25 design points is given as

$$\xi_{21} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 \\ -1 & 1 & 1 & -1 \\ 0 & 1 & -1 & 0 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 0 \\ 1 & -1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ 0 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 0 \\ 1 & 1 & -1 & -1 \\ 0 & 1 & 1 & -1 \\ 0 & -1 & 1 & -1 \\ 0 & -1 & -1 & 0 \\ -1 & -1 & -1 & -1 \end{pmatrix}; \quad \xi_{25} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 0 & 0 & -1 & 1 \\ 0 & -1 & 1 & -1 \\ 0 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 \\ -1 & -1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & -1 & -1 & 0 \\ -1 & -1 & -1 & 0 \\ -1 & 1 & 1 & 0 \\ 1 & 1 & -1 & 0 \\ -1 & -1 & 1 & -1 \\ 0 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & 1 & -1 & -1 \\ 0 & -1 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & -1 & 1 & -0.06 \\ 1 & -1 & 1 & 0 \\ 0 & 1 & 1 & -1 \end{pmatrix}$$

The Custom D-optimal design with 21 and 25 design points is given as

$$\xi_{21} = \begin{pmatrix} -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 0 \\ -1 & -1 & -1 & -1 \\ -1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 0 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 \\ -1 & 1 & -1 & -1 \\ 0 & -1 & -1 & -1 \\ 0 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & 0 \\ 1 & -1 & -1 & 0 \end{pmatrix}; \qquad \xi_{25} = \begin{pmatrix} 1 & -1 & -1 & 0 \\ 1 & -1 & -1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 0 \\ -0.06 & -1 & 1 & 0 \\ -1 & -1 & -1 & 0 \\ 1 & -1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 0 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 0 & -1 & -1 & -1 \\ 0 & -1 & -1 & -1 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 0 \end{pmatrix}$$

Custom I-optimal design with 21 and 25 design points is given as

$$\xi_{21} = \begin{pmatrix} 1 & 1 & -1 & 0 \\ 0 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 0 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ 0 & -1 & -1 & 1 \\ -1 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 1 & -1 & 1 \end{pmatrix}; \qquad \xi_{25} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 0 \\ -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ 0 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 0 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ 0 & -1 & 1 & 0 \\ -0.17 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 0 & -1 & 1 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

Table 6: Efficiency Values of Second-order Designs for the 9-parameter Non-standard Model in Four Variables

Design Size (N)	Design Type	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)
25	CCD ($\alpha = 1$)	52.14	88.53	31.60
	BBD ($n_c = 1$)	34.96	64.34	27.18
	Custom A-optimal Design	57.67718	79.99164	44.21452
	Custom D-optimal Design	61.47872	89.83834	37.93374
	Custom I-optimal Design	57.08659	66.10358	43.44466
21	MCCD ($\alpha = 1$)	53.40	83.19	25.29
	Custom A-optimal Design	58.53976	72.40759	43.80603
	Custom D-optimal Design	61.47599	82.6686	34.77996
	Custom I-optimal Design	58.53976	72.40759	43.80603

4. Discussion

Regarding Table 1, the result of the efficiency metrics for the second-order designs with a design size of 15 (except for the BBD) using the three-variable standard second-order model showed that custom designs are as efficient as the commonly used CCD. Specifically, custom A-optimal design and custom I-optimal design with D-, G- and A-efficiency values of 44. 71631%, 83.62369%, and 31.29074% respectively performed as well as the CCD. This implies that the custom A- and I-optimal designs are as efficient as the CCD. Also, the D-optimal design had the best D-efficiency value of 45.51884%. Thus, custom designs performed better than the BBD and are as efficient as the CCD. Again, considering the four-variable standard second-order model, it is observed from the result in Table 2 that the CCD had the highest G-efficiency of 91%. This justifies its usefulness in second-order models for process optimisation and prediction. Next to it is the A-optimal design with a G-efficiency of 74.25987% and the highest A-efficiency of 32.82217%. The D-optimal design had the highest D-efficiency of 47.16184%. From the result, it is seen that custom designs are efficient in standard second-order models in three variables.

Table 3 shows the efficiency result of second-order designs with 15 and 13 design points using the 5-parameter non-standard model in three variables. For the 15-point design, it is observed that the custom D-optimal design performed best with a D and G-efficiency of 65.64985% and 93.83373%, respectively. The BBD with 3 centre points had the second-highest G-efficiency of 84.85%. While the custom A- and I-optimal designs had the highest A-efficiency value of 48.9083%. For the 13-point design, the custom D-optimal design performed best with D-efficiency and G-efficiency of 65.88084%, and 92.307693%

respectively, and the second highest A-efficiency of 47.09576%. Next to it is the custom A-optimal design with D-efficiency and G-efficiency of 63.43927% and 92.31354% respectively, and with the highest A-efficiency of 47.5631%. Custom I-optimal design had the third highest D- and A-efficiency values. The MCCD performed the least in terms of D-, G-, and A-efficiency. Hence, custom designs are efficient designs.

The result in Table 4 using the 6-parameter non-standard model showed that for the 15-point design, the custom D-optimal design had the highest D- and G-efficiency of 66.61465% and 80%, respectively. The CCD had the second-highest G-efficiency value of 76.19%. Custom A- and I-optimal designs had the highest A-efficiency of 49.01293%. For the 13-point design, the custom D-optimal design had the best D-efficiency of 65.66822%; custom A- and I-optimal designs had the best G- and A-efficiency values of 85.2071% and 49.01293%, respectively. The MCCD performed better than the BBD in all the efficiency values. Thus, custom A-, D-, and I-optimal designs are more appropriate for the 6-parameter non-standard model in three variables with 15 and 13 design points. Regarding Table 5, the result revealed that the custom D-optimal design performed best with D- and G-efficiency of 67.23916% and 80%, respectively. The BBD with 3 centre points and the custom A-optimal had the second highest G-efficiency of 74.67%, followed by the full CCD with a G-efficiency of 71.79%. Custom A- and I-optimal designs had the highest A-efficiency value of 50.09585% and the second highest D-efficiency value of 61.21732%. For the 13-point design, the custom D-optimal design had the highest D-efficiency value of 66.51036% and the second highest G-efficiency of 85.34107%. The BBD with one centre point had the highest G-efficiency of 86.15%. Custom A- and I-optimal designs had the best A-efficiency value of 50.48077%. Generally, for the 7-parameter non-standard model, custom designs outperformed the CCD, BBD, and MCCD.

Table 6 shows the efficiency values of CCD, BBD, custom A-, D-, I-optimal design, and MCCD for a 9-parameter non-standard model in four variables with 25 and 21 design points. For the 25-point design, the custom D-optimal design performed the best in terms of D- and G-efficiency at 61.47872% and 89.83834%, respectively. The full CCD had the second-highest G-efficiency of 88.53%, and the custom A-optimal design had the highest A-efficiency of 44.21452%. For the 21-point design, the MCCD had the best G-efficiency of 83.19%, followed by the custom D-optimal design with a G-efficiency of 82.6686%. Custom D-optimal designs had the highest D-efficiency of 61.47599%. Custom A- and I-optimal designs had the highest A-efficiency value of 43.80603% and the second highest D-efficiency of 58.53976%. Generally, we can say that custom designs performed better than the CCD, BBD, and MCCD for the non-standard model. Nevertheless, based on the non-standard models considered in this study, it is observed that the custom designs, namely, custom D-, A-, and I-optimal designs, performed better or are more efficient in terms of D-efficiency, G-efficiency, and A-efficiency than the CCD, BBD, and MCCD. This result supports Iwundu & Otaru (2019), and Akinlana (2022) that computer-generated designs are efficient designs.

Conclusion

The efficiency of custom A-, D-, and I-optimal designs to the CCD, BBD, and MCCD have been thoroughly examined and demonstrated in this research work on second-order standard and non-standard models. D-, G-, and A-efficiency metrics are utilised to assess the quality of these designs. Comparatively, custom A-, D-, and I-optimal designs are efficient designs for standard and non-standard models.

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Appendix A: Hat Matrix of the CCD for the 5-parameter Non-standard Model with $k = 3$, $n_c = 1$, and $\propto = 1.0$

0.4000	0.2000	0.2000	-0.0000	0.2000	-0.0000	-0.0000	-0.2000	-0.0000	0.2000	-0.1000	0.1000	-0.1000	0.1000	0
0.2000	0.4000	-0.0000	0.2000	-0.0000	0.2000	-0.2000	-0.0000	0.2000	-0.0000	-0.1000	0.1000	-0.1000	0.1000	0
0.2000	-0.0000	0.4000	0.2000	-0.0000	-0.2000	0.2000	-0.0000	-0.0000	0.2000	0.1000	-0.1000	-0.1000	0.1000	0
-0.0000	0.2000	0.2000	0.4000	-0.2000	-0.0000	-0.0000	0.2000	0.2000	-0.0000	0.1000	-0.1000	-0.1000	0.1000	0
0.2000	-0.0000	-0.0000	-0.2000	0.4000	0.2000	0.2000	-0.0000	-0.0000	0.2000	-0.1000	0.1000	0.1000	-0.1000	0
-0.0000	0.2000	-0.2000	-0.0000	0.2000	0.4000	-0.0000	0.2000	0.2000	-0.0000	-0.1000	0.1000	0.1000	-0.1000	0
-0.0000	-0.2000	0.2000	-0.0000	0.2000	-0.0000	0.4000	0.2000	-0.0000	0.2000	0.1000	-0.1000	0.1000	-0.1000	0.1000
-0.2000	-0.0000	-0.0000	0.2000	-0.0000	0.2000	0.2000	0.4000	0.2000	-0.0000	-0.1000	0.1000	-0.1000	0	0
-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	0.2000	-0.0000	0	0	0	0	0
0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	-0.0000	0.2000	0	0	0	0	0
-0.1000	-0.1000	0.1000	0.1000	-0.1000	-0.1000	0.1000	0.1000	0	0	0.3000	0.1000	0.2000	0.2000	0.2000
0.1000	0.1000	-0.1000	-0.1000	0.1000	0.1000	-0.1000	-0.1000	0	0	0.1000	0.3000	0.2000	0.2000	0.2000
-0.1000	-0.1000	-0.1000	-0.1000	0.1000	0.1000	0.1000	0.1000	0	0	0.2000	0.2000	0.3000	0.1000	0.2000
0.1000	0.1000	0.1000	0.1000	-0.1000	-0.1000	-0.1000	-0.1000	0	0	0.2000	0.2000	0.1000	0.3000	0.2000
0	0	0	0	0	0	0	0	0	0	0.2000	0.2000	0.2000	0.2000	0.2000

Appendix B: Hat Matrix of the CCD for the 6-parameter Non-standard Model with $k = 3$, $n_c = 1$, and $\propto = 1.0$

0.5250	0.3250	0.0750	-0.1250	0.0750	-0.1250	0.1250	-0.0750	0.1000	-0.1000	0.1000	-0.1000	0.2000	-0.0000	0
0.3250	0.5250	-0.1250	0.0750	-0.1250	0.0750	-0.0750	0.1250	-0.1000	0.1000	0.1000	-0.1000	0.2000	-0.0000	0
0.0750	-0.1250	0.5250	0.3250	0.1250	-0.0750	0.0750	-0.1250	0.1000	-0.1000	-0.1000	0.1000	0.2000	-0.0000	0
-0.1250	0.0750	0.3250	0.5250	-0.0750	0.1250	-0.1250	0.0750	-0.1000	0.1000	-0.1000	0.1000	0.2000	-0.0000	0
0.0750	-0.1250	0.1250	-0.0750	0.5250	0.3250	0.0750	-0.1250	0.1000	-0.1000	0.1000	-0.1000	-0.0000	0.2000	0
-0.1250	0.0750	-0.0750	0.1250	0.3250	0.5250	-0.1250	0.0750	-0.1000	0.1000	0.1000	-0.1000	-0.0000	0.2000	0
0.1250	-0.0750	0.0750	-0.1250	0.0750	-0.1250	0.5250	0.3250	0.1000	-0.1000	-0.1000	0.1000	-0.0000	0.2000	0
-0.0750	0.1250	-0.1250	0.0750	-0.1250	0.0750	0.3250	0.5250	-0.1000	0.1000	-0.1000	0.1000	-0.0000	0.2000	0
0.1000	-0.1000	0.1000	-0.1000	0.1000	-0.1000	0.1000	-0.1000	0.3000	0.1000	0.2000	0.2000	0	0	0.2000
-0.1000	0.1000	-0.1000	0.1000	-0.1000	0.1000	-0.1000	0.1000	0.1000	0.3000	0.2000	0.2000	0	0	0.2000
0.1000	0.1000	-0.1000	-0.1000	0.1000	0.1000	-0.1000	-0.1000	0.2000	0.2000	0.3000	0.1000	0	0	0.2000
-0.1000	-0.1000	0.1000	0.1000	-0.1000	-0.1000	0.1000	0.1000	0.2000	0.2000	0.1000	0.3000	0	0	0.2000
0.2000	0.2000	0.2000	0.2000	-0.0000	-0.0000	-0.0000	-0.0000	0	0	0	0	0.2000	-0.0000	0
-0.0000	-0.0000	-0.0000	-0.0000	0.2000	0.2000	0.2000	0.2000	0	0	0	0	-0.0000	0.2000	0
0	0	0	0	0	0	0	0	0.2000	0.2000	0.2000	0.2000	0	0	0.2000

Appendix C: Hat Matrix of the CCD for the 7-parameter Non-standard Model with $k = 3$, $n_c = 1$, and $\propto = 1.0$

0.6500	-0.0500	0.2000	-0.0000	0.2000	-0.0000	-0.2500	0.0500	0.2000	-0.0000	0.1000	-0.1000	0.1000	-0.1000	0
-0.0500	0.6500	-0.0000	0.2000	-0.0000	0.2000	0.0500	-0.2500	-0.0000	0.2000	0.1000	-0.1000	0.1000	-0.1000	0
0.2000	-0.0000	0.6500	-0.0500	-0.2500	0.0500	0.2000	-0.0000	0.2000	-0.0000	-0.1000	0.1000	0.1000	-0.1000	0
-0.0000	0.2000	-0.0500	0.6500	0.0500	-0.2500	-0.0000	0.2000	-0.0000	0.2000	-0.1000	0.1000	0.1000	-0.1000	0
0.2000	-0.0000	-0.2500	0.0500	0.6500	-0.0500	0.2000	-0.0000	0.2000	-0.0000	0.1000	-0.1000	-0.1000	0.1000	0
-0.0000	0.2000	0.0500	-0.2500	-0.0500	0.6500	-0.0000	0.2000	-0.0000	0.2000	0.1000	-0.1000	-0.1000	0.1000	0
-0.2500	0.0500	0.2000	-0.0000	0.2000	-0.0000	0.6500	-0.0500	0.2000	-0.0000	-0.1000	0.1000	-0.1000	0.1000	0
0.0500	-0.2500	-0.0000	0.2000	-0.0000	0.2000	-0.0500	0.6500	-0.0000	0.2000	-0.1000	0.1000	-0.1000	0.1000	0
0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0	0	0	0	0
-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	0	0	0	0	0
0.1000	0.1000	-0.1000	-0.1000	0.1000	0.1000	-0.1000	-0.1000	0	0	0.3000	0.1000	0.2000	0.2000	0.2000
-0.1000	-0.1000	0.1000	0.1000	-0.1000	-0.1000	0.1000	0.1000	0	0	0.1000	0.3000	0.2000	0.2000	0.2000
0.1000	0.1000	0.1000	0.1000	-0.1000	-0.1000	-0.1000	-0.1000	0	0	0.2000	0.2000	0.3000	0.1000	0.2000
-0.1000	-0.1000	-0.1000	-0.1000	0.1000	0.1000	0.1000	0.1000	0	0	0.2000	0.2000	0.1000	0.3000	0.2000
0	0	0	0	0	0	0	0	0	0	0.2000	0.2000	0.2000	0.2000	0.2000

s

Appendix 4.4: Hat Matrix of the CCD for the 9-parameter Non-standard Model with $k = 4$, $n_c = 1$, and $\propto = 1.0$

0.4066 0.1705 0.0455 0.0594 0.1705 -0.0656 0.0594
0.0733 0.2955 0.0594
0.1705 0.4066 0.0594 0.0455 -0.0656 0.1705 0.0733
0.0594 0.0594 0.2955
0.0455 0.0594 0.4066 0.1705 0.0594 0.0733 0.1705 -
0.0656 -0.0656 -0.0517
0.0594 0.0455 0.1705 0.4066 0.0733 0.0594 -0.0656
0.1705 -0.0517 -0.0656
0.1705 -0.0656 0.0594 0.0733 0.4066 0.1705 0.0455
0.0594 0.0594 -0.1767
-0.0656 0.1705 0.0733 0.0594 0.1705 0.4066 0.0594
0.0455 -0.1767 0.0594
0.0594 0.0733 0.1705 -0.0656 0.0455 0.0594 0.4066
0.1705 -0.0517 -0.0378
0.0733 0.0594 -0.0656 0.1705 0.0594 0.0455 0.1705
0.4066 -0.0378 -0.0517
0.2955 0.0594 -0.0656 -0.0517 0.0594 -0.1767 -0.0517 -
0.0378 0.4066 0.1705
0.0594 0.2955 -0.0517 -0.0656 -0.1767 0.0594 -0.0378 -
0.0517 0.1705 0.4066
-0.0656 -0.0517 0.2955 0.0594 -0.0517 -0.0378 0.0594 -
0.1767 0.0455 0.0594
-0.0517 -0.0656 0.0594 0.2955 -0.0378 -0.0517 -0.1767
0.0594 0.0594 0.0455

-0.0656 -0.0517 0.0594 -0.1767 -0.0517 -0.0378 -0.0308
0.0803 -0.0655 0.0457 -0.0517 -0.0656 -0.1767 0.0594 -
0.0378 -0.0517 0.0803 -0.0308 -0.0655 0.0457
0.2955 0.0594 -0.0517 -0.0378 0.0594 -0.1767 -0.0308
0.0803 0.0457 0.0655
0.0594 0.2955 -0.0378 -0.0517 -0.1767 0.0594 0.0803 -
0.0308 0.0457 0.0655
-0.0517 -0.0378 0.2955 0.0594 -0.0656 -0.0517 -0.0308
0.0803 -0.0655 0.0457
-0.0378 -0.0517 0.0594 0.2955 -0.0517 -0.0656 0.0803 -
0.0308 -0.0655 0.0457
0.0594 -0.1767 -0.0656 -0.0517 0.2955 0.0594 -0.0308
0.0803 0.0457 0.0655
-0.1767 0.0594 -0.0517 -0.0656 0.0594 0.2955 0.0803 -
0.0308 0.0457 0.0655
0.0455 0.0594 0.1705 -0.0656 0.0594 0.0733 -0.0308
0.0803 -0.0655 0.0457
0.0594 0.0455 -0.0656 0.1705 0.0733 0.0594 0.0803 -
0.0308 -0.0655 0.0457
0.4066 0.1705 0.0594 0.0733 0.1705 -0.0656 -0.0308
0.0803 0.0457 -0.0655
0.1705 0.4066 0.0733 0.0594 -0.0656 0.1705 0.0803 -
0.0308 0.0457 -0.0655

-0.0655 0.0457 -0.0308 0.0803
-0.0099
-0.0655 0.0457 -0.0308 0.0803
-0.0099
-0.0655 0.0457 -0.0308 0.0803
-0.0099
-0.0655 0.0457 -0.0308 0.0803
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-0.0655 0.0457 0.0803 -0.0308
-0.0099
-0.0655 0.0457 0.0803 -0.0308
-0.0099
-0.0655 0.0457 0.0803 -0.0308
-0.0099

0.0594 -0.1767 -0.0517 -0.0378 0.2955 0.0594 -0.0656 -
0.0517 0.1705 0.0656
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