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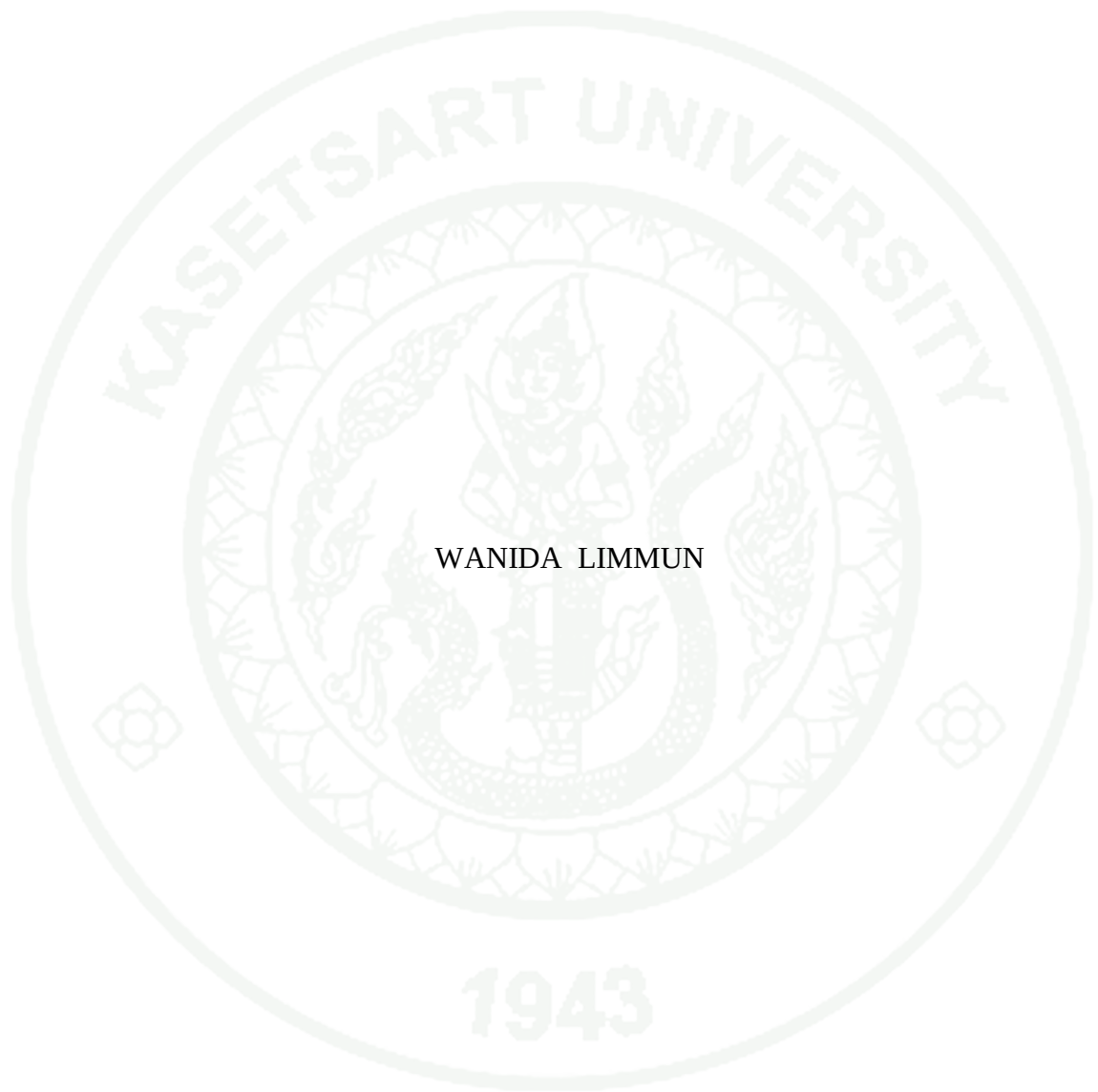
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THESIS

EXAMINING MODEL ROBUSTNESS IN MIXTURE EXPERIMENTS



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In this dissertation, the major objective is to develop a genetic algorithm (GA) for generating weighted D - and G -optimal exact designs for mixture experiments having model robustness properties where the experimental mixture region is defined by only single-component constraints or by single and multiple component constraints. For the GA, new versions of two crossover operators and a mutation operator are developed to handle the component constraints when generating mixture designs for an irregularly-shape polyhedron region. Two new objective functions which are the weighted D - and G - design optimality criteria are developed for evaluating the fitness of a design over sets of reduced models based on weak and strong heredity principles. This approach allows exploration and searching for points through a highly-constrained continuous mixture region and does not require selection of points from a user-defined candidate set of mixtures which is a limitation for current design-generating algorithms.

The results are focused on the examination of model robustness properties of the GA-generated mixture designs. The weighted optimal exact designs which have interior points and a point near the overall centroid have good prediction variance properties. However, not all of the weighted D -optimal exact designs have good prediction variance properties, whereas all of the weighted G -optimal exact designs have good prediction variance properties. The designs which have good prediction variance properties also appear to have good robustness properties. The weighted G -optimal exact designs are superior to the weighted D -optimal exact designs in terms of the scaled prediction variance and appear to be more robust designs than the weighted D -optimal exact designs.

Student's signature

Thesis Advisor's signature

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EXAMINING MODEL ROBUSTNESS IN MIXTURE EXPERIMENTS

INTRODUCTION

Response surface methodology (RSM) is a collection of statistical and mathematical techniques that are used to develop new processes, optimize process performance, and improve the design and the formulation for new products. The performance measure or quality characteristic is typically selected as the response used to study the behavior of the process. The response variables are influenced by input variables which sometimes are referred to as independent variables that can be controlled by engineers or scientists for testing or experimenting purposes. In a typical response surface design, the levels chosen for any factor are independent of those chosen for other factors (Myers *et al.*, 2009).

Response surface methodology is mostly concerned with approximating a complex unknown function with a lower order polynomial, normally either a first-order model or second-order model. Therefore, the choice of design for model fitting is very important. When selecting a design, there are many criteria and characteristics that could be considered. Myers *et al.* (2009) suggest that a good design should:

1. yield in a good fit of the model to the data.
2. give sufficient information to allow a test for lack of fit.
3. allow models of increasing order to be constructed sequentially.
4. provide an estimate for “pure” experiment error.
5. be insensitive (robust) to the presence of outliers in the data.
6. be robust to error in control of design levels.
7. be cost-effective, that is, not require too many experimental trials (runs).
8. allow for experiments to be conducted in blocks.
9. provide a check on the homogeneous variance assumption.

10. provide a good distribution of variances of the predicted response throughout the design region.

The problem of selecting a suitable design can be difficult because of the dependence on the experimental circumstances. A good design does not require all of the stated characteristics be satisfied. However, most of all properties should be seriously considered when designing an experiment. The design that is optimal for one particular property is often not similar to the design that is optimal for another property. Thus, there are tradeoffs that almost always exist when one selects an appropriate design. The well-known bias-variance tradeoff is a very important issue in data modeling; ignoring it is a frequent cause of model failure. As the model complexity increases, the bias usually decreases while the variance rises. Generally, neither the bias nor the variance should be too large, but usually, minimizing one tends to increase the other. Underfitting a model may result in large biased predictions of the response and the design will be unable to estimate the true model, while overfitting a model may lead to an inflation of the prediction variance and efficiency is lost by devoting resources to estimate unnecessary parameters. Choosing between competing designs involves many tradeoffs as this decision is based on several goals for a good design.

The standard error of predicted values gives a rough idea of the quality of the predicted response values across the various locations in the design region. The distribution of prediction variances throughout the region of interest is very important for comparing competing designs (Myers *et al.*, 2009). The distribution of prediction variances is a reflection of how well the model can predict responses for a chosen design. Box and Hunter (1957) emphasized that assessing the quality of a design should be based on the distribution of prediction variances over the region. Because the experimenter does not know a specific location in the design space where he or she might wish to predict a response, a reasonably stable prediction variance over the whole region is desired. Therefore, the best design should be the design that produces the optimal prediction variance distribution throughout the constrained region of

interest where ‘optimal’ implies the distribution of the prediction variances should be stable and uniformly low throughout the experimental region.

The objective of many experiments is to obtain an understanding about an unknown underlying relationship between input variables and responses variables. In practice, the assumed model is, in general, only a reasonable approximation to the true but unknown model for the response of interest. Critically, if the assumed model has insufficient complexity to adequately approximate the true underlying function and a check for lack of fit cannot be made, then the experimenter does not realize that an inappropriate model was fitted to data. The construction of a design should be very efficient for a set of potential or candidate models because choosing a design depends on the specific type of model. For example, the central composite design is commonly used for the second order model because its structure allows for good estimation of all parameters in that model (Ozol-Godfrey *et al.*, 2005).

Before beginning an experiment, the practitioners must decide which type of design he or she wants to use to fit the approximating model. Typically, when an experimenter chooses a design, the first step is to specify the model that is proposed for analysis once the data have been collected. Frequently, after the data have been collected, the researcher may subsequently modify the model because the original model is inappropriate. When the initial model for which the design was chosen does not turn out to be the final model used in the analysis phase, the initial design may no longer have desirable prediction variance properties with respect to the final model. Therefore, the experimenter might need a method for selecting a good design regardless of the final model selected. Therefore, the robustness of a design to model change, known as model robustness, plays a crucial role for addressing this problem.

One common approach for comparing designs is to consider design optimality criteria which are characterized by various letters (e.g. *D*, *A*, *G*, or *I*) of the alphabet. They are often called alphabetical optimality criteria. The *D*, *A*, *G*, and *I* criteria each attempt to summarize one important characteristic of the design. Specifically, for any design, an optimality criterion produces a single value that expresses a property of the

variance of predictions. Typically, for a design, the optimality criteria values will vary. Thus, no one optimality criterion completely reflects the prediction variance characteristics of the design. For example, when the experimenter evaluates two designs by using the G optimality criterion, two competing designs can have the same G -efficiency value, and then the question is which one should be chosen?. Therefore, the experimenter needs additional information to help in the design selection process. Graphical methods come into play here because they are highly effective and informative tools for evaluating competing designs (Anderson-Cook *et al.*, 2009 and Borkowski, 2009).

Designs for mixture experiments are a special type of response surface designs where the factors are the components or the ingredients of a mixture. The response is a function of the proportions of each component that are typically measured by weight, volume, molar ratio and so on. In other words, the mixing or the blending of ingredients in an effort to get a more desirable final product is known as a mixture experiment. In the typical mixture experiment, the response is assumed to depend only on the relative proportion of the components rather than the total amount of the mixture. Mixture experiments involve varying the proportions of two or more components and study the resulting changes that occur in the measured response that is assumed to be functionally related to ingredient compositions. In mixture experiments, the component proportions must sum to one; therefore, the levels chosen for any component are dependent on the levels chosen for the other components.

Mixture experiments are commonly encountered in many fields, including industrial processes such as agricultural, chemical and pharmaceutical drug formulation, food processing, and textile fiber production. The results of mixture experiments are all around us but we often do not realize their existence. For example: (a) the delectable taste of salad dressing that is the product of mixing proportions of oil, vinegar, and some spices; (b) the fluffiness of a cake that is relative to the blending proportions of baking power, shortening, flour, sugar, and water and (c) the fruitiness flavor of punch that depends on the relative proportions of orange, pineapple, and other juices. In general, suppose that the mixture experiment consists

of q ingredients or components, and let x_i be the proportion of the i th component. Then the proportions must satisfy the following constraints:

$$0 \leq x_i \leq 1 \quad \forall i = 1, 2, \dots, q \quad (1)$$

and

$$\sum_{i=1}^q x_i = 1. \quad (2)$$

The first constraint keeps each mixture component proportion between 0% and 100%, and the second constraint makes sure that at any point in the mixture space, the sum of component proportions is always equal to unity. In many experiments, additional constraints are placed on the component proportions, and the experimental region takes on the form of an irregular polyhedron.

For example, in manufacturing flares, the objective is to find the mixture that gives out the maximum illumination (McLean and Anderson, 1966). The chemical components consist of magnesium(x_1), sodium nitrate(x_2), strontium nitrate(x_3), and binder(x_4) and their proportions sum to 1. Engineering experience indicated that the individual components should have the following constraints:

$$0.40 \leq x_1 \leq 0.60, \quad 0.10 \leq x_2 \leq 0.50, \quad 0.10 \leq x_3 \leq 0.50, \quad 0.03 \leq x_4 \leq 0.08.$$

The flare experiment region is an irregular polyhedron and is shown in Figure 1.

In optimization problems, to increase the possibility of finding the optimal solution where uncertainty in the solution exists, it is necessary to apply a method that is both efficient and effective. Thus, the evolutionary approach that requires a certain amount of randomness is often used. The genetic algorithm is the one of the evolutionary approaches and is based on the survival of the fittest biological imperative. That is, individuals adapt themselves to their environment and then evolve themselves into more desirable individuals (Sivanandam and Deepa, 2008). The genetic algorithm is very effective procedure for constructing designs in a constrained

region because the genetic algorithm does not require an explicit candidate set of points (Heredia-Langner *et al.*, 2004).

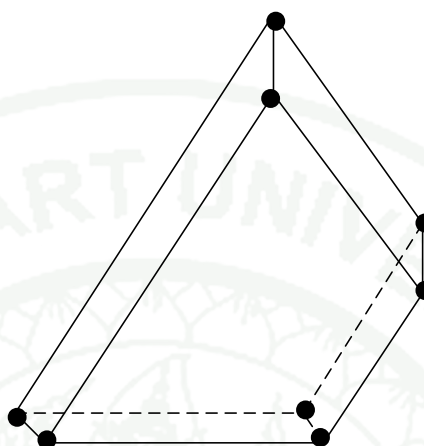


Figure 1 Shape of regular polyhedron mixture space for the flare experiment.

Source: McLean and Anderson (1966).

Although there have been many studies on the problem of model robustness in response surface design that are focused on how to find the best design, relatively little attention has been paid to the problem of the robustness of the design to model misspecification, known as model robustness. In general, a researcher is interested in constructing designs that have good efficiency across a set of candidate models to assist him/her to choose the best design regardless of the final model selected. In this dissertation, the genetic algorithm will be used to generate model-robust designs for mixture experiments and graphical approaches will be developed for evaluating the designs in terms of prediction variance properties and aiding the exploration of the design performance when model misspecification exists.

OBJECTIVES

The objectives of this dissertation are classified as follows:

1. To develop computational methodology for generating mixture designs for model robustness based on a genetic algorithm.

1.1 Develop new mutation and reproduction operators for a GA for generating mixture designs.

1.2 Develop new versions of two crossover operators for real-number encoded genes for generating mixture designs.

2. To develop statistical techniques for examining and assessing model robustness in mixture experiments in constrained regions based on two criteria.

2.1 Alphabetical optimality criteria approach (such as D -efficiency and G -efficiency)

2.2 Graphical approach (such as variance dispersion graphs (VDGs), componentwise VDGs (CVDGs), and fraction of design space plots (FDS plots)).

3. To evaluate and assess the prediction variance properties of a design throughout the design space in mixture experiments in constrained regions.

4. To apply the graphical approach for choosing the best design for model robustness in mixture experiments in constrained regions.

Scope of the Research

The research involves the determination of design efficiency and examination of model misspecification in mixture experiments within the following means and conditions:

1. Two models are considered as key or “full” models. These two models are the Scheffé quadratic and special cubic model which can be expressed as;

Quadratic model :

$$y = \sum_{i=1}^q \beta_i x_i + \sum_{i<j}^q \beta_{ij} x_i x_j + \varepsilon, \quad (3)$$

Special Cubic model :

$$y = \sum_{i=1}^q \beta_i x_i + \sum_{i<j}^q \beta_{ij} x_i x_j + \sum_{i<j<k}^q \beta_{ijk} x_i x_j x_k + \varepsilon, \quad (4)$$

where y is an observed response, the β 's correspond to the parameter coefficients to be estimated, $x_1, x_2, \dots, x_q$ are the explanatory mixture proportions, and ε is a normally distributed error term having an expectation of zero and variance σ^2 .

2. The constraints imposed on the single component proportions have the form of lower (L_i) and upper bounds (U_i),

$$0 \leq L_i \leq x_i \leq U_i \leq 1 \quad ; i = 1, 2, \dots, q \quad (5)$$

and experiments with and without linear multi-component constraints of the form

$$C_j \leq A_{1j}x_1 + A_{2j}x_2 + \dots + A_{qj}x_q \leq D_j \quad ; j = 1, 2, \dots, h \quad (6)$$

are considered where A_{ij}, C_j and D_j are scalar constants, and h is the number of linear multi-component constraints.

3. Mixture experiments consisting of three and four mixture components ($q = 3$ and 4) with only single-component constraints and experiments consisting of three mixture components ($q = 3$) with single and multiple component constraints are considered in this dissertation.

4. A genetic algorithm is used for the construction of mixture designs and the resulting design is then assessed for suitability with respect to model robustness and prediction variance properties.

5. The strong heredity (SH) principle and the weak heredity (WH) principle are used to produce all possible reduced models. When the full model is the Scheffé quadratic model, the number of possible reduced models for 3 and 4 components are equal to 8 and 64, respectively, for SH and WH. For SH, if the full model is the special cubic model, then the number of possible reduced models for 3 and 4 components are equal to 9 and 113, respectively. For WH, if the full model is the special cubic model, then the number of possible reduced models for 3 and 4 components are equal to 15 and 809, respectively.

6. We employ alphabetical optimality criteria and graphical approaches for evaluating model robustness with respect to the prediction variance. Specifically, D - and G -alphabetical optimality criteria as well as variance dispersion graphs (VDGs), componentwise VDGs (CVDGs), and fraction of design space plots (FDS plots) are considered.

Expected Results of the Research

1. To provide the statistical methodology that will help experimenters generate a model-robust design when there exists prior uncertainty with the choice of final model in mixture experiments.

2. To develop and demonstrate how to use alphabetical optimality criteria and the graphical techniques for experimenters in choosing a design that will perform well across a set of specified models.

3. To propose an alternative approach for generating an efficient design in situations where conventional exchange algorithms fail to find a near-optimal design.

LITERATURE REVIEW

This chapter provides background information on the key topics of this dissertation. It is divided into two parts. The first part contains a discussion of the relevant statistical methodology and the second part contains a review of previous studies related to the research proposed in this dissertation.

Relevant Statistical Methodology

This part provides a brief review for the statistical methodology that will be used in the proposed dissertation.

1. Introduction to Mixture Experiments

In this dissertation, a mixture experiment is defined to be an experiment in which the response is a function only of the proportions of the components in the mixture and is not a function of the total amount of the mixture. In a mixture experiment, the factors are the ingredients or the components of a mixture. These components cannot be varied independently, and the measured response is an “intensive” property. The proportion of each ingredient, $x_i, i=1,2,\dots,q$, of a q -component mixture must satisfy the following constraints:

$$0 \leq x_i \leq 1 \quad \forall i = 1, 2, \dots, q \quad \text{and} \quad (7)$$

$$\sum_{i=1}^q x_i = 1. \quad (8)$$

The level of the final component, x_q , is defined by and can be calculated from the levels of the other $q-1$ components. That is,

$$x_q = 1 - \sum_{i=1}^{q-1} x_i. \quad (9)$$

because the components cannot be varied independently of each other (Cornell, 2002). The constraints in equation (7) and (8) represent the fundamental constraints underlying any mixture problem. The first constraint keeps each mixture component proportion between 0% and 100%, and the second constraint makes sure that at any point in the mixture space, the sum of the component proportions is unity. The constraint in (8) reduces the dimension of the mixture space from q to $q-1$. Specifically, given the constraints in (7) and (8), the experimental region for a q component mixture system is a $q-1$ dimensional simplex with q vertices.

For $q = 2$ components, the experimental region is a straight line segment (1-dimensional simplex) between $(0, 1)$ and $(1, 0)$; for $q = 3$ components, the experimental region is an equilateral triangle (2-dimensional simplex) with vertices at $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$; and for $q = 4$ components the experimental region is a tetrahedron (3-dimensional simplex) with vertices at $(1, 0, 0, 0)$, $(0, 1, 0, 0)$, $(0, 0, 1, 0)$, and $(0, 0, 0, 1)$. The simplex regions for $q = 2, 3$, and 4 are shown in Figure 2. The coordinate system for the values of the x_i , $i=1,2,\dots,q$, is called a simplex coordinate system. The simplex coordinate system for $q=3$ is shown in Figure 3.

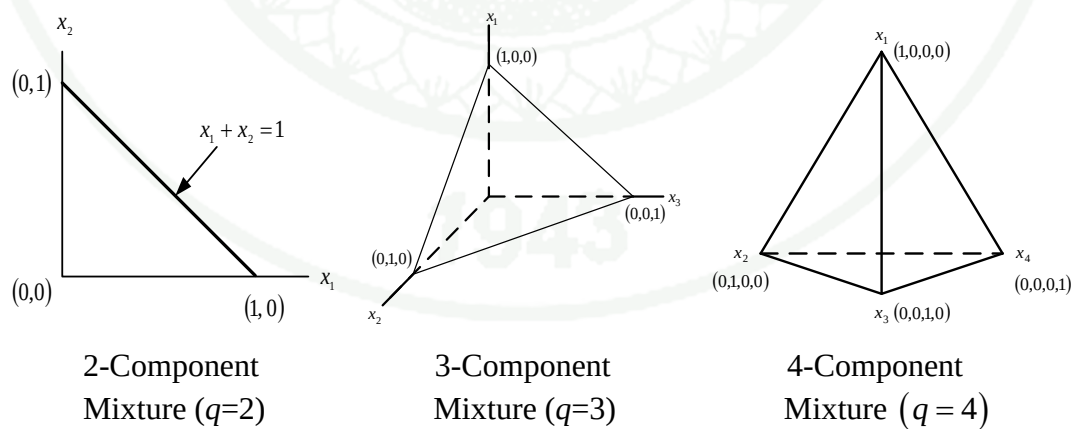


Figure 2 Two-, three-, and four-component simplex experimental regions for mixture experiments.

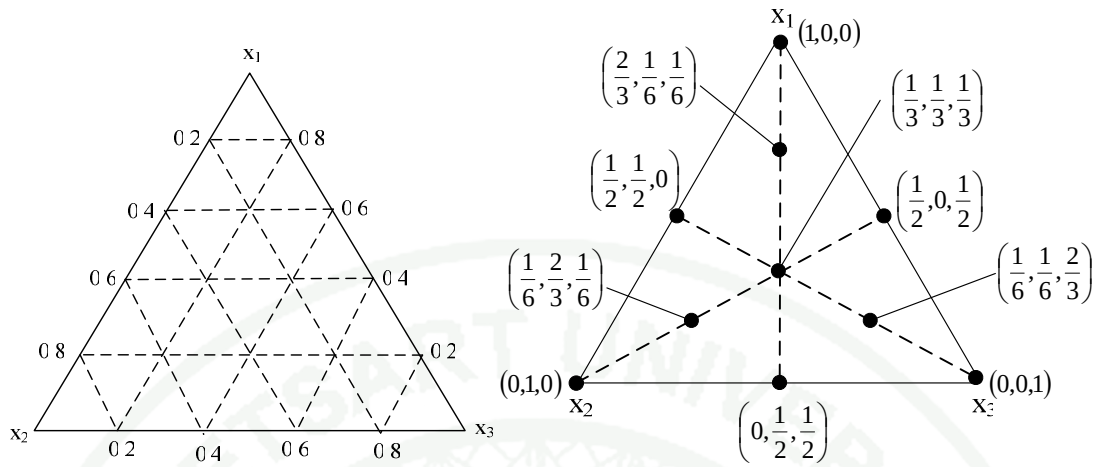


Figure 3 Triangular coordinate system for the 3-component simplex.

The experimental design space of the q components consists of all points on or inside the boundaries of the simplex. The boundary of a regular $(q-1)$ -dimensional simplex contains the vertices, edges, faces, etc. The vertices represent mixtures consisting of a single-component or ‘pure’ mixture. The interior points are the result of combining all the components (each $x_i > 0$). The points on the vertices, edges, and faces represent mixtures where only two or more of the components are presented. The simplex centroid corresponds to the mixture with equal proportion from each of the components (Cornell, 2002). For example, the triangle with vertices $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ represent a single-component or pure mixture and the interior points of the triangle represent mixtures in which all component proportions are positive; that is $0 < x_i < 1$ for $i = 1, 2$ and 3 ; and the centroid of the triangle is the mixture with equal proportions $(x_1, x_2, x_3) = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$ for each component.

2. Constraints and Experimental Region

In many mixture systems, physical and economic considerations often impose lower (L_i) and upper (U_i) bounds,

$$0 \leq L_i \leq x_i \leq U_i \leq 1 \quad ; i = 1, 2, \dots, q, \quad (10)$$

on the levels of some or all the components known as single-component constraints or SCCs. Given the constraints in (10), the shape of a design region in a mixture experiment is an irregularly-shaped polyhedron that is determined by the upper and lower bound constraints that are imposed on the component proportions. An example is shown in Figure 4 for a 3-component mixture with lower and upper bounds.

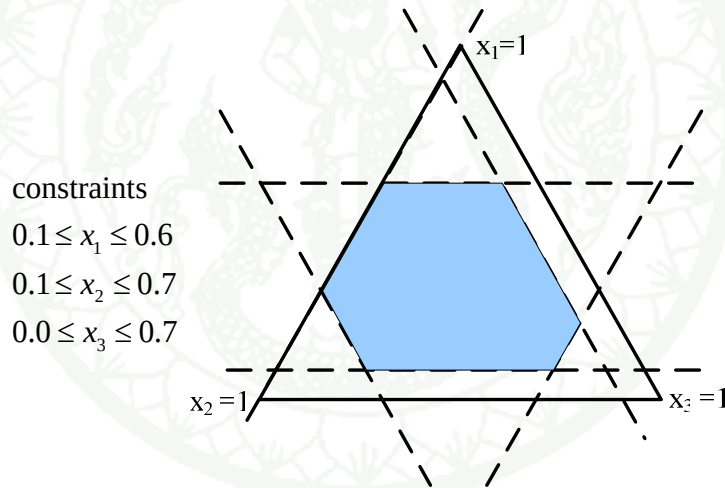


Figure 4 The irregular shape region of a three component mixture system with lower and upper bounds on the components and unequal component ranges.

In addition to the lower and upper bound restrictions on the component proportions, some mixture systems have linear constraints of the form,

$$C_j \leq A_{1j}x_1 + A_{2j}x_2 + \dots + A_{qj}x_q \leq D_j \quad ; j = 1, 2, \dots, h, \quad (11)$$

which are known as linear multi-component constraints or MCCs. In (11), the A_{ij} , C_j and D_j are scalar constants, and C_j and D_j are the lower and upper bounds, respectively, for the j -th linear MCC, and h is the number of linear MCCs. In mixture problems that include both single-component and linear multi-component constraints on the levels of some or all components, the experimental region will be an irregular polyhedron. That is, it is a subspace of the simplex. An example of an irregularly shaped region for three components with lower and upper bound SCCs as well as one linear MCC is shown in Figure 5.

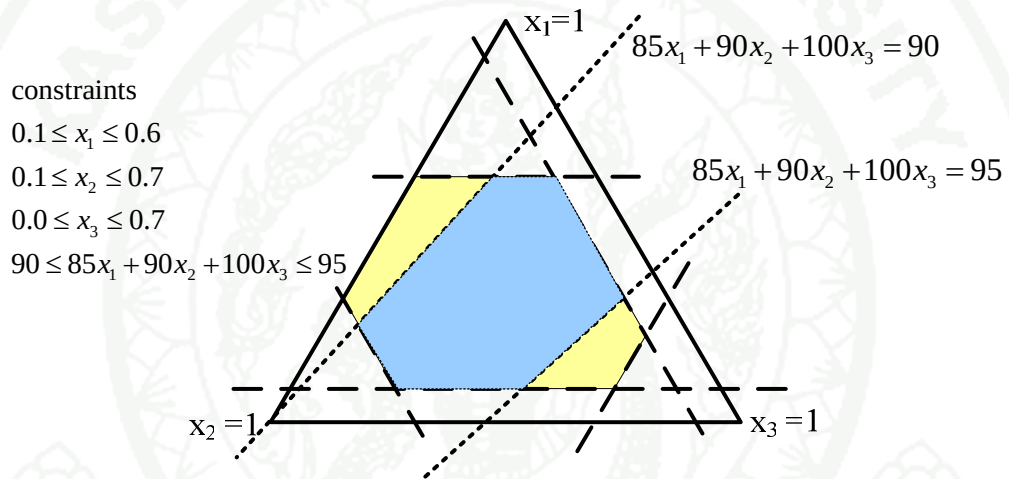


Figure 5 An irregularly shaped region of a three component mixture system with lower and upper bounds as well as one multi-component constraint on the components.

If only lower bounds are placed on the levels of the components, then the feasible region is always a smaller simplex within the original simplex and the pseudocomponent transformation is appropriate (Crosier, 1984). That is, the coordinates of mixtures in the subregion can be redefined as a new set of components known as ‘pseudocomponents’. When the lower bounds are used to define the pseudocomponents, the redefined components are called as ‘ L -pseudocomponents’. The L -pseudocomponent x'_i is defined by using the linear transformation as

$$x'_i = \frac{x_i - L_i}{1 - L_i} \quad (12)$$

where $L = \sum_{i=1}^q L_i < 1$. Because the feasible region is still a simplex but with vertices contained within the $(q-1)$ simplex, the set of pseudocomponents will take on the values 0 to 1 over the feasible region (Cornell, 2002). The experimental region is redefined as a simplex in the L -pseudocomponents x'_i . An example for three components and pseudocomponents is displayed in Figure 6.

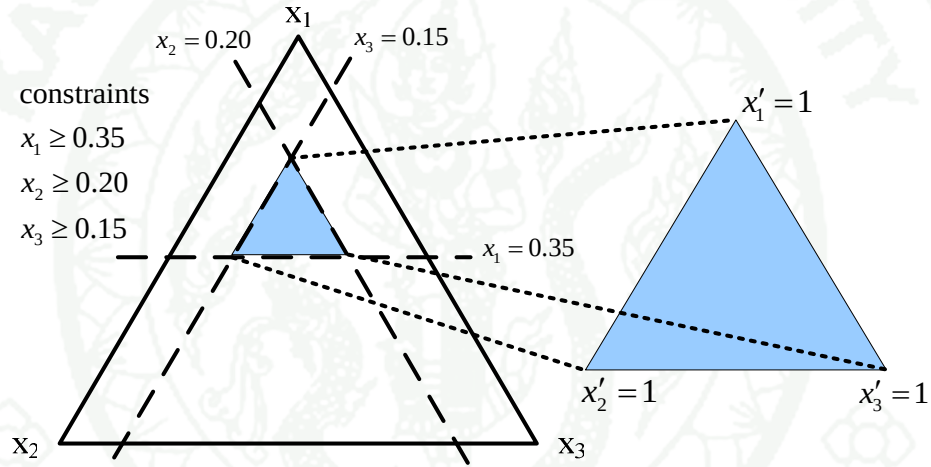


Figure 6 The subregion of the original simplex redefined as a simplex in the L -pseudocomponents x'_i for three components.

On the other hand, if only upper bounds are placed on the levels of the components, then the design region will be points in an inverted simplex that are contained inside the original simplex, and a pseudocomponent transformation is appropriate (Crosier, 1984). The feasible region is an inverted simplex that lies entirely inside the original simplex if and only if

$$\sum_{i=1}^q U_i - U_{\min} \leq 1 \quad (13)$$

where $U_{\min}$ is minimum of q upper bounds. On the contrary, when $\sum_{i=1}^q U_i - U_{\min} > 1$, the feasible region is the intersection of the original simplex and an inverted simplex containing points outside the original simplex (called the U -simplex). When the upper bounds are used to define the pseudocomponents, the redefined components are called as ' U -pseudocomponents'. The U -pseudocomponent u_i is defined by using the linear transformation:

$$u_i = \frac{U_i - x_i}{U - 1} \quad (14)$$

where $U = \sum_{i=1}^q U_i > 1$. The values of each pseudocomponent range from 0 to 1 (Cornell, 2002). For example, if three components are restricted by

$$x_1 \leq 0.4, \quad x_2 \leq 0.6, \quad x_3 \leq 0.3,$$

then the U -simplex is the inverted simplex inside the original simplex and is shown in Figure 7 (Cornell, 2002). In this situation, we have

$$\sum_{i=1}^3 U_i = 0.4 + 0.6 + 0.3 = 1.3$$

and $U_{\min} = 0.3$, so $\sum_{i=1}^q U_i - U_{\min} = 1.3 - 0.3 = 1$. Thus, the feasible region is an inverted simplex and is represented by the shaded region in Figure 7.

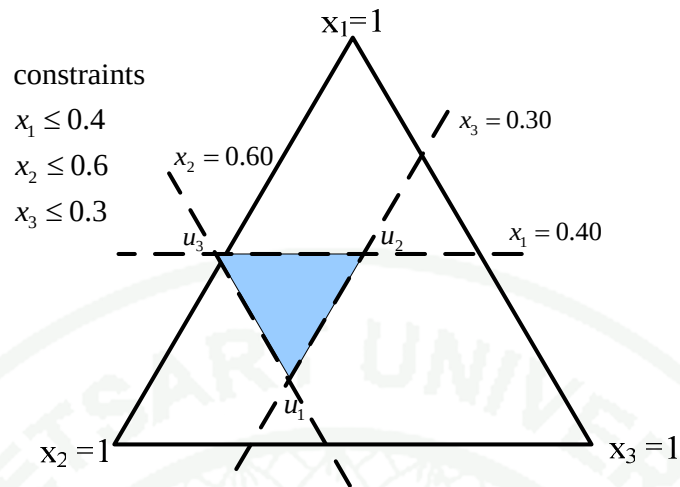


Figure 7 The inverted U -pseudocomponents u_i simplex lies entirely inside the original simplex for three components.

On the other hand, if three components are restricted by

$$x_1 \leq 0.7, \quad x_2 \leq 0.6, \quad x_3 \leq 0.8,$$

then the U -simplex is the inverted simplex that contains points outside the original simplex, and is the large inverted triangle displayed in Figure 8 (Cornell, 2002). In this case, we have

$$\sum_{i=1}^3 U_i = 0.7 + 0.6 + 0.8 = 2.1$$

and $U_{\min} = 0.6$, so $\sum_{i=1}^q U_i - U_{\min} = 2.1 - 0.6 = 1.5$. Thus, the feasible region is not a simplex. The feasible region is the intersection of the inverted simplex and the original simplex, and is shown in the shaded region in Figure 8.

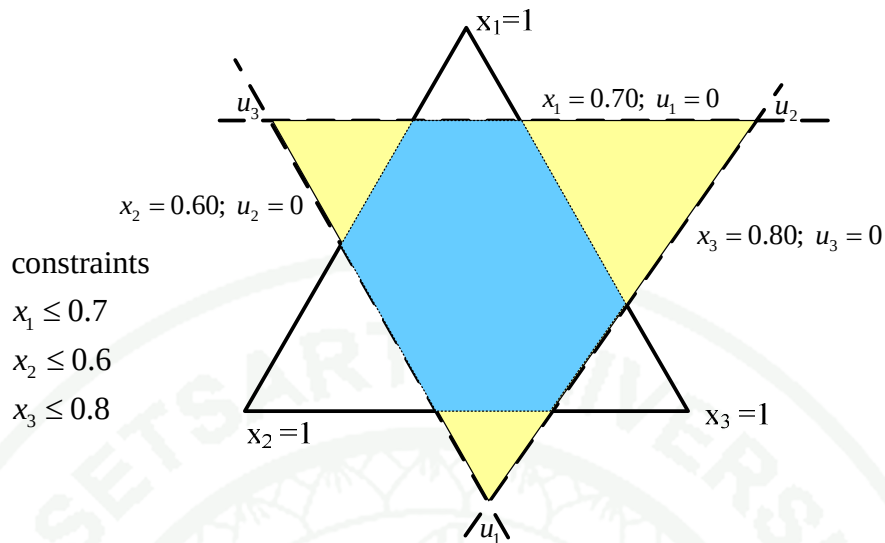


Figure 8 The inverted U -pseudocomponents u_i simplex lies entirely outside the original simplex for three components.

Piepel (1983) proposed a technique for checking the consistency of the single and multiple component constraints. In practice, for the mixture experiment, the initial constraints specified by the experimenter are often modified to eliminate inconsistencies (e.g. $\sum_{i=1}^q x_i > 1$). To determine a feasible mixture design space, the single component and multi-component constraints must be consistent. In the case of multi-component constraints, although a set of them may be consistent, they might modify the experimental region in a fashion different from that desired. When developing single component constraints, two obvious conditions must be met:

$$\sum_{i=1}^q L_i \leq 1 \quad \text{and} \quad \sum_{i=1}^q U_i \geq 1. \quad (15)$$

These conditions guarantee that the set of mixtures in the constraint region is not empty. The set of single component constraints is consistent if there exists some mixture $\mathbf{x} = (x_1, x_2, \dots, x_q)$ in the constraint region such that $x_i = L_i$ and $x_i = U_i$ for each $i = 1, 2, \dots, q$. Similarly, the set of multiple components constraints is consistent if

there exist mixtures $\mathbf{x} = (x_1, x_2, \dots, x_q)$ and $\mathbf{x}' = (x'_1, x'_2, \dots, x'_q)$ in the constraint region such that $A_{1j}x_1 + A_{2j}x_2 + \dots + A_{qj}x_q = C_j$ and $A_{1j}x'_1 + A_{2j}x'_2 + \dots + A_{qj}x'_q = D_j$ for each j .

For SCCs, an inconsistency occurs if for some constraint i ,

$$R'_i > 1 \ ; i = 1, 2, \dots, q \quad (16)$$

or

$$\sum_{j \neq i}^q R'_j < 1 \ ; \text{for some } i = 1, 2, \dots, q \quad (17)$$

where $R'_j = \frac{(U_j - L_j)}{\left(1 - \sum_{k=1}^q L_k\right)}$ is the pseudocomponent range of component j .

For example, the following shows one type of inconsistency for three components:

$$\begin{aligned} 0.0 &\leq x_1 \leq 0.1 \\ 0.1 &\leq x_2 \leq 0.2 \\ 0.6 &\leq x_3 \leq 0.8. \end{aligned} \quad (18)$$

Specifically, the constraint region is empty because each $R'_i < 1$

$$\begin{aligned} R'_1 &= \frac{(0.1 - 0.0)}{1 - (0.0 + 0.1 + 0.6)} = \frac{1}{3} < 1, \quad R'_2 = \frac{(0.2 - 0.1)}{1 - (0.0 + 0.1 + 0.6)} = \frac{1}{3} < 1, \text{ and} \\ R'_3 &= \frac{(0.8 - 0.6)}{1 - (0.0 + 0.1 + 0.6)} = \frac{2}{3} < 1, \end{aligned}$$

while for $i = 1$, $\sum_{j \neq i}^3 R'_j = R'_2 + R'_3 = \frac{1}{3} + \frac{2}{3} = 1$, for $i = 2$, $\sum_{j \neq i}^3 R'_j = R'_1 + R'_3 = \frac{1}{3} + \frac{2}{3} = 1$,

$$\text{and } i = 3, \sum_{j \neq i}^3 R'_j = R'_1 + R'_2 = \frac{1}{3} + \frac{1}{3} = \frac{2}{3} < 1.$$

Thus, these constraints are inconsistent. Given the constraints for x_1 and x_2 , the minimum value of x_3 must be $x_3 = 1 - U_1 - U_2 = 1 - 0.1 - 0.2 = 0.7$.

For MCCs, the inconsistency occurs if for some constraint j ,

$$Q'_j > 1 \quad (19)$$

and

$$\sum_{i \neq j}^k Q'_i < 1 \quad (20)$$

where $Q'_j = \frac{(D_j - C_j)}{\left(1 - \sum_{k=1}^q C_k\right)}$ is the pseudocomponent range of component j .

When the experiment has inconsistent constraints, experimental mixtures may not be investigated in a portion of the mixture space important to scientists, and may be found to produce unacceptable blends $\left(\sum_{i=1}^q x_i \neq 1\right)$. The consistent bounds are necessary for determining the shape (number of vertices, edges, faces, etc) and the size of the experimental region of feasible mixture proportions. Some design generating and analysis procedures, such as the extreme vertices algorithm of McLean and Anderson (1966), Snee and Marquardt (1974), and Snee (1979), are not adversely affected by inconsistent constraints.

Crosier (1984) pointed out that the upper bounds (U_i) create implied lower bounds (L_i^*) , and the lower bounds (L_i) create implied upper bounds (U_i^*) for detecting inconsistencies. Any upper bound larger than the corresponding implied upper bound is inconsistent or unattainable. While, any lower bound less than the corresponding implied lower bound is inconsistent or unattainable. The minimum value of x_i or implied lower bound is

$$\begin{aligned}
L_i^* &= U_i - R_U \\
&= U_i - \left(\sum_{i=1}^q U_i - 1 \right) \\
&= 1 - U_1 - U_2 - \dots - U_{i-1} - U_{i+1} - \dots - U_q \\
&= 1 - \sum_{j \neq i}^q U_j.
\end{aligned} \tag{21}$$

The maximum value of x_i or implied upper bound is

$$\begin{aligned}
U_i^* &= L_i - R_L \\
&= L_i - \left(1 - \sum_{i=1}^q L_i \right) \\
&= 1 - L_1 - L_2 - \dots - L_{i-1} - L_{i+1} - \dots - L_q \\
&= 1 - \sum_{j \neq i}^q L_j.
\end{aligned} \tag{22}$$

Another method of detecting inconsistencies is from the component ranges

$$R_i = U_i - L_i \tag{23}$$

First, calculate the component ranges of each constraint (R_i). Then, any R_i being greater than R_L indicates an inconsistent upper bound. While, any R_i being greater than R_U indicates an inconsistent lower bound.

The properties of mixture designs for irregular regions is affected by many factors such as the number of design variables, the shape of the irregular region, the number of design points, the distribution of the design points over the irregular region, the number of replicates, the presence or absence of a centroid(s), and the model form employed to construct the design (Piepel *et al.*, 1993b).

3. The General Form of Mixture Models

We now consider models for mixture experiments which will be presented in a general linear models framework. That is, the relationship between the explanatory factors and the response of interest can be written as

$$\mathbf{y} = [\eta(x_1), \eta(x_2), \dots, \eta(x_n)] + \boldsymbol{\varepsilon}, \quad (24)$$

where $\mathbf{y}$ is the $n \times 1$ vector of responses, $\eta(x_i)$ is the true but unknown function value at the i^{th} mixture vector x_i of component proportions (the explanatory variables) ($i=1,2,\dots,n$), and $\boldsymbol{\varepsilon}$ is the $n \times 1$ vector of error terms representing sources of variability not accounted for. Thus, $\boldsymbol{\varepsilon}$ represents the deviation of $\mathbf{y}$ about η . The error terms are assumed to have zero mean and variance-covariance matrix $\sigma^2 \mathbf{I}$. That is $E(\boldsymbol{\varepsilon}) = 0$ and $\text{Var}(\boldsymbol{\varepsilon}) = \sigma^2 \mathbf{I}$.

The general linear model of a mixture experiment in matrix form is given as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \quad (25)$$

$$\text{where } \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{bmatrix}, \quad \text{and } \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

In general, $\mathbf{y}$ is a $n \times 1$ vector of observed responses, $\mathbf{X}$ is an $n \times p$ model matrix consisting of the levels of the independent variables expanded to a p -parameter model form that contains n -row vectors of terms $\mathbf{x}_i$, $\boldsymbol{\beta}$ is a $p \times 1$ vector of regression model coefficients, and $\boldsymbol{\varepsilon}$ is an $n \times 1$ vector of errors with zero mean and variance-covariance matrix $\sigma^2 \mathbf{I}_n$ where σ^2 is the observation error variance and $\mathbf{I}_n$ is a $n \times n$ identity matrix, n is the number of observations and p is the number of parameters in the model. Thus, we are also assuming that the errors are independent with constant

variance. Hence $E(\mathbf{y}) = \boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ where $\boldsymbol{\mu}$ is a column vector of all expected responses. The parameters in the model (vector $\boldsymbol{\beta}$) are usually estimated by the method of least squares (Cornell, 2002). The vector of least square estimators that minimizes the error sums of squares L :

$$\begin{aligned} L &= \boldsymbol{\varepsilon}'\boldsymbol{\varepsilon} \\ &= (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \\ &= \mathbf{y}'\mathbf{y} - \boldsymbol{\beta}'\mathbf{X}'\mathbf{y} - \mathbf{y}'\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta} \\ &= \mathbf{y}'\mathbf{y} - 2\boldsymbol{\beta}'\mathbf{X}'\mathbf{y} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta} \end{aligned} \quad (26)$$

because scalars $\mathbf{y}'\mathbf{X}\boldsymbol{\beta} = (\boldsymbol{\beta}'\mathbf{X}'\mathbf{y})'$. The least squares estimator for $\boldsymbol{\beta}$ must satisfy

$$\left. \frac{\partial L}{\partial \boldsymbol{\beta}} \right|_{\mathbf{b}} = -2\mathbf{X}'\mathbf{y} + 2\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{0} \quad (27)$$

which is simplified to

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{y} . \quad (28)$$

Therefore, the least squares estimator for $\boldsymbol{\beta}$ is

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{y} . \quad (29)$$

The expectation of $\mathbf{b}$ is $E(\mathbf{b}) = \boldsymbol{\beta}$. Thus $\mathbf{b}$ is unbiased estimator of $\boldsymbol{\beta}$. The variance-covariance matrix of $\mathbf{b}$ is $\text{var}(\mathbf{b}) = (\mathbf{X}'\mathbf{X})^{-1} \sigma^2$, and the unbiased estimator of σ^2 is given by

$$\hat{\sigma}^2 = \frac{SSE}{n - p} \quad (30)$$

where $SSE = \mathbf{y}'\mathbf{y} - \mathbf{b}'\mathbf{X}'\mathbf{y}$, n is the number of observations, and p is the number of parameters in the model. The fitted model is

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{b} \quad (31)$$

The objective of any mixture experiment is to construct blending models that are applicable in a region of interest. Thus, within the mixture region of interest, we can make predictions and estimate the effects of any ingredients or combinations of ingredients on the response.

In response surface methodology (RSM), the general form of an m th-degree polynomial is given by

$$y = \beta_0 + \sum_{i=1}^q \beta_i x_i + \sum_{i \leq j}^q \sum_{j=1}^q \beta_{ij} x_i x_j + \sum_{i \leq j \leq k}^q \sum_{j=1}^q \sum_{k=1}^q \beta_{ijk} x_i x_j x_k + \dots + \varepsilon. \quad (32)$$

where the highest order term has degree = m . The number of terms in Eq. (32) is $\binom{q+m}{m}$. For example, when $q = 2$ and $m = 2$,

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \varepsilon.$$

For a mixture experiment, however, the m th-degree polynomial model is overparameterized because of the mixture constraint $\sum_{i=1}^q x_i = 1$. When this constraint is introduced, the general polynomial for degree m in q components is modified by multiplying certain terms in Eq. (32) by the constraint $\sum_{i=1}^q x_i = x_1 + x_2 + \dots + x_q = 1$, and is then simplified. The resulting equation is the so-called the ‘canonical’ polynomial or the ‘Scheffé’ polynomial or the $\{q, m\}$ polynomial that has degree m in q components. For example, the standard first-order RSM polynomial model for a q factor response surface design is

$$y = \beta_0^* + \sum_{i=1}^q \beta_i^* x_i + \varepsilon. \quad (33)$$

When the constraint $\sum_{i=1}^q x_i = 1$ is applied to Eq. (33), the resulting mixture model is

$$\begin{aligned} y &= \beta_0^* \left(\sum_{i=1}^q x_i \right) + \sum_{i=1}^q \beta_i^* x_i + \varepsilon \\ &= \sum_{i=1}^q \beta_i x_i + \varepsilon, \end{aligned} \quad (34)$$

where $\beta_i = \beta_0^* + \beta_i^*$ for all $i = 1, 2, \dots, q$. The standard second-order RSM polynomial model for a q factor response surface design is

$$y = \beta_0^* + \sum_{i=1}^q \beta_i^* x_i + \sum_{i=1}^q \beta_{ii}^* x_i^2 + \sum_{i < j}^q \beta_{ij}^* x_i x_j + \varepsilon. \quad (35)$$

When the mixture constraints $\sum_{i=1}^q x_i = 1$ and $x_i^2 = x_i \left(1 - \sum_{\substack{j=1 \\ j \neq i}}^q x_j \right)$ are applied to (35), the

resulting model is the canonical or Scheffé form of the quadratic mixture model :

$$\begin{aligned} y &= \beta_0^* \left(\sum_{i=1}^q x_i \right) + \sum_{i=1}^q \beta_i^* x_i + \sum_{i=1}^q \beta_{ii}^* x_i \left(1 - \sum_{j \neq i}^q x_j \right) + \sum_{i < j}^q \beta_{ij}^* x_i x_j + \varepsilon \\ &= \sum_{i=1}^q (\beta_0^* + \beta_i^* + \beta_{ii}^*) x_i - \sum_{i=1}^q \beta_{ii}^* x_i \left(\sum_{j \neq i}^q x_j \right) + \sum_{i < j}^q \beta_{ij}^* x_i x_j + \varepsilon \\ &= \sum_{i=1}^q \beta_i x_i + \sum_{i < j}^q \beta_{ij} x_i x_j + \varepsilon, \end{aligned} \quad (36)$$

where $\beta_i = \beta_0^* + \beta_i^* + \beta_{ii}^*$ is the expected response at the pure component i , and $\beta_{ij} = \beta_{ij}^* - \beta_{ii}^* - \beta_{jj}^*$ is the measure of the quadratic (or binary) mixing behavior of components i and j ; $i < j$. The second-order canonical mixture model is the most popular in documented case studies. Generally, the canonical or Scheffé mixture model in terms of $E(y)$ can be classified as follows :

Linear model:

$$E(y) = \sum_{i=1}^q \beta_i x_i \quad (37)$$

Quadratic model :

$$E(y) = \sum_{i=1}^q \beta_i x_i + \sum_{i < j}^q \beta_{ij} x_i x_j \quad (38)$$

Full Cubic model :

$$E(y) = \sum_{i=1}^q \beta_i x_i + \sum_{i < j}^q \beta_{ij} x_i x_j + \sum_{i < j}^q \delta_{ij} x_i x_j (x_i - x_j) + \sum_{i < j < k}^q \beta_{ijk} x_i x_j x_k \quad (39)$$

Special Cubic model :

$$E(y) = \sum_{i=1}^q \beta_i x_i + \sum_{i < j}^q \beta_{ij} x_i x_j + \sum_{i < j < k}^q \beta_{ijk} x_i x_j x_k \quad (40)$$

The number of terms for the models in Eq. 37 to 40 is given in Table 1.

Generally, a canonical or Scheffé polynomial model is adequate for modeling well-behaved data. For some situations, there may be better model forms than the canonical or Scheffé polynomial models which can be used. Alternative model schemes developed by Scheffé and other authors have been reviewed in Cornell (2000). Among them are the additive polynomial models proposed by Darroch and Waller (1985). Becker (1968) introduced three models for the situation where some components are inert or have additive effects. Draper and St. John (1977) proposed models with inverse terms when the value of the response increases rapidly as the value of one or more components converges to the boundary of the simplex.

If the design region is small, it may be possible to estimate the response by the canonical or Scheffé first-order model. If the design region is large, a quadratic or higher-order model may be needed to estimate the response (Snee, 1981).

Table 1 Number of the terms in the canonical polynomial mixture model.

Number of components : q	linear	quadratic	full cubic	special cubic
2	2	3	-	-
3	3	6	10	7
4	4	10	20	14
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
q	q	$\frac{q(q+1)}{2}$	$\frac{q(q+1)(q+2)}{6}$	$\frac{q(q^2+5)}{6}$

Source: Cornell (2002).

4. Designs in Mixture Experiments

Response surface designs such as factorial, fractional factorial, Plackett-Burman, central composite, and Box-Behnken are generally applicable to cuboidal or spherical regions. Hence, they will not be applicable in mixture experiments because the experimental region is the simplex or an irregular subspace of the simplex. Experimental designs such as the simplex lattice design, and simplex-centroid designs, were developed when the design space is a regular simplex (Cornell, 2002).

The $\{q, m\}$ simplex-lattice design (Scheffé, 1958) can be employed to fit a polynomial of degree m in q components. The points are selected so that proportions of each of q components are selected from the set of $m+1$ equally spaced values from 0 to 1. All possible combinations of $(x_1, x_2, \dots, x_q)$ are employed to set up the design points where

$$x_i \in 0 \left\{ \frac{1}{m}, \frac{2}{m}, \dots, \frac{m}{m} \right\} ; i = 1, 2, \dots, q \quad (41)$$

The number of points in the $\{q, m\}$ simplex-lattice design is $\binom{q+m-1}{m}$. For example, the $\{4, 2\}$ simplex lattice design would consist of the 10 design points,

$$\begin{aligned} (x_1, x_2, x_3, x_4) = & (1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1), \\ & \left(\frac{1}{2}, \frac{1}{2}, 0, 0\right), \left(\frac{1}{2}, 0, \frac{1}{2}, 0\right), \left(\frac{1}{2}, 0, 0, \frac{1}{2}\right), \\ & \left(0, \frac{1}{2}, \frac{1}{2}, 0\right), \left(0, \frac{1}{2}, 0, \frac{1}{2}\right), \left(0, 0, \frac{1}{2}, \frac{1}{2}\right). \end{aligned}$$

The $\{4, 2\}$ simplex lattice points are illustrated in Figure 9 .

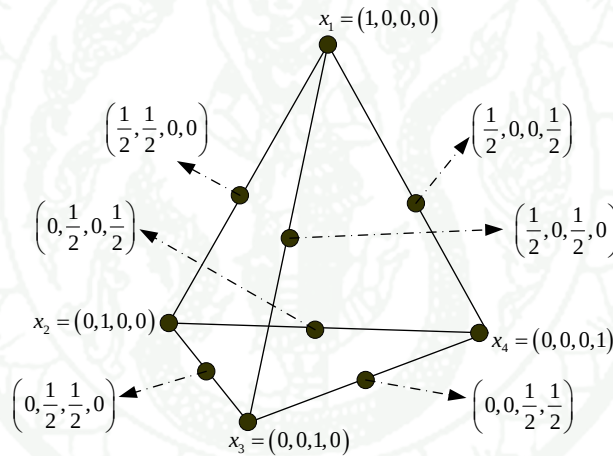


Figure 9 The $\{4, 2\}$ simplex lattice design.

The simplex-centroid design (Scheffé, 1963) consists of all mixtures located at the centroids of each simplex confined within the q component simplex. The points correspond to the $\binom{q}{1}$ permutations of $(1, 0, \dots, 0)$ or q single component blends, the $\binom{q}{2}$ permutations of $\left(\frac{1}{2}, \frac{1}{2}, 0, \dots, 0\right)$ or all the binary blends, the $\binom{q}{3}$ permutations of

$\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0, \dots, 0\right)$ or all the ternary blends and so on, with finally the $\binom{q}{q}$ permutations of $\left(\frac{1}{q}, \frac{1}{q}, \frac{1}{q}, \frac{1}{q}, \frac{1}{q}, \frac{1}{q}\right)$ or the overall centroid. The number of points in the simplex-centroid design is $\sum_{i=1}^q \binom{q}{i} = 2^q - 1$. For example, the simplex centroid design for $q = 4$ components would consist of the 15 design points,

$$\begin{aligned} (x_1, x_2, x_3, x_4) = & (1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1), \\ & \left(\frac{1}{2}, \frac{1}{2}, 0, 0\right), \left(\frac{1}{2}, 0, \frac{1}{2}, 0\right), \left(\frac{1}{2}, 0, 0, \frac{1}{2}\right), \left(0, \frac{1}{2}, \frac{1}{2}, 0\right), \left(0, \frac{1}{2}, 0, \frac{1}{2}\right), \left(0, 0, \frac{1}{2}, \frac{1}{2}\right), \\ & \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0\right), \left(\frac{1}{3}, \frac{1}{3}, 0, \frac{1}{3}\right), \left(\frac{1}{3}, 0, \frac{1}{3}, \frac{1}{3}\right), \left(0, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right), \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right). \end{aligned}$$

The point of this simplex-centroid design are displayed in Figure 10. For further information of these two types of designs as well as other designs, consult Cornell (2002).

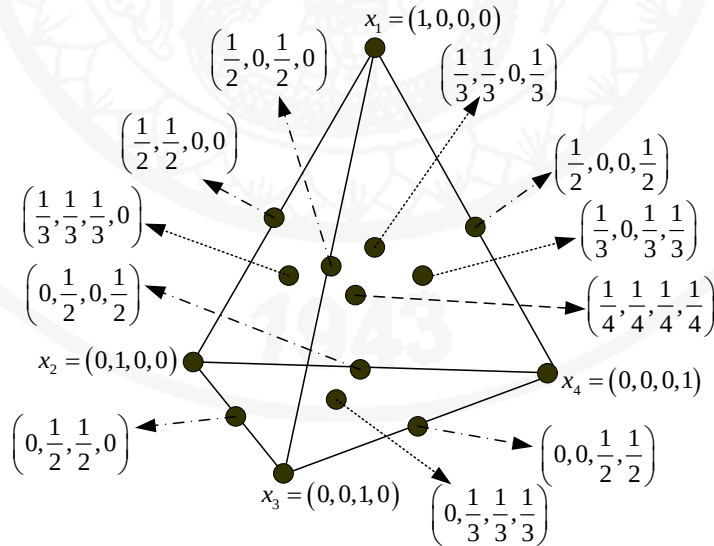


Figure 10 The simplex centroid design with four components.

The mixture designs that are commonly used for a simplex mixture design region (such as the simplex lattice design and the simplex-centroid design) are inappropriate for an irregularly-shaped design region. One reason is that these designs assume all single component mixtures are possible, but this is not possible in an irregularly-shaped region. For constrained mixture experiments where the feasible region is irregularly-shaped, computer-aided experimental designs are often used (Smith, 2005). Computer-aided experimental designs are commonly generated using point-exchange algorithms to select design points from a list of candidates. The ‘candidate list’ is a list composed of some or all of the vertices that define the boundary of the feasible mixture space, the one-dimensional centroids, the two-dimensional centroids,..., the $(q-1)$ -dimensional centroid. The centroids are calculated by averaging vertices are called ‘averaged-extreme-vertices centroids’. The selection of design points also depends on the model selected. Some of the algorithms used to generate designs for irregularly-shaped experimental regions are shown in Table 2. Further information for each algorithm in Table 2 can be found in Section 10 of the literature review of the research.

Table 2 Algorithms for generating designs an irregularly-shaped mixture experimental region.

Year	Name	Author (s)
1966	EV (Extreme Vertices)	McLean and Anderson
1974	DETMAX	Mitchell
1974	XVERT	Snee and Marquardt
1979	CONSIM	Snee

Source: Smith (2005).

5. Genetic Algorithms

Experimental designs for computer experiments have received a great deal of attention given the increased use of computer simulation models in scientific research. Computer search algorithms are often employed to find a suitable design and are widely available in commercial software. Many procedures have been developed to improve the search for solutions. Heuristic optimization has been used in design of experiments to solve a variety of problems. Generally, the heuristic search algorithm refers to a practical and quick procedure based on strategies that are likely to lead to a solution that is approximately optimal or near optimal, while avoiding being trapped at a locally optimal solution. One of the most famous heuristic search methods based on the general principle of local improvement is the genetic algorithm (GA). The use of a genetic algorithm that is designed to solve a complex combinatorial optimization problem is motivated by an analogy of natural evolution and heredity.

The genetic algorithm (GA) was first described by Holland (1975) and has been popularized through the work of Goldberg (1989). The method has often been viewed from a biological perspective, with a wide range of applicability in scientific and industrial applications. More recently, the GA has also been successfully applied to experimental design problems using various optimality criteria. For an optimization problem, the overall effectiveness of a GA depends on several factors such as the choice of design region, encoding scheme, choice of the evaluation function, and the manner in which the experiments are constructed within the design region. A GA does not guarantee the optimal design (solution) will be found, and getting trapped at a locally optimal design is possible due to complex combinatorial conditions. The GA, however, can be an excellent alternative search method for constructing optimal designs for several experimental situations.

A genetic algorithm is a method for moving from one population of individuals to a new population by simulating a kind of natural selection based on genetic operators such as crossover, mating, mutation, and inversion to optimize an objective function. A GA also has specific terminology that is commonly-used. A

chromosome is a potential solution that can be encoded as a string of length n . The variable in a position on the chromosome is known as the **gene** at that position. For example, if $n=5$, a general chromosome is $x=(x_1, x_2, x_3, x_4, x_5)$ where x_1, x_2, x_3, x_4 , and x_5 are the genes on this chromosome. The flowchart of a commonly-used genetic algorithm is shown in Figure 11.

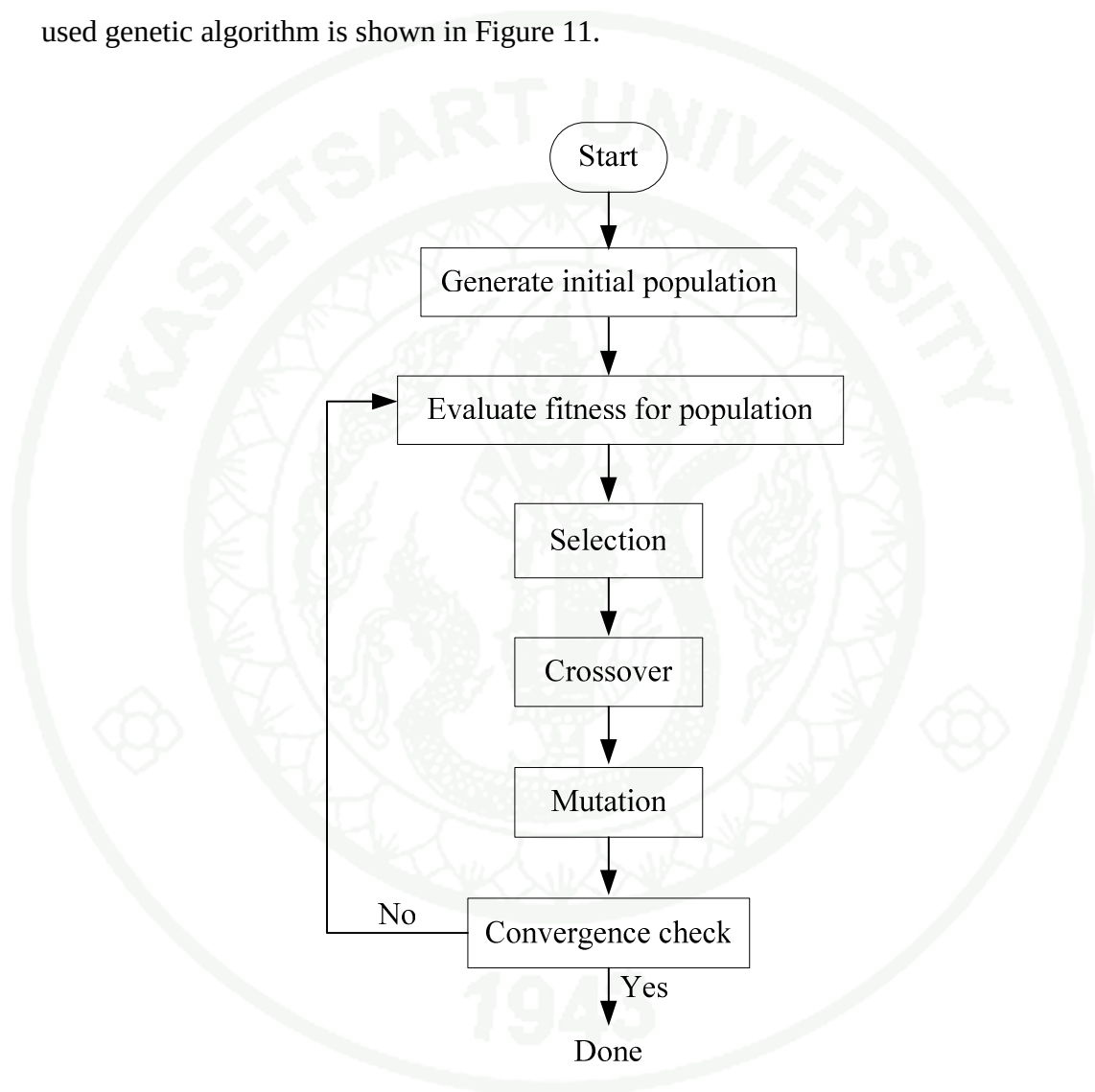


Figure 11 The flowchart of a genetic algorithm.

In general, a genetic algorithm proceeds in the following steps:

5.1 Encoding

The first step of a genetic algorithm is to represent a solution in an encoded form. This process can be performed using binary encoding, real number encoding, or any other user-defined encoding (Sivanandam and Deppa (2008)). The choice of encoding depends on the type of problem. In binary encoding, genes are encoded 0 or 1, and each chromosome is a binary string. An example is shown in Figure 12. For some applications, however, it is natural to use real number encoding to form chromosomes such as when the number of variables is large, and, thus, the size of the chromosome is also large. In this case, 1s and 0s are inappropriate to represent a variable. In this dissertation, the use of real numbers for encoding is adopted. Each chromosome is a string of numbers and an example is shown in Figure 13. One of the advantages of real value encoding is that it requires less storage than that of binary encoding. Borkowski (2003) cited Davis (1991) who stated that GAs using real value encoding have outperformed GAs using binary encoding in a numerical optimization problems.

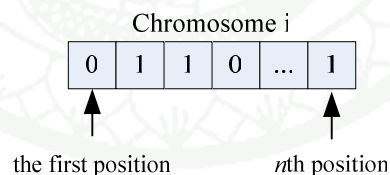


Figure 12 Binary encoding scheme.

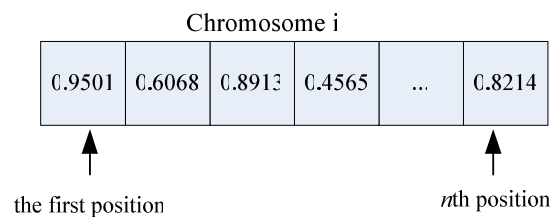


Figure 13 Real value encoding scheme.

In this dissertation, the genetic algorithm starts with a group of C chromosomes known as the **population** and is shown in Figure 14 where each row in the population is a chromosome. A **chromosome** will be an $n \times q$ design matrix where n is the number of mixture design points, and q is the number of mixture components. A **gene** x_{ij} is the i th row of chromosome j and is the coded setting of the i th mixture component in the j th experimental run.

$$population = \begin{bmatrix} \text{chromosome 1} \\ \text{chromosome 2} \\ \vdots \\ \text{chromosome } C \end{bmatrix}$$

Figure 14 Population consisting of C chromosomes.

5.2 Selection and Reproduction

Selection is the process of choosing two chromosomes from the population called **parents**, in order to produce two new chromosomes, called **offspring**. In the **reproduction** process good genes are passed to the next generation of the population. The reproductive operation simulates the survival of chromosomes for more than one generation as would happen in a natural population. The selection drives the genetic algorithm to improve the population fitness over successive generations.

After completing the selection and reproduction processes, chromosomes with higher “fitness” relative to the existing population are selected. Different fitness measures are discussed in the Methods chapter. The chromosomes that have higher fitness values can be passed on to the next generation of chromosomes, while, the chromosomes with lower fitness values are removed from the population.

The convergence rate of a genetic algorithm relies largely on the selection pressure, with higher selection pressure resulting in faster convergence rates (Haupt

and Haupt (2004). The selection pressure is the degree to which the better chromosomes are selected. There are many methods for selecting chromosomes for the reproduction process such as elitist selection, roulette wheel selection, random selection, rank selection, tournament selection, Boltzmann selection, and so on (Sivanandam and Deepa (2008) and Haupt and Haupt (2004)). Some selection methods are now discussed:

5.2.1 Elitist selection

The best chromosome or several of the best chromosomes are retained to the population in the next generation. The best chromosome or chromosomes are called **elite** chromosomes and do not participate in the selection process. The selection process is then applied to remaining chromosomes.

5.2.2 Roulette wheel selection

Roulette wheel selection simulates a linear search through a roulette wheel with the wheel weights in proportion to the fitness values. That is, each chromosome is assigned a slice of the roulette wheel, the size of the slice being proportional to the chromosome's fitness. The wheel is spun N times, where N is the number of the chromosomes in the population. On each spin, the chromosome under the wheel's marker is selected to be in the pool of parents for the next generation. Parents are selected according to their fitness. Variations on roulette wheel selection exist based on whether or not a parent can be selected multiple times, and if so, one parent can be paired with itself. Another variation uses weights that are based on ranks.

5.2.3 Tournament selection

This selection provides selective pressure by holding a tournament among a small number k (often 2 or 3) chromosomes, where k is the tournament size. The winner chromosome from the tournament is the chromosome with the

higher fitness of the k tournament chromosomes, and the winner is then inserted into the mating pool for the reproduction process. This procedure is repeated until the required number of parents (usually N) is obtained.

5.2.4 Random pairing

Random pairing selection uses a uniform random number generator to select parent chromosomes from the population. The parent chromosomes are randomly partitioned into $\frac{C}{2}$ pairs where C is the number of chromosomes.

5.3 Recombination

After the selection process, the goal is to improve the current population with the selected chromosomes. **Mating** is the creation of one or more offspring from the parents selected in the selection process. The recombination operator allows the exchange of the information contained in a chromosome by its transmission to the next generation. For a pair of two parent chromosomes, the recombination operator is used to modify the gene structure to create offspring chromosomes having the potential of becoming members of the population for the next generation. The **crossover** is the most commonly used form for the recombination process. The crossover chooses one or more crossover points which partition the encoded chromosomes, and then creates the offspring by swapping corresponding portions of the parents formed by the partition. The crossover points are randomly selected between the string length of the parent's chromosomes. There are several different types of crossovers such as single point crossover, two points crossover, and uniform crossover. For more information on the recombination process see Sivanandam and Deepa (2008). Three crossover methods are now discussed:

5.3.1 Single point crossover

Two new offspring are obtained by copying the portion of the chromosome from one parent determined from a single crossover point, with the rest of the chromosome replaced with a copy from the second parent. Two new offspring are produced and the process is shown in Figure 15.

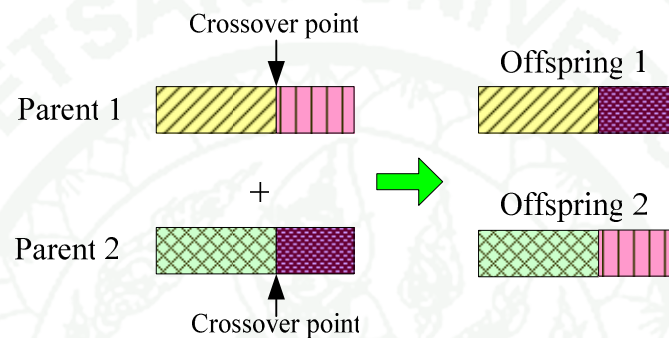


Figure 15 Two new offspring as created by single point crossover.

5.3.2 Two points crossover

Two new offspring are obtained by copying the beginning and end portions of the chromosome determined by two crossover points from one parent, with the middle part of the chromosome replaced with a copy from the second parent. Two new offspring are produced and the process is shown in Figure 16.

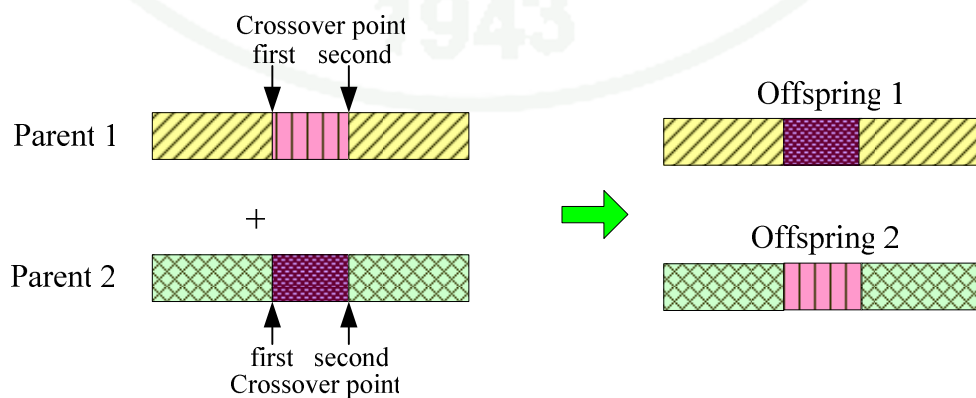


Figure 16 Two new offspring as created by a two point crossover.

5.3.3 Uniform crossover

Two new offspring are obtained by randomly copying from the first or from the second parent. Two new offspring are produced and the process is displayed in Figure 17.

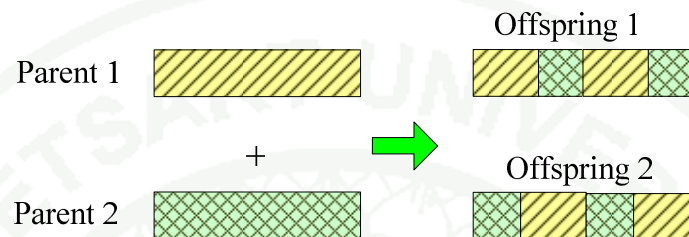


Figure 17 Two new offspring as created by uniform crossover.

5.4 Mutation

After crossover, a chromosome is subject to mutation. Mutation alters one or more gene values of a chromosome in a random fashion for improving the diversity of the population, and, in certain applications, expanding the volume of the current search space. With these new mutated gene values, the genetic algorithm may be able to arrive at a better solution than was previously possible. Mutation is an important part of the genetic search because it helps escaping from a local minima trap. Mutation occurs during evolution according to a user-definable mutation probability. This probability should usually be set fairly low in order to avoid the disruption and divergence of the solution. There are many variation of mutation such as flipping, interexchange, random uniform, Gaussian, and so on (Sivanandam and Deepa (2008) and Heredia-Langner *et al.* (2003)). Several mutation methods are now discussed:

5.4.1 Uniform mutation

One or more genes from the parent are randomly selected and replaced with other genes that are randomly generated.

5.4.2 Gaussian mutation

Gaussian mutation is the most popular mutation technique. Genes are altered by normally distributed random values with zero mean and standard deviation σ to create a new offspring. The choice of σ is selected based on the problem at hand.

5.5 Replacement

Replacement is the last stage of any reproduction cycle. This is used in a GA to determine how each offspring chromosome has adapted to the population in the next generation. After the mutations take place, the fitness value of each offspring chromosome is calculated. Two parents produce two offspring, but only two of these four chromosomes return to the next generation while two are removed. The basic generation update consists of producing n offspring from the population of n parents and a replacement criterion is used to form the population at the next generation. Replacement criteria include random replacement, weak parent replacement, and both parent replacement (Sivanandam and Deepa (2008)). Two methods are discussed:

5.5.1 Weak parent replacement

For four chromosomes consisting of two parent and two offspring, a weaker parent is replaced by a stronger offspring, leaving only the fittest two (parent or offspring) to return to the next generation.

5.5.2 Both parent replacement

Both parents are replaced by the two offspring.

5.6 Convergence Criteria

Termination or convergence is the criterion by which the genetic algorithm decides whether to continue searching or to stop the search. The various

stopping conditions include maximum generation, no improvement, stall generation and local optimizer (Haupt and Haupt (2004)). Two common methods are now discussed:

5.6.1 Maximum generation

If the specified number of generations has been reached, then the algorithm will end.

5.6.2 No improvement

If the fitness values for a population at generation t equal the fitness values of the population at generation $t+1$, then the algorithm stops. The researcher must be careful because the final population may be stuck in a local minimum.

6. Prediction Variance Function

In mixture experiments, the p -parameter-variable linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ is assumed. All assumptions and notation for this linear model were presented in Section 3 of the Literature Review. Recall that the least squares estimator for $\boldsymbol{\beta}$ is

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{y} \quad (42)$$

where $\mathbf{X}$ is design matrix expanded in the form of the model. $\mathbf{X}$ is also called the model matrix. The variance-covariance matrix of the elements of $\mathbf{b}$ is given by

$$\text{var}(\mathbf{b}) = (\mathbf{X}'\mathbf{X})^{-1} \sigma^2 \quad (43)$$

where $\mathbf{X}'\mathbf{X}$ is a $p \times p$ matrix of rank $= p$.

The predicted value of a response at a mixture $\mathbf{x} = (x_1, x_2, \dots, x_q)$ in the experimental mixture region is expressed in matrix notation as

$$\hat{y}(\mathbf{x}) = \mathbf{x}_m' \mathbf{b} \quad (44)$$

where $\mathbf{x}_m$ is the mixture point of interest $\mathbf{x}$ expanded to model form. Thus, $\mathbf{x}_m$ is a $1 \times p$ vector (Cornell, 2002). The $\mathbf{m}$ in $\mathbf{x}_m$ reflects the model.

For the linear model : $\mathbf{x}_m = (x_1, x_2, \dots, x_q)'$

For the quadratic model : $\mathbf{x}_m = (x_1, x_2, \dots, x_q, x_1x_2, x_1x_3, \dots, x_{q-1}x_q)'$.

The prediction variance at point $\mathbf{x}$ is

$$\begin{aligned} PV(\mathbf{x}) &= \text{var}(\hat{y}(\mathbf{x}_m)) \\ &= \text{var}(\mathbf{x}_m' \mathbf{b}) \\ &= \mathbf{x}_m' \text{var}(\mathbf{b}) \mathbf{x}_m \\ &= \mathbf{x}_m' (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_m \sigma^2. \end{aligned} \quad (45)$$

To compare competing designs, it is often convenient to scale the prediction variance to what is known as the scaled prediction variance (SPV). The scaled prediction variance (SPV) is calculated for each point, $\mathbf{x}$ according to

$$SPV(\mathbf{x}_m) = \frac{n \text{var}(\hat{y}(\mathbf{x}_m))}{\sigma^2} = n \mathbf{x}_m' (\mathbf{X}'\mathbf{X}) \mathbf{x}_m \quad (46)$$

where n is the number of runs in the mixture design. The division by σ^2 makes the quantity scale-free, and the multiplication by n allows the quantity to reflect variance on a per observation basis (Myers *et al.*, 2009).

In the case when the prediction variance has been scaled by a number of design points, the assumption is that the cost of the experiment is proportional to the number of observations collected. Using the scaled prediction variance, we find the best design after penalizing for their different costs. In some cases, it is not as

important to consider the quality of the design as a function of cost. In those cases, the unscaled prediction variance might be more appropriate.

7. Design Optimality Criteria

Design optimality criteria are single value criteria which represent different variance properties of a design. They are also called **alphabetical optimality criteria** because they are characterized by letters of the alphabet. Kiefer and Wolfowitz (1959) were among the first authors to develop these optimality criteria. Notationally, $\mathbf{X}$ is the model matrix, $\mathbf{X}'\mathbf{X}$ is the information matrix, $\mathbf{x}$ is the any point in the design region R , p is the number of parameters in the model, $\mathbf{x}_m = (x_1, x_2, \dots, x_p)'$ is a vector of p real-value functions based on the terms in the model, and n is the total number of runs in the design, and. For a summary of design optimality criteria, see Atkinson *et al.* (2007) and Myers *et al.* (2009).

7.1 D-Optimality

The best known and most popular design criterion is the D -optimality criterion which focuses on the variances of the model parameters through good attributes of the **moment matrix**, defined as

$$\mathbf{M}(X) = \frac{\mathbf{X}'\mathbf{X}}{n}. \quad (47)$$

Under the standard normality assumptions, $|\mathbf{X}'\mathbf{X}|$ is inversely proportional to the square of the volume of the confidence region for the regression coefficients. Hence, larger $|\mathbf{X}'\mathbf{X}|$, or equivalently, smaller $|(\mathbf{X}'\mathbf{X})^{-1}|$, implies better estimation of the model parameters. The goal of D -optimality is to

$$\text{Maximize } |\mathbf{X}'\mathbf{X}|, \text{ or equivalently to minimize } |(\mathbf{X}'\mathbf{X})^{-1}|.$$

The theoretical D -efficiency of a design D^* is defined as

$$D\text{-efficiency} = \left(\frac{|\mathbf{M}(D^*)|}{\max_{\zeta \in \chi} |\mathbf{M}(D)|} \right)^{1/p} \quad (48)$$

where χ is the space of all possible designs for a given design region. A D -optimal design is defined as one in which the determinant of the moment matrix is maximized; that is

$$\max_{\zeta \in \chi} |\mathbf{M}(D)|. \quad (49)$$

A D -efficiency measure that is commonly output by many computer programs (Mitchell, 1974) such as SAS, MINITAB, and JMP is

$$D\text{-efficiency} = 100 \frac{|\mathbf{X}'\mathbf{X}|^{\frac{1}{p}}}{n} \quad (50)$$

7.2 G -Optimality

In industrial situations, the objective of the practitioner is good prediction performance at various locations in the design space or throughout the entire design space which can be important for assessing the choice of design. Box and Hunter (1957) defined the scaled prediction variance function (SPV) which provides a measure of how precise the estimated response is at any particular location in the design space. A good design should have as small and stable SPV values as possible throughout the entire region. G -optimality makes use of the scaled prediction variance directly. The goal of G -optimality is to minimize the maximum SPV throughout the design region. That is, the goal is to find a design ζ that minimizes the following:

$$G(\zeta) = \max_{\mathbf{x} \in R} [n\mathbf{x}'_m (\mathbf{X}'\mathbf{X}) \mathbf{x}_m] = \max_{\mathbf{x} \in R} v(\mathbf{x}_m)$$

where $v(\mathbf{x}_m) = n\mathbf{x}'_m (\mathbf{X}'\mathbf{X}) \mathbf{x}_m$. The G -efficiency of a design ζ can be expressed as

$$G\text{-efficiency} = \frac{p}{\max_{\mathbf{x} \in R} \nu(\mathbf{x}_m)} = \frac{p}{G(\zeta)} \quad (51)$$

A G -optimal design ζ^* is one which satisfies

$$\min_{\zeta \in \chi} \left(\max_{\mathbf{x} \in R} \nu(\mathbf{x}_m) \right) \quad (52)$$

where R is the region of interest and χ is the space of all possible designs for design region R . That is,

$$G(\zeta^*) = \max_{\zeta \in \chi} G(\zeta). \quad (53)$$

7.3 I -Optimality

Another design optimality criterion that addresses prediction variance directly is I -optimality, also called Q -optimality, V -optimality and IV -optimality, and is based on properties of the scaled prediction variance function (SPV). I -optimality attempts to minimize the average SPV over the entire design region of interest. That is, the goal is to find a design that minimizes the following:

$$\text{average}_{\mathbf{x} \in R} \left[n\mathbf{x}'_m (\mathbf{X}'\mathbf{X}) \mathbf{x}_m \right] = \text{average}_{\mathbf{x} \in R} \nu(\mathbf{x}_m)$$

where R is the region of interest and χ is the space of all possible designs for design region R . An I -optimal design ζ^* is one that satisfies

$$\min_{\zeta \in \chi} \frac{1}{K} \int_R \nu(\mathbf{x}_m) d\mathbf{x}_m = \max_{\zeta \in \chi} I(\zeta) \quad (54)$$

where K is the volume of the region of interest, and

$$\begin{aligned}
 I(\zeta) &= \frac{1}{K_R} \int v(\mathbf{x}_m) d\mathbf{x}_m \\
 &= \frac{n}{K_R} \int \mathbf{x}_m' (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_m d\mathbf{x}_m.
 \end{aligned} \tag{55}$$

The I -efficiency of design ζ is defined as

$$I\text{-efficiency} = \frac{I(\zeta^*)}{I(\zeta)} \tag{56}$$

8. The Method of Model Reduction

In practice, an experimenter often selects a design based on a model proposed before data collection. When the data are collected and the model is fitted, the experimenter finds that some effects are not statistically significant, and then decides to use a reduced model. Hence, the experimenter should consider selecting a design that is robust over the set of potential reduced models. Many different strategies have been developed for examining a set of potential reduced models. The most basic and commonly-used algorithm defined classes of reduced models containing two-way interactions and higher-order polynomial terms (Chipman 1996). Chipman, however, only reviewed models with two-way interactions. The reduced models formed by removing terms based on hierarchy of two-way interactions led to two specific classes of reduced models. The two classes are based on two heredity principles.

1. The strong heredity (**SH**) principle requires that if a model contains the interaction term $(x_i x_j)$, then it must also contain both of the corresponding x_i and x_j main effects.

2. The weak heredity (**WH**) principle requires that if a model contains the interaction term $(x_i x_j)$, then it must contain one or more of the corresponding x_i or x_j main effects.

Strong and weak heredity are called ‘inheritance principles’ because the higher order terms depend only on the lower order terms. A main effect is **active** if its corresponding term is in the model. Otherwise, it is inactive. Thus, for **SH**, if $x_i x_j$ is active, then both x_i **and** x_j are also active. For **WH**, if $x_i x_j$ is active, then either main effect x_i **or** x_j or both are active.

The model can be defined by a vector δ where the entries of δ are either ‘1’ or ‘0’. The ‘1’ indicates an active effect, while ‘0’ indicates an inactive effect. Let δ_i , and δ_{ij} represent the indicator function values of the i^{th} first order effect and the ij^{th} interaction effect, respectively. In a model with two-way interactions and 3 potential main effects, the vector $\delta = (\delta_1, \delta_2, \delta_3, \delta_{12}, \delta_{13}, \delta_{23})$ defines a particular model. For instance, the reduced response surface model $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon$ has corresponding $\delta = (1, 1, 0, 1, 0, 0)$. For any 3-component mixture model, there is no intercept term, so $\beta_0 \equiv 0$.

Suppose that there are m main effects, and all possible two factor interactions are considered in the model. Then the number of non-intercept terms in the model are $p = m + \binom{m}{2}$, and the number possible models without any restriction is 2^p . For

strong heredity, however, the number of all possible response surface models is

$\sum_{i=0}^m \binom{m}{i} 2^{\binom{i}{2}}$. While, for weak heredity, the number of all possible response surface

models is $\sum_{i=1}^m \binom{m}{i} 2^{m - \frac{i(i+1)}{2}}$. For mixture experiments, however, there is no intercept

and the condition that the all components (main effect) must occur in each reduced model is added to define SH and WH for mixtures. Thus, for quadratic mixture models, there are 2^{p-m} reduced models for both strong heredity and weak heredity. Table 3 contains the 8 possible mixture models for three components and the Scheffé quadratic mixture model for both strong and weak heredity. In Table 3, the 1’s and 0’s

in the ‘Terms in model’ columns represent the presence or absence of the terms in the reduced model, respectively. The column p is the number of model parameters, and cp is the number of 2-way interaction (or binary blending or quadratic) terms.

Table 3 Reduced models of the quadratic mixture model for strong and weak heredity in $q = 3$ components.

model	Terms in model						p	cp
	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3		
1	1	1	1	1	1	1	6	3
2	1	1	1	0	1	1	5	2
3	1	1	1	1	0	1	5	2
4	1	1	1	1	1	0	5	2
5	1	1	1	0	0	1	4	1
6	1	1	1	0	1	0	4	1
7	1	1	1	1	0	0	4	1
8	1	1	1	0	0	0	3	0

9. Graphical Methods for Mixture Experiments

The alphabetical optimality criteria are often employed for evaluating designs. It is recommended, however, for the decision of a best design to be based on the distribution of the scaled prediction variance (SPV) over the region of interest because it provides more information than a criterion based on a single number summary. That is, optimality criteria do not, in general, provide enough information for design comparisons because a single value does not reveal the true complexities of design prediction capability over all the region of interest. If the experimenter has no prior knowledge about the locations in the design region that are most important for prediction, then the prediction variance properties of the design should be assessed throughout the entire design region prior to running an experiment. Therefore, the performance of competing designs should be considered over the region entire of interest for concluding which is the best design.

Graphical techniques are very informative for the exploration of properties of competing designs and allows for detailed understanding of prediction variance properties throughout the design region for competing designs. Several commonly used graphical methods will be reviewed in the following sections.

9.1 Variance Dispersion Graphs (VDGs)

The variance dispersion graph (VDG) was proposed by Giovannitti-Jensen and Myers (1989) to evaluate the prediction variance properties of response surface designs for a spherical region S_k defined as the set of points $\mathbf{x} = (x_1, x_2, \dots, x_k)$ satisfying

$$S_k = \left\{ \mathbf{x} : \sum_{i=1}^k x_i^2 \leq k \right\} \quad (57)$$

where k is the number of design variables. These graphs display properties of the distribution of the SPV throughout a multidimensional region on two-dimensional graphs. The standard VDG consists of three curves per design with the maximum, average and minimum SPV values plotted against r over the region of interest where r is the radius of a hypersphere $U_r = \left\{ (x_1, x_2, \dots, x_k) : \sum_{i=1}^k x_i^2 = r^2 \right\}$ centered at the origin $(0, 0, \dots, 0)$. The x -axis represents the radius r for $0 \leq r \leq \sqrt{k}$, while the y -axis represents the scaled prediction variance. The minimum of SPV is defined as

$$\min_{\mathbf{x} \in U_r} [v(\mathbf{x})] = \min_{\mathbf{x} \in U_r} \frac{N \text{var}(\hat{y}(\mathbf{x}))}{\sigma^2}. \quad (58)$$

The maximum of SPV is defined

$$\max_{\mathbf{x} \in U_r} [v(\mathbf{x})] = \max_{\mathbf{x} \in U_r} \frac{N \text{var}(\hat{y}(\mathbf{x}))}{\sigma^2}. \quad (59)$$

The average of SPV (also called the spherical variance) is defined as

$$V^r = N \frac{\psi}{\sigma^2} \int_{U_r} \text{var}(\hat{y}(\mathbf{x})) d\mathbf{x} = \psi \int_{U_r} v(\mathbf{x}) d\mathbf{x} \quad (60)$$

for any $0 \leq r \leq \sqrt{k}$, $\psi^{-1} = \int_{U_r} d\mathbf{x}$ is the surface area of a sphere of radius r , and $v(\mathbf{x})$

is the scaled prediction variance. A VDG typically includes two horizontal lines at p and $2p$ that correspond to the 100% and 50% G-efficiencies, respectively, where p is the number of the parameters in the model.

Rozum and Myers (1991) adapted the spherical region VDG for designs in cuboidal regions. A cuboidal region C_k is defined as the set of points $\mathbf{x} = (x_1, x_2, \dots, x_k)$ satisfying

$$C_k = \{\mathbf{x} : -1 \leq x_i \leq 1; i = 1, \dots, k\} \quad (61)$$

where k is the number of design variables. They plotted the maximum, average, and minimum SPV in U_r^* against r where $U_r^* = \{\mathbf{x} : -r \leq x_i \leq r, i = 1, 2, \dots, k; x_j = \pm r \text{ for at least one } j, j \in \{1, 2, \dots, k\}\}$ is the surface of the hypercube C_r for $0 \leq r \leq 1$. The minimum, maximum, and average of SPV are defined respectively as

$$\min_{\mathbf{x} \in U_r^*} [v(\mathbf{x})] = \min_{\mathbf{x} \in U_r^*} \frac{N \text{var}(\hat{y}(\mathbf{x}))}{\sigma^2}. \quad (62)$$

$$\max_{\mathbf{x} \in U_r^*} [v(\mathbf{x})] = \max_{\mathbf{x} \in U_r^*} \frac{N \text{var}(\hat{y}(\mathbf{x}))}{\sigma^2}. \quad (63)$$

$$V^{r*} = N \frac{\psi^*}{\sigma^2} \int_{U_r^*} \frac{\text{var}(\hat{y}(\mathbf{x}))}{\sigma^2} d\mathbf{x} = \frac{\psi^*}{\sigma^2} \int_{U_r^*} v(\mathbf{x}) d\mathbf{x} \quad (64)$$

where $(\psi^*)^{-1} = \int_{U_r^*} d\mathbf{x}$ is the surface area of U_r^* and $v(\mathbf{x})$ is the scaled prediction variance.

Piepel and Anderson (1992) and Piepel, Anderson and Redgate (1993a) extended VDGs to mixture designs with and without constraints on polyhedral regions. The polyhedral regions is defined by lower bound, upper bound, and linear multi-component constraints. They plotted the maximum, average and minimum SPV for each shrunken version of the polyhedral region against values of the shrinkage factor. The shrinkage factors is varied with equal distance from a shrinkage point to the boundary of the polyhedral region ($0 \leq s \leq 1$). They recommended that the appropriate choice of the shrinkage point is the centroid of the polyhedral region. An example of a VDG is shown in Figure 18.

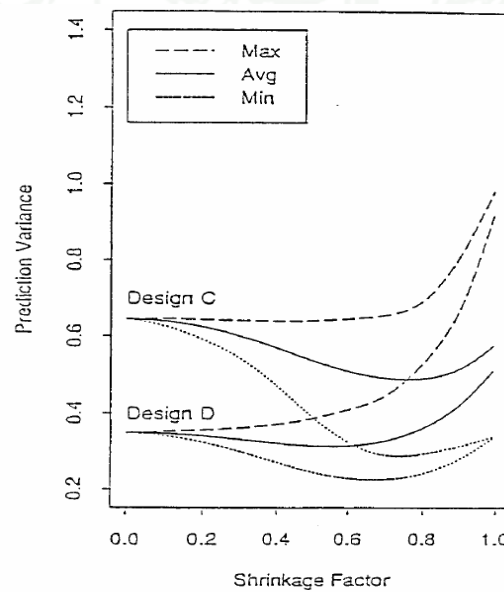


Figure 18 Variance dispersion graph for two designs for the McLean and Anderson flare mixture experiment.

Source: Piepel and Anderson (1992).

9.2 Quantile Dispersion Graphs (QDGs)

Quantile dispersion graphs (QDGs), introduced by Khuri, Kim and Um (1996), can be used to compare response surface designs by studying properties of the distribution of the prediction variance on concentric spheres within a spherical region on two-dimensional graphs with a single curve plotted per design. QDGs display the quantiles of the SPV (including the minimum and the maximum values) on the surface of the hypersphere $S(r)$ against the radius r . This method uses quantiles of the scaled prediction variance to describe the distribution of SPV at each radius in the entire design region. A QDG requires converting rectangular coordinates to spherical coordinates. Any point $\mathbf{x} = (x_1, \dots, x_k)'$ in rectangular coordinates can be represented by spherical coordinates $(r, \psi_1, \psi_2, \dots, \psi_{k-1})$. The relationship between $(r, \psi_1, \psi_2, \dots, \psi_{k-1})$ and $(x_1, x_2, \dots, x_k)$ is given by

$$\begin{aligned} x_1 &= r \cos \psi_1, \\ x_2 &= r \sin \psi_1 \cos \psi_2, \\ &\vdots \\ x_{k-1} &= r \sin \psi_1 \sin \psi_2 \dots \sin \psi_{k-2} \cos \psi_{k-1}, \\ x_k &= r \sin \psi_1 \sin \psi_2 \dots \sin \psi_{k-2} \sin \psi_{k-1} \end{aligned} \tag{65}$$

for $r^2 = \sum_{i=1}^k x_i^2$ and $0 \leq \psi_i \leq \pi; i = 1, \dots, k-2, 0 \leq \psi_{k-1} \leq \pi$. A QDG is constructed by first sampling a large number of points at random locations on a sphere of radius r by using spherical coordinates and then evaluating the SPV at the selected points. Then all corresponding SPV values obtained are ordered and plotted against the empirical quantiles. The x -axis gives the quantiles of the design space ranging from 0 to 1, while the y -axis gives the scaled prediction variance.

Khuri, Harrison and Cornell (1999) extended QDGs to mixture designs. They employed the scaled prediction variance quantile (SPVQ) plots for a mixture experiment in irregularly-shaped convex polyhedral region that is defined by

lower and upper component bounds. These plots display the quantiles of the empirical distribution of the SPV (including the minimum and the maximum values) within the shrunk regions that are centered at the centroid of the region. The shrunk region maintains its shape by using a shrinkage factor, λ , ($0 \leq \lambda \leq 1$). It is constructed by generating random points from a Dirichlet distribution inside the L -pseudocomponent simplex using Rubinstein's algorithm. The generated points are mapped from the pseudocomponent simplex onto the simplex of the original components. Therefore, any point might fall inside or outside the original region. The x -axis gives the cumulative percentage of the design space ranging from 0 to 100, while the y -axis gives the scaled prediction variance quantile. An example of a QDG is shown in Figure 19.

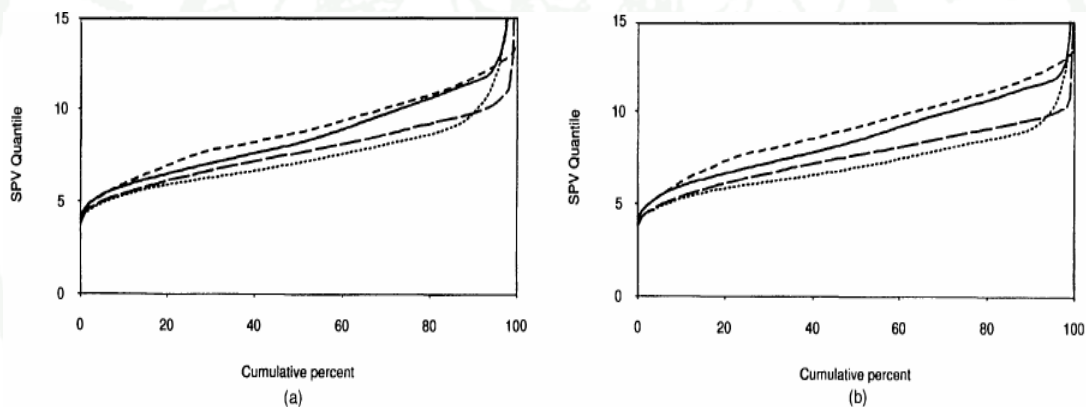


Figure 19 Quantile dispersion graph for four designs and two value of the shrinkage factor : (a) shrinkage factor 1 and (b) shrinkage factor 0.9.

Source: Khuri *et al.* (1999).

9.3 Fraction of Design Space (FDS) plots

The fraction of design space (FDS) plots were first introduced by Zahran, Anderson-Cook and Myers (2003) to complement the variance dispersion graphs on spherical and cuboidal regions. An FDS plot displays the distribution of the SPV throughout a multidimensional region on two-dimensional graphs with a single curve.

The x -axis gives the fraction of the design space value ranging from 0 to 1, while the y -axis gives the SPV values ranging from the minimum to the maximum of the SPV. The plot also shows two horizontal lines at p and $2p$ that are the 100% and 50% G-efficiencies for a design of interest, respectively, where p is the number of the parameter in the model. Therefore, the FDS plot quantifies the cumulative distribution of the SPV function. The exact fraction of the design space is calculated as

$$FDS(x) = \frac{1}{\psi} \int_D \cdots \int I(x) dx_k \cdots dx_1 \quad (66)$$

where D is the total design space, ψ is the volume of the design region,

$$I(x) = \begin{cases} 0.5 \frac{(|g| - g)}{g} & ; g \neq 0 \\ 0 & ; g = 0 \end{cases}, \quad (67)$$

$g = v(x) - x$, and v is any predetermined value of the SPV. Thus, $I(x)$ is either 1 or 0. The FDS plot can be used to evaluate the prediction performance of a design (or the prediction capability).

Goldfarb, Anderson-Cook, Borror, and Montgomery (2004) modified the FDS plot for mixture and mixture-process designs with irregularly-shaped mixture regions. Their procedure requires sampling a large number of points on the boundary corresponding to various shrinkage levels proportional to the relative volume associated with that portion of the total design space, as well as uniformly sampling over the entire space where the boundary of the region was determined by constraints on the individual components. For lower dimensional spaces, with four or fewer factors, an accurate FDS plot can be constructed within the range of 2,000 to 5,000 points. For higher dimensional spaces, with five to eight, simulations have shown that 10,000 points is adequate (Anderson-Cook and Ozol-Godfrey, 2006). Shrinkage values at intervals of 0.1 were considered. As a result, the points that are selected on the boundaries of the shrinkage regions provide a fairly evenly distributed grid over the entire design space. Once the points are generated, the SPV is calculated for each

point. Then, for each design, the empirical cumulative distribution function is calculated for all of the SPV values and plotted on a global FDS plot. The minimum value of SPV occurs at $FDS = 0$ and the maximum value of SPV occurs at $FDS = 1$. The better design is one that starts with small values and remains relatively flat throughout the region. When comparing designs, the desirable designs have a large fraction of the design space for SPV values which are close to the minimum and a flatter line indicates the more stable the SPV distribution is for the design. An example of FDS plots is shown in Figure 20.

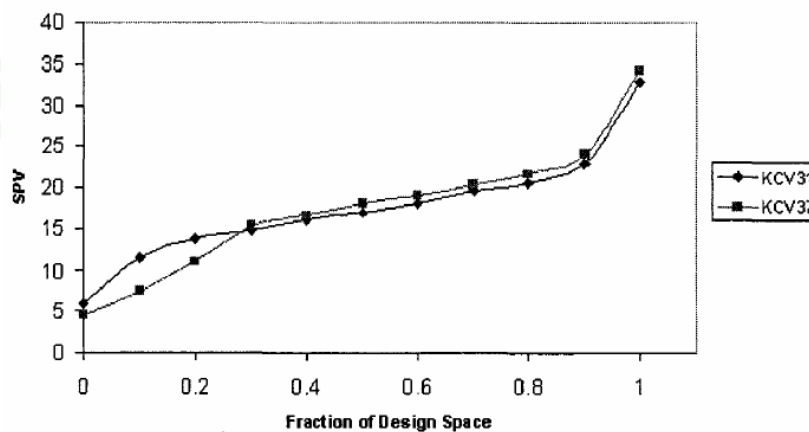


Figure 20 Fraction of design space plots for four designs obtained from the McLean and Anderson flare mixture experiment.

Source: Goldfarb *et al.* (2004).

9.4 Componentwise Variance Dispersion Graphs (CVDGs)

Borkowski (2006) proposed componentwise variance dispersion graphs for mixture designs that summarize the scaled prediction variance throughout an irregularly-shaped design region. CVDGs display the variability of the SPV throughout an irregularly-shaped multidimensional region on two-dimensional graphs with three curves for each mixture component. They are constructed by plotting the average, minimum, and maximum of the scaled prediction variance over the space of

mixtures at component proportion $x_i = a_i$ against the set of feasible values of x_i for $i=1, \dots, q$ where q is the number of the mixture components. For the i^{th} mixture component, fix a component proportion $x_i = a_i$ with $L_i \leq a_i \leq U_i$. The x -axis gives the component proportion $x_i = a_i$, while the y -axis gives the SPV values. The graph can be plotted with either one component per plot or by overlaying all component plots in one graph. The author recommends plotting one component at a time. An example of CVDGs is shown in Figure 21.

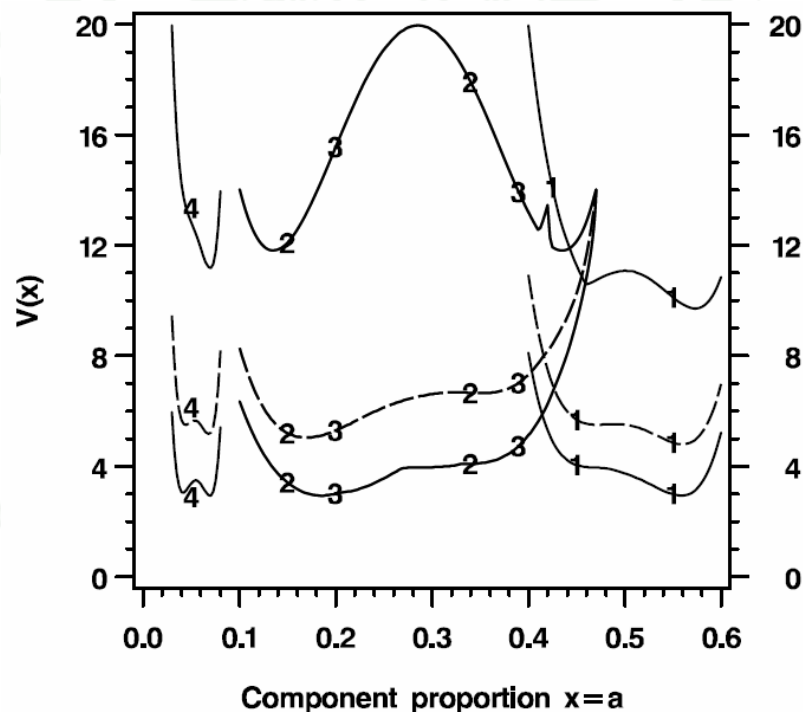


Figure 21 Componentwise variance dispersion graphs for the McLean and Anderson flare mixture experiment where all components are plotted in one graph.

Source: Borkowski (2006).

Each graphical method has limitations. The VDG cannot provide complete information about the distribution of the SPV on the given sphere because these plots only consider the maximum, average and minimum SPV regardless of the volume of the sphere at any radius. That is, a VDG does not account for the proportion of the

total design space at various distances from the center of the design space. Hence, it might be impossible to differentiate between two designs that have almost similar patterns in the VDGs but have quite different distributions of SPV values throughout a region of interest (Khuri *et al.*, 1996).

The QDG provides a better depiction of the degree of rotatability of the design based on the flatness of the plots and more information about the prediction capability of a design than that of VDG because the curves of these plots are the cumulative distribution of the SPV at a given radius. If the design is a rotatable design, then QDG for each radius will be perfectly parallel with horizontal lines. However, the QDG has the same problems as the VDG. That is, it might be impossible to differentiate between two designs that have almost similar the patterns in the QDGs but have quite different distributions of SPV values throughout a region of interest (Zahran *et al.*, 2003). QDGs, however, are computationally more difficult to produce than VDGs.

The FDS plot provides more detailed information about the distribution of the SPV in the region of interest and allows comparison of the global minimum and maximum of the SPV for each design. The plot takes into account the volume of the region which is proportionally large near the boundary of the design space. The FDS plot can be used to show the distributions of the SPV over the design space for different models for the chosen design on the same graph (Zahran *et al.*, 2003).

In summary, although VDGs and QDGs provide more information than alphabetical optimality criteria, they do not provide complete information because they do not consider the volume of the sphere and the proportion of the total design space at various distances from the center of the design space. VDGs and QDGs weight each radius or shrinkage factor equally. It is more informative if information on SPV values is weighted with weights corresponding to the volume of the design space (Zahran *et al.*, 2003). This is the advantage of FDS plots over VDGs and QDGs.

Background Review

The remaining sections of this chapter provides a review of the literature on algorithms used to generate experimental designs and model robustness. Approaches for generating and examining models in mixture experiments will be discussed.

10. Algorithm for Constructing Designs for Irregularly-Shape Regions in Mixture Experiments

McLean and Anderson (1966) introduced the extreme vertices design when there are only single-component constraints in a mixture experiment. The points in an extreme vertices design consists of the vertices of the polyhedron and one or more subsets of the centroids of its various faces. When the boundary is constrained by only the single components of $(q-1)$ components, the extreme vertices of the design may be found by using the following two step procedure:

1. List all possible two-level combinations of the values of L_i and U_i for each set of $(q-1)$ components and leave the value of the remaining component blank. This procedure generates $q2^{q-1}$ possible combinations with one component's level blank in each combination.
2. Go through all $q2^{q-1}$ possible combinations in step 1 and fill in those blanks that are admissible. That is, it represents a mixture that satisfies all single component constraints. Each admissible q component mixture is an extreme vertex.

Once the extreme vertices are found, the next step is to define sets of centroids on the faces and the edges and so on. There is one centroid point located in each two-dimensional face, three-dimensional face,..., r -dimensional face ($r \leq q-2$), and the overall centroid of polyhedron. The centroid of a two-dimensional face is found by grouping the extreme vertices into groups of vertices that have $(q-3)$ identical

component proportions and then averaging the component proportions of each of the three remaining factors. All remaining centroids are found in a similar manner using all vertices that have $(q-r-1)$ identical component proportions for r -dimensional face where $3 \leq r \leq q-2$.

Snee and Marquardt (1974) proposed the XVERT algorithm for selecting a subset of mixtures from the extreme vertex design for linear mixture models that generally gives the best design in terms of the trace $(\mathbf{X}'\mathbf{X})^{-1}$. The extreme vertices of the XVERT design can be found by using the following five step procedure:

1. Rank the components in order of increasing ranges $(U_i - L_i)$ and then label the ordered components as $X_1, X_2, \dots, X_q$ where X_1 has the smallest range, and X_q has the largest range.
2. Set up a two-level design from the upper and lower component constraints of $X_1, X_2, \dots, X_{q-1}$ (the $q-1$ components with the smallest range). There are 2^{q-1} combinations.
3. Calculate the level of the omitted component X_q :

$$X_q = 1 - \sum_{i=1}^{q-1} X_i \quad (68)$$

4. If the value of X_q in step 3 falls inside its acceptable bounds $(L_q \leq X_q \leq U_q)$, then the given mixture is an extreme vertex and is known as a core point. If the value of X_q in step 3 falls outside its acceptable bounds, then the given point needs to be adjusted in step 5.

5. For each of the points that X_q falls outside its original bounds, the experimenter generates additional points (a candidate subgroup) by adjusting the level of one component X_i ; $(1 \leq i \leq q-1)$ by an amount equal to the difference between the computed value for X_q and the substituted lower or upper bound. Each point that fell

outside its original bounds can generate at most $q-1$ additional feasible points. The design thus consists of the core points and one point from each candidate subgroup.

The authors suggested that when it is necessary to support terms in a quadratic mixture model, the experimenter can add the centroid of the faces of polyhedron. The centroids are useful for modeling a surface that is nonlinear in the mixture components.

Snee (1975) showed that an efficient design can be constructed from a subset of vertices and centroids of the extreme vertices design for quadratic mixture models where there are only single-component constraints. The design points in an efficient design for a quadratic model should consist of the vertices, edge centroids, $(q-2)$ -dimensional face centroids, and the overall centroid. A good design for three components consists of the vertices and the overall centroid. If long edges are present on the polyhedron and/or the number of vertices is less than or equal to four, then the centroids of the long edges are added. A good design for four component mixtures consists of the vertices, the $(q-2)$ -dimensional face centroids, the centroids of any long edges, and the overall centroid. The best design for a five or more components can be found by using the Wynn and exchange algorithms to select design points from a candidate list consisting of the vertices, edge centroids, $(q-2)$ -dimensional constraint plane centroids, and the overall centroids. In case of five components, a good design consists of the vertices selected by the XVERT algorithm, the $(q-2)$ -dimensional face centroids, and overall centroid with G -efficiencies $\geq 50\%$.

Snee cited that Wheeler (1972) found that designs that have G -efficiencies $\geq 80\%$ also have high efficiencies for most other optimality criteria. Wheeler suggested that any design with G -efficiencies $\geq 50\%$ can be considered a good design.

Mitchell (1974) introduced the DETMAX algorithm for constructing designs that are D -optimal. That is, $|\mathbf{X}'\mathbf{X}|$ is maximized. This algorithm is the most widely-

used optimal design search algorithm. Although it was originally developed for generating non-mixture designs, it is also applicable to generating mixture designs. This algorithm does not guarantee D -optimality, but it has performed well in many cases where D -optimal designs are known.

First, an initial design is constructed either randomly or using a sequential search algorithm. This DETMAX algorithm is a modification of the single point exchange algorithm that allows the replacement of more than one point in the original design for each iteration. The single point exchange algorithm adds one candidate point to an initial n -point design that increases $|\mathbf{X}'\mathbf{X}|$ to its maximum, and then removes one of the $(n+1)$ points that results in the minimum possible decrease in $|\mathbf{X}'\mathbf{X}|$. The DETMAX algorithm, however, does not immediately require that one of the $(n+1)$ points be removed. It allows for ‘excursions’ to other design sizes before returning to an n -point design. If $|\mathbf{X}'\mathbf{X}|$ is not improved during an excursion, then all designs constructed on that excursion form F , the set of all “Failure designs”. F is then used to determine the direction of the next excursion. Each excursion starts by using the currently-best n -point design. Let D be the current design at any time during an excursion and let n_D be the number of points in D . The rules of an excursion are as follows:

1. If $n_D > n$, then either remove a point from D if $D \notin F$ or add a point to D if $D \in F$.
2. If $n_D < n$, either add a point to D if $D \notin F$ or remove a point from D if $D \in F$.

To determine if $D \in F$, only values of $|\mathbf{X}'\mathbf{X}|$ are compared. During an excursion, the number of points in the design may vary between $n_D + n$ and $n_D - n$. Computationally, the DETMAX algorithm does not consider $|\mathbf{X}'\mathbf{X}|$ directly, but it

attempts to minimize $\left| \mathbf{X}'\mathbf{X} + \alpha \left(\frac{\mathbf{X}_0'\mathbf{X}_0}{N_0} \right) \right|$, where N_0 is the number of candidate points, $\mathbf{X}_0$ is the design consisting of all N_0 candidate points, and α is a very small positive number. The author used the value of α is 0.005.

Snee (1979) developed the CONSIM algorithm for construction of the extreme vertices design in linear and quadratic mixture models where there are single-component and multi-component constraints. This algorithm selects vertices and centroids as follows:

1. Express each constraint in the following form:

$$\theta_1 x_1 + \theta_2 x_2 + \dots + \theta_q x_q \geq 0. \quad (69)$$

For example, in three components, the constraint

$$c_j \leq A_1 x_1 + A_2 x_2 + A_3 x_3 \quad (70)$$

can be rewritten as

$$A_1 x_1 + A_2 x_2 + A_3 x_3 \geq c_j (x_1 + x_2 + x_3) \quad (71)$$

or

$$(A_1 - c_j) x_1 + (A_2 - c_j) x_2 + (A_3 - c_j) x_3 \geq 0. \quad (72)$$

Therefore, $\theta_i = A_i - c_j$.

2. Determine which vertices lie inside and outside the constraint.
3. Form new points by combining a suitable linear combination of each point outside the constraint with a point that is inside the constraint and lies on the same one-dimensional edge. The new point is the intersection of the constraint plane and the one-dimensional edge.
4. After all the new points have been generated, the points that are outside the constraint are deleted, and then the next constraint is introduced.

The process continues until all constraint planes have been considered. The points that remain are the vertices of the region defined by the constraints. The edge centroid is the average of any two vertices that lie on the same $(q-2)$ -dimensional constraint plane. The overall centroid is the average of all the vertices. The constraint plan centroid is the average of all points that lie on the given constraint.

Cook and Nachtsheim (1980) introduced a modification of the Fedorov algorithm which was originally developed for non-mixture settings. This algorithm is based on simultaneously adding and deleting points. Usually, this algorithm finds a better design than those obtained from other design algorithms and it is recommended for generating highly efficient designs. Each step involves a search over all possible pairs of candidate and design points but it requires longer computing time.

An initial n -point starting design is constructed (often randomly) from the design space $\mathcal{X}$, and then $\mathbf{M}$, $\mathbf{M}^{-1}$, and $|\mathbf{M}|$ are found. At stage i , the algorithm removes support point $\mathbf{x}_i$ from the current n point design and adds the point $\mathbf{x}^*$ in the candidate list such that

$$\max_{\mathbf{x} \in \mathcal{X}} \Delta(\mathbf{x}_i, \mathbf{x}) = \Delta(\mathbf{x}_i, \mathbf{x}^*) \quad (73)$$

where $\Delta(\mathbf{x}_i, \mathbf{x}) = \mathbf{x}'\mathbf{M}^{-1}\mathbf{x} - \mathbf{x}_i'\mathbf{M}^{-1}\mathbf{x}_i + (\mathbf{x}'\mathbf{M}^{-1}\mathbf{x}_i)^2 - \mathbf{x}'\mathbf{M}^{-1}\mathbf{x}\mathbf{x}_i'\mathbf{M}^{-1}\mathbf{x}_i$ is Fedorov's delta function, $\mathbf{M} = \mathbf{X}'\mathbf{X}$ and it is assumed that $\mathbf{M}^{-1}$ exists. Then $\mathbf{x}_i$ is replaced by $\mathbf{x}^*$, so that it is possible to switch each point $\mathbf{x}$ in the design with the candidate point $\mathbf{x}_i^*$. If, for any j ,

$$\max_{\mathbf{x} \in \mathcal{X}} \Delta(\mathbf{x}_j, \mathbf{x}) = \Delta(\mathbf{x}_j, \mathbf{x}^*) > 0,$$

then an improvement is the exchange of point $\mathbf{x}_j$ in the n point design and $\mathbf{x}^*$ in the candidate list. The algorithm stops when there are no further improvements in the respective optimality criterion.

Piepel *et al.* (1993) considered five approaches for constructing designs in irregularly-shaped regions consisting of the variance optimal design approach (VOD), the bias/MSE optimal design approach (BMOD), the central composite analogue design approach (CCAD), the layer design approach (LS), and the distance optimal design approach (DOD).

The variance optimal design approach (VOD) involves selecting design points to minimize an alphabetical optimality criterion (e.g. D, G, V) for a specified model form. This approach may be the best choice if the assumed model form provides a very good approximation to the true response surface. The bias/MSE optimal design approach (BMOD) is similar to the VOD approach, except the criterion involves bias and the mean square error. The central composite analogue design approach (CCAD) involves selecting an appropriate subset of the vertices on the shrunken version of the polyhedral region, and axial points on the boundary of the polyhedral region. The layer design approach (LS) is merely a design with its points on one or more shrunken version (layers) of the polyhedron region. The boundary of the polyhedron region is the outer layer that contains no shrinkage, while the centroid of the polyhedron is the layer with complete shrinkage. This design consists of points on the outer layer (boundary), on one or more of the inner layers, and the centroid. This approach provides for good coverage of the polyhedral region by spreading design points over multiple layers as well as at the centroid. D -, G -, and V -optimality criteria were used to select design points. In some cases, selecting outer layer points first seems to yield better prediction variance and bias properties. The distance optimal design approach (DOD) involves selecting design points that are spread uniformly over the region of interest. The criterion for constructing designs using the DOD approach is to minimize the maximum distance and Euclidean distance.

Borkowski and Piepel (2009) introduced two number-theoretic methods for generating space-filling designs for constrained mixture experiments defined by single and multiple component constraints. Thus, the experimental region is an irregularly-shaped region. The approach consists of the one-pass exchange algorithm and the powers-modulo-a-prime method. The goal of a space-filling design is to

uniformly scatter the design points in the experimental region. If the set of all possible a number-theoretic mixture designs is evaluated, the best design is called the uniform mixture design. Let $d(\mathbf{x}, \mathbf{D})$ be the rescaled distance between $\mathbf{x} \in R$ and the nearest design point in design $\mathbf{D}$ where R is the mixture region. The three distance-based criteria that were used to evaluate a design's uniformity of the scatter can be expressed as

1. The root mean squared distance $\left(\sqrt{E\left[\left(d(\mathbf{x}, \mathbf{D}) \right)^2 \right]} \right)$ is the square root of the expected value of the squared distance $\left(d(\mathbf{x}, \mathbf{D}) \right)^2$.
2. The average distance $\left(E\left[d(\mathbf{x}, \mathbf{D}) \right] \right)$ is the expected value of the distance $d(\mathbf{x}, \mathbf{D})$.
3. The maximum distance $\left(\max_{\mathbf{x}} d(\mathbf{x}, \mathbf{D}) \right)$ is the maximum distance between any $\mathbf{x}$ in the region and the design point of $\mathbf{D}$ nearest to $\mathbf{x}$.

These three distance-based criteria were approximated from random sets of points in the mixture space. The authors did not claim that the methods proposed will yield uniform mixture designs, but merely that the generated designs will have good uniformity of scatter over the constrained region.

11. General Algorithms for Construction of Designs

Borkowski (2003) employed a genetic algorithm (GA) to generate near-optimal D , A , G , and IV exact N -point designs in the hypercube. The author created a catalog of D , A , G , and IV optimal exact N -point designs for the second order model for 1 factor having 3 to 9 points, 2 factors having 6 to 12 points, and 3 factors having 10 to 16 points. The optimal exact designs were found by applying a local search to near-optimal designs. Objective function values of the optimal exact N -point designs were used to calculate relative design efficiencies to help the experimenter realize how good a proposed design's D , A , G and IV criterion values

are relative to the best exact N -point design. Relative design efficiencies were calculated for central composite designs, small composite designs, Box-Draper designs, Notz designs, and designs generated by the Optex procedure in SAS.

In this paper, the author used the real-valued encoding to form chromosomes because it worked effectively on the mathematical optimization problem and allowed the use of numerical reproduction operators. He used a five step GA.

- (1) An initial population of M chromosomes is created.
- (2) An objective function to evaluate the fitness of M chromosomes in the initial population was used. The objective function F_i measured a chromosome's fitness as a solution in the search for an exact design relative to optimality criterion i where $F_D = D(\mathbf{X})$, $F_A = A(\mathbf{X})$, $F_G = G(\mathbf{X})$, $F_{IV} = IV(\mathbf{X})$ for $i = D, A, G, IV$ and $\mathbf{X}$ was the model matrix corresponding to design chromosome C . The design optimality goal can be expressed in term of maximization of one of the following:

$$D(\mathbf{X}) = \frac{100|\mathbf{X}'\mathbf{X}|^{1/p}}{N}, \quad A(\mathbf{X}) = \frac{100p}{\text{trace}[\mathbf{N}(\mathbf{X}'\mathbf{X})^{-1}]},$$

$$G(\mathbf{X}) = \frac{100p}{\max_{\mathbf{x} \in \chi} [\mathbf{N}\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}]}, \text{ and } IV(\mathbf{X}) = \frac{V}{\int_{\chi} \mathbf{N}\mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x} dx_1 dx_2 \dots dx_k}$$

where χ is the k -dimensional hypercube $[-1,1]^k$, N is the design size, p is the number of parameters in the model, $V = 2^k$ is the volume of design space χ , and $\mathbf{x}' = [1, x_1, \dots, x_k, x_1x_2, \dots, x_{k-1}x_k, x_1^2, \dots, x_k^2]$ is the vector corresponding to the terms in the second-order model.

- (3) Offspring chromosomes are created by mating chromosomes using a linear combination of two runs (genes) called 'blending' for the reproduction process. Additonal reproduction operators (zero gene, extreme gene, and creep) were also applied to genes. The objective function was calculated for each parent/offspring pair, and the parent or offspring that has the larger objective function F_i was retained for

the next generation while the other was removed. The next generation of M chromosomes consisted of 2 elite and $M - 2$ future parents.

(4) The selection and reproduction process in step 3 was iterated for a large number of generations.

(5) The process was stopped when the iteration limits of 12,000, 18,000, and 21,000 for 1, 2, and 3 factors, respectively were reached.

A local grid search was employed to find the most fit chromosome, yielding the optimal exact designs. A local grid search increased the objective function F_i values slightly until no further improvement can be found.

Heredia-Langner *et al.* (2003) also presented a technique for generating D-optimal designs using GAs. D-optimal designs are often used when the experimental design region is irregular in shape, or the experimenter wishes to fit a non-standard model, or a non-standard experiment is required because of the number of runs and/or the number and type of blocks. GAs can be used when the traditional factorial, fractional factorial or other standard designs cannot be used, such as in highly constrained regions. In their GAs, they used the real-valued encoding to form chromosomes because it is simple, the ease for performing operations, easy to understand and used to develop crossover and mutation procedures. A benefit of using a GA to generate D-efficient designs for a variety of practical situations is that a GA does not need to explicitly consider a candidate set of experimental runs in the region. The good performance of a GA is the result of allowing multiple exchanges during the mating procedure, the alteration of the coordinate points in the mutation procedure, and the presence of multiple potential solutions at every generation. The GA also allows selecting points at the vertices without the use of an exchange algorithm.

The authors compared a GA to traditional algorithms for many situations, such as designs in factorial regions, a mixture problem with one process variable, a constrained mixture problem, and a quadratic model for a mixture problem. In the factorial region situation, they evaluated the performance of the coordinate exchange, k-exchange, modified-Fedorov and genetic algorithms for D-efficiency. Good

performance was observed for the modified-Fedorov because of the long and extensive search time. The modified-Fedorov algorithm produces high efficiencies as long as a sufficiently large candidate set of runs is available. The performance of the GA was at least as good as the other procedures. In a mixture problem with one process variable situation, they evaluated the performance of the modified DETMAX, modified-Fedorov, and genetic algorithm for D-efficiency. As a consequence, the GA yielded as good a performance as the modified DETMAX, while the modified-Fedorov was poor. In a constrained mixture problem, they evaluated the performance of the modified XVERT, CADEX, modified-Fedorov, and genetic algorithms for D-efficiency. The result showed that the GA was superior to the modified XVERT, CADEX, and the modified-Fedorov algorithms. Overall the study concluded that the GA performed comparably relative to other algorithms.

Drain *et al.* (2004) proposed the use of a genetic algorithm for simulated annealing (GASA). It is a hybrid heuristic optimization algorithm used in situation where traditional designs cannot be employed, exchange methods are ineffective, and simple heuristics fail to find good solutions. Hybrid heuristic optimization methods combine two or more features of simple heuristics to create a more powerful algorithm. The GASA was used to take the advantage of the exploration ability of the genetic algorithm (GA) and the exploitation ability of simulated annealing (SA). For the GASA, the chromosomes resulting from the GA after performing the mutation operation in every generation were modified by SA. SA depends on algorithm parameters, such as the starting and ending ‘temperature’, the definition of a neighborhood, the temperature reduction of the search range, and the number of annealing steps. Temperature is a measure which determines whether or not a poor solution will be selected.

Each step of the GASA was initiated by reading all parameters for GA and SA and defining the rules for parameters in each iteration. Then, an initial population was created by randomly generating a set of candidate designs (chromosomes) and then checking to assure that a set of candidate designs met experimental constraints. An objective function was calculated for each candidate design and the performance was

evaluated for the population. A roulette wheel was used for the selection process of the GA. For each iteration, the elite chromosomes were selected for the next generation. The candidate designs that had the best objective function values were always selected while the candidate designs that had a poor objective function values, however, might be selected with a probability inversely proportional to the temperature. The midpoint was used for the crossover operator to generate an offspring chromosome. By applying the mutation operator to the new population and letting the resulting population be the new population, the minimization of the objective function was found by using SA to optimize every member of the new population. If the convergence criterion was satisfied, the process was terminated. Otherwise, the entire population at the last generation and the winning designs from each iteration were taken as the starting point for the next step of GASA.

The first iteration of the GASA used the initial temperature of SA as a starting condition for the first iteration of the GA and the final GASA iteration used the initial temperature of the SA at the last iteration as that for the GA. The early iterations of SA had higher temperatures, and then the temperature was gradually decreased until the final iteration. In SA, the greater the temperature, the greater the probability that a poor objective function was selected. This was an advantage of the SA algorithm. This advantage can be applied to the GASA for evaluation the objective function which was the average prediction variance over the region of interest that was difficult to calculate. As a result, the GASA was computationally more efficient than a simple genetic algorithm. A case study showed that the GASA approach can achieve highly satisfactory results.

Park *et al.* (2006) employed a GA for finding cost or resource-constrained *G*-efficient designs for a second order model over cuboidal regions. Two situations were studied: (i) experimental runs having a certain level of a factor is costly and (ii) when budget constraints exist. The *G*-optimality criterion was implemented to evaluate the quality of the experimental design while considering the measurement cost. The best (i.e., non-dominated) design is selected from the set of efficient designs that satisfy all cost constraints. Immediately, after the non-dominated designs are determined, a

method for selecting a final design among the set of all efficient designs is needed. The genetic algorithm was employed to develop or to modify and improve the dominated designs instead of ignoring them when the design space was investigated. All feasible experimental arrangements are not equally attractive because any experimental arrangement that was very efficient could be very expensive. The final experimental design will be different depending on the choice of design optimality criterion. A non-dominated design may or may not be found for a certain cost constraint because different random seeds were used in different simulations.

The authors created an initial population of 1,000 designs and the number of iterations was 50 for all cases. The initial population of experimental designs consisted of v treatments out of T possible treatments, and then the generated designs were checked for the feasibility, and next the G -efficiency of the design and cost were computed to find the best designs. Next, in the reproduction procedure, they produced offspring by using the cloning rate of 0.32, crossover rate of 0.16, and mutation rate of 0.52. The process was stopped when the convergence criterion was satisfied.

The authors used the real-valued encoding genetic algorithm for finding the experimental runs when a certain level of a factor is costly, and used the binary encoding GA for finding the budget constraint because this problem can be formulated as a 0-1 knapsack problem. The experimental cost for each experimental run depends on the factor levels. The objective is to minimize the cost for G -efficient response surface designs for each experimental run. The total experiment cost can be expressed as:

$$TC = pc + qm_1c, \quad (74)$$

where p is the number of runs constructed at the low level of X_1 , c is the standard cost c for a design variable X_1 , q is the number of runs constructed at the high level of X_1 , and m_1 is the multiplier of the standard cost at the high level of X_1 in comparison to the other levels of X_1 . In the situation where a budget constraint exists,

the objective is to maximize G-efficiency that is subject to a budget constraint of the form $\sum_{i=1}^n c_i x_i = B$, $x_i = 0$ or 1 for $i=1,2,\dots,n$ total treatment combinations, c_i is the cost per observation at i^{th} treatment combination, and B is the budget for the experiment.

12. Model Robustness

Heredia-Langner *et al.* (2004) presented a technique to obtain model-robust optimal designs using genetic algorithms to optimize a desirability function of D-or I-optimality criteria for a given set of potential models. This technique is useful in the situation where a computer-generated design is most likely to be utilized, and does not require linearity, smoothness, or continuity of the objective functions or constraints. A model robust design has high efficiency with respect to a particular optimization criterion for every member of a set of candidate models that is of interest to experimenter.

The authors employed real-valued encoding to form chromosomes and created a parent population of 50 designs. Then, the recombination step produced 350 offspring. Next, in a selection process, the best 50 offspring become members of the next parent population. Finally, they applied the Gaussian mutation procedure to up to 15% of the new parent population. Usually, the total number of generations needed to achieve the convergence was between 50 and 100 generations. They employed a desirability function as a tool for multiobjective function optimization that was constructed for every candidate in the set of potential models. For D-optimality, the individual desirability functional d was

$$d = \begin{cases} 1 & ; y \geq B \\ \left(\frac{y-A}{B-A} \right)^s & ; A \leq y \leq B \\ 0 & ; otherwise \end{cases} \quad (75)$$

For Q-optimality, the individual desirability function was of the form

$$d = \begin{cases} 1 & ; y \leq B \\ \left(\frac{y-C}{B-C} \right)^t & ; B \leq y \leq C \\ 0 & ; otherwise \end{cases} \quad (76)$$

where y was the value of the function being optimized, B was the maximum value of $|\mathbf{X}'\mathbf{X}|$ of the model (the target value of response), A was a lower performance bound (in this paper, $A=0$), C was an upper bound on the average scaled prediction variance, and s and t were weights that allow for linear or nonlinear behavior between a bound and the target (B) (in this paper, $s=t=1$). The value of any individual desirability (d) was between 0 and 1, where a higher value of d indicated that the response value(y) was more desirable. Generally, the overall desirability D^* was the geometric mean of individual desirability functions where

$$D^* = \{d_1 \cdot d_2 \cdots d_m\}^{1/m} ; i=1, \dots, m ; 0 \leq D^* \leq 1 \quad (77)$$

where d_i was the individual desirability for the i th candidate model. Thus, the optimization became a maximization on D^* . The author suggested that the values of C and A should be set close to the average objective function value of the individuals in the initial population.

The authors compared the genetic algorithm and the exchange algorithm for four cases: a constrained response surface problem, a set of nested polynomial models in one variable, a constrained mixture problem, and a formulation of a household product. The result showed that the best design for the most complex model did not necessarily produce good efficiencies for the simpler model. In general, a model robust design, which is employed in situations where there is uncertainty in the exact form of the final model, has high efficiency with respect to a particular optimization criterion for every member of a set of candidate models.

Ozol-Godfrey *et al.* (2005) presented a graphical method using fraction of design space (FDS) plots for examining design robustness relative to the scaled prediction variance (SPV) values to the choice of potential nested models for different designs. After the data were collected, and the effects of individual were tested, some model terms may be insignificant. Then the experimenter may decide to use a reduced model in the analysis phase. When a reduced model is used, the initial design might have undesirable prediction variance properties for that reduced model. Therefore, the experimenter needs a tool to help select the best design regardless of the final model selected. The FDS plot was used to compare several models for several designs on the same graph, showed the distribution of the SPV throughout the design space for a specific model, and considered the addition of points to the design to obtain better prediction variance properties as well as a check for lack of fit.

The authors determined G – and V –efficiencies based on the FDS plot. The V –average was estimated by averaging all the sampled SPVs in the region of interest. G –efficiency seeks to minimize the maximum SPV over the region of interest, while V –efficiency seeks to minimize the average SPV throughout the region of interest. The V -efficiency was estimated by averaging a random sample of SPV values taken from the region of interest. The authors also used $\frac{SPV}{p}$ for scaling each of the FDS curves where p is called the G -optimal bound. The scaled FDS plot for each model helped the experimenter when comparing models that have a different number of terms and when comparing any designs for a specific model on the similar scale. If all of the curves associated with different models for a specific design are close to one another on the G -scaled FDS plot, then the design is robust to the model considered and the model considered has similar prediction performance. The G -scaled FDS plot may change the order of the unscaled FDS curves. The new adaptation of the FDS plots adds more detail into the relative performance of the various designs for a small number of nested models. In this paper, the authors used three examples consisting of three-factor designs on a cuboidal region, four-factor designs on a cuboidal region, and mixture designs.

For three-factor designs on a cuboidal region, the authors considered designs that had much flatter and lower FDS curves because such designs have better prediction variance properties. In this case, they selected designs that had considerably higher G – efficiencies and lower V – averages. For the CCD, the FDS curve of the first order model with interactions had a slope that was flatter than that of other models that had a similar number of terms. Therefore, the interaction terms had much larger effects on the stability of the distribution of the SPV. For the second order model, the FDS curve for the CCD performed better than that of the Hoke D6 for most of the design space. However, for the first-order and first-order with interactions model, the FDS curve for the Hoke D6 performed better than that of the CCD for most of the design space. For the G -scaled FDS plot, the first order with interactions model for the CCD and the Hoke D6 had the lowest values for most of the design space. If the experimenter desired the second order model, then the CCD performs best based on the G - and V - efficiency. If some terms in the second order model were insignificant and the experimenter decided to use the reduced model such as the first order or first order with interaction model, then the Hoke D6 may be more suitable.

For four-factor designs on a cuboidal region, the authors were more interested in the average SPV value over the design region. For the second order model, the CCD and PBCD had similar performance for small SPV values; however, the CCD was more stable for the large values of SPV. For the first-order with interactions model, the CCD and Hoke D5 were quite similar in performance. For first order model, the Hoke D5 had slightly lower SPV values than that of the CCD and PBCD, but all three designs seemed to perform quite similarly. For the G -scaled FDS plot, the first order with interaction model had the lowest values for most of the design space for the three designs. All three designs had good robustness properties. The CCD performed best based on the G - and V - efficiency for the second-order, the first-order with interaction, and the first-order model.

When comparing mixture designs, the authors examined the simplex centroid and the simplex lattice designs. The simplex centroid design was augmented with

interior points supported the fitting of a special quadratic model with 9 parameters, while the $\{3,3\}$ simplex lattice supported the fitting of a general cubic model with 10 parameters. The full model was the special cubic model. The G -scaled SPV values of the simplex centroid and the $\{3,3\}$ simplex lattice design were nearly identical. However, the simplex centroid design was the more robust design because the G -scaled SPV values of the special cubic, second order, and first order models were more similar. When the experimenter had no idea about candidate models, the authors suggested a few common classes of models such as the second order model, the first order with interaction model, and the first order model because the FDS curve of these models contains the terms of the other model considered.

Anderson-Cook *et al.* (2009) developed a methodology for evaluating the robustness of designs to model misspecification, with respect to an assumed model on the expected mean square error (EMSE) over cuboidal regions of interest. The expected mean square error (EMSE) is the sum of prediction variance (PV) and expected squared bias (ESB). The authors used fraction of design space (FDS) plots and boxplots to examine the relative contribution of bias and PV under various assumed levels of the model misspecification. The type of model misspecification can have a significant effect on prediction and optimization. The authors focused on the median of PV and ESB.

Suppose the assumed model can be written as

$$\mathbf{Y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\varepsilon}, \quad (78)$$

while the true model had an additional q terms and was given by

$$\mathbf{Y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon}, \quad (79)$$

where $\mathbf{Y}$ is an $n \times 1$ vector of observed response, $\mathbf{X}_1$ is the $n \times p$ matrix expanded to the assumed model form, $\boldsymbol{\beta}_1$ is the vector of coefficients of the assumed model, $\mathbf{X}_2$ is the $n \times q$ matrix expanded to the true model form but with the absence of the assumed

model form, β_2 is the vector of coefficients of the true model form but with the absence of the assumed model form, and ε is a $n \times 1$ vector of independent and identically distributed errors, $\varepsilon \sim N(0, \sigma^2)$. The response model at an observed design point, x_0 , is given by

$$Y | (x = x_0) = w'\beta_1 + z'\beta_2 + \varepsilon, \quad (80)$$

where w is a $p \times 1$ matrix expanded to the assumed model form at an observed design point x_0 , z is a $q \times 1$ matrix expanded to the true model form but with the absence of the assumed model form at an observed design point x_0 . The coefficients in β_1 can be estimated using ordinary least squares or some other estimation approach. The coefficients in β_2 are not fully estimable so they were excluded in the estimation process. Normally, the coefficients of β_2 are unknown, thus, the assessment of a design needed additional assumptions that the coefficients of β_2 were independent and identically distributed random variables, $\beta_2 \sim N(0, \Sigma_{\beta_2})$. If the variances of missing terms are all assumed to be equal, then Σ_{β_2} is given by

$$\Sigma_{\beta_2} = \begin{bmatrix} \sigma_B^2 & 0 & \dots & 0 \\ 0 & \sigma_B^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \sigma_B^2 \end{bmatrix}.$$

The mean square error (MSE) of prediction can be written as

$$MSE[\hat{y}(x_0)] = \sigma^2 w' (X_1' X_1)^{-1} w + \beta_2 (w'A - z')(z - w'A) \beta_2', \quad (81)$$

where $A = (X_1' X_1)^{-1} X_1' X_2$ is the alias matrix, and $\hat{y}(x_0)$ is the prediction response at an observed design point. The square of bias is $\beta_2 (w'A - z')(z - w'A) \beta_2'$ and the prediction variance (PV) is $\sigma^2 w' (X_1' X_1)^{-1} w$. The authors used the prediction

variance because they were interested in a direct measure of quality of prediction in the design space.

In this paper, the authors used fraction of design space (FDS) plots and boxplots for evaluating the performance of designs. Four cases were studied: of a two-factor response surface model, a three-factor response surface model, a four-factor response surface model, and an eight-factor screening design. In the response surface case, the true model was a cubic model, while the assumed model was a quadratic model. In the screening experiment case, the true model was a quadratic model, while the assumed model was the first-order model. The CCD was the reference design for the response surface experiments, but in the screening experiment, the 2^{8-4} fractional factorial was the reference design.

In the two-factor response surface model case, the quadratic *I*-optimal designs (Q *I*-opt) corresponded to the central composite design (CCD) which performed best based on minimizing the maximum EMSE, had a good robustness to bias, and had the best mean PV. If the quadratic model was correct, then the quadratic *I*-optimal design was a good choice for the mean and maximum PV. The cubic *I*-optimal design (C *I*-opt) and the cubic Bayesian *I*-optimal design (C Bays *I*-opt) had the lowest mean ESB and performed well for the mean, median, and 95th percentiles of the EMSE. When some cubic terms were present, the cubic *I*-optimal design (C *I*-opt) and the cubic Bayesian *I*-optimal design (C Bays *I*-opt) were good choices. The *I*-optimal designs can have poor performance for the maximum PV, ESB, and EMSE, but they affected only a small proportion of the design space.

In the three-factor response surface model case, the CCD was the best design based on the mean and 95th percentile of PV and for minimizing the maximum value of EMSE. If the quadratic model was correct, then the CCD performed the best in terms of PV. The BBD was the best design for minimizing the mean PV and performed well for the mean, median, and 95th percentiles of ESB and EMSE. When some cubic terms were present, the BBD was a good choice. The C Bays *I*-opt

design performed well for the mean, median, and 95th percentiles except for the maximum of EMSE.

In the four-factor response surface model case, the Q *I*-opt design was a strong choice based on the PV and best based on the mean and 95th percentile of EMSE. The CCD performed well for PV and best for the 95th percentile and minimizing the maximum value of EMSE. The BBD was best based on the median of EMSE. When some cubic terms were present, the BBD was a good choice. If the quadratic model was correct, then the CCD and Q *I*-opt design were best in the terms of EMSE.

In the eight-factor screening design case, the *D*-optimal design was best for PV, but worst for the mean, median, 95th percentile, and the maximum of ESB and EMSE. If the first order model was correct, then the *D*-optimal design was best in terms of PV. On the other hand, if the second order model was correct, then the *D*-optimal design was worst in terms of PV. The Bayes *I*-optimal design was best for the mean, median, and 95th percentile except for the maximum of ESB and EMSE. When some second order terms were present, this design was the best choice. The 2^{8-4} fractional factorial was best for PV and ESB. This design dominated the other designs based on the mean, median, 95th percentile, and maximum EMSE.

For the screening design and the response surface design, different conclusions were drawn about the robustness of designs. For a response surface design, the central composite designs (CCD) has excellent performance when the quadratic model is correct; however, the Box-Behnken designs are superior when the missing cubic terms are present. In a screening design, the *D*-optimal design has the best performance when the first order model is correct; however, the Bayes *I*-optimal design is superior when the missing quadratic terms are present. The authors selected the value of the variance of omitted cubic terms, σ_B^2 , that makes the median of PV and ESB approximately equal. If the difference between the number of terms in the assumed and true models increased, then the size of σ_B^2 required to balance contributions of PA and ESB value decreased.

MATERIALS AND METHODS

Materials

1. High performance personal computer (Intel® Core™2 Duo Processor P8600, 4.0 GB of RAM) for running the coded program.

2. MATLAB (Matrix Laboratory) student version 2010a is used for execution of the code developed and used in this research.

Methods

This chapter gives a detailed definition of the scope of the research and introduces a methodology for construction and evaluation of mixture experiments. The main objective of this dissertation is to generate model robust designs for mixture experiments using a genetic algorithm. Model robustness will be examined and assessed using a graphical approach and an alphabetical optimality criteria approach. The specific details about the research methods are the following:

1. Consider mixture experiments with constraints that are imposed on the component proportions in the form of lower and upper bounds:

$$0 \leq L_i \leq x_i \leq U_i \leq 1 \quad ; \quad i = 1, 2, \dots, q. \quad (82)$$

where L_i is the lower bound and U_i is the upper bound for the i th component. Also, consider mixture experiments with and without linear multiple component constraints:

$$C_j \leq A_{1j}x_1 + A_{2j}x_2 + \dots + A_{qj}x_q \leq D_j \quad ; \quad j = 1, 2, \dots, h \quad (83)$$

where A_{ij} , C_j and D_j are scalar constants such that C_j and D_j are lower and upper bounds, respectively, for the j -th two-sided constraint.

This dissertation focuses on mixtures with three and four components. Two cases are considered: experiments with only single component constraints (SCCs) and experiments with both SCCs and with linear multiple component constraints (MCCs). Specifically, the following mixture experiment problems results are considered:

- SCCs in three-component mixture experiments.
- SCCs in four-component mixture experiments.
- SCCs and MCCs in three-component mixture experiments.

The following three case studies are based on particular examples selected from the statistical literature for mixture experiments, and are considered for this dissertation:

Case 1: An example of three components with only SCCs comes from Snee and Raynor (1982) and deal with a poultry feed blend experiment. The objective of the experiment is to evaluate the effects of the components on the weight gain of chicks consuming the feed. In making the poultry feed blend, there are three mixture components (maize = x_1 , fish = x_2 , soybean = x_3). The SCCs for the mixture components are given by:

$$\begin{aligned} 0.3 &\leq x_1 \leq 0.8 \\ 0.0 &\leq x_2 \leq 0.3 \\ 0.0 &\leq x_3 \leq 0.5. \end{aligned} \tag{84}$$

Case 2: A four-component example with only SCCs is from McLean and Anderson (1966) and deals with the illumination produced by flares. The objective of the experiment is to determine the formulation of the flare components that gives maximum illumination level. The flare consists of four components: magnesium (x_1), sodium nitrate (x_2), strontium nitrate (x_3), and binder (x_4). The SCCs for these components are

$$\begin{aligned}
0.4 &\leq x_1 \leq 0.6 \\
0.1 &\leq x_2 \leq 0.47 \\
0.1 &\leq x_3 \leq 0.47 \\
0.03 &\leq x_4 \leq 0.08.
\end{aligned} \tag{85}$$

Case 3: A hypothetical three-component mixture example with SCCs and MCCs taken from Snee (1979). The experimental region is defined by the following set of three SCCs and two MCCs:

$$\begin{aligned}
0.1 &\leq x_1 \leq 0.5 \\
0.1 &\leq x_2 \leq 0.7 \\
0.0 &\leq x_3 \leq 0.7 \\
0.9 &\leq 0.85x_1 + 0.9x_2 + x_3 \leq 0.95 \\
0.4 &\leq 0.7x_1 + x_3.
\end{aligned} \tag{86}$$

2. Construct the key models, referred to as the “full” models. Two models are proposed: the Scheffé quadratic mixture model and the special cubic mixture model for q -component mixture experiments which consist of three and four component mixture problems. The full models can be mathematically expressed as

Quadratic model :

$$E(y) = \sum_{i=1}^q \beta_i x_i + \sum_{i<j}^q \beta_{ij} x_i x_j. \tag{87}$$

Special Cubic model :

$$E(y) = \sum_{i=1}^q \beta_i x_i + \sum_{i<j}^q \beta_{ij} x_i x_j + \sum_{i<j<k}^q \beta_{ijk} x_i x_j x_k. \tag{88}$$

In this dissertation, the goal is to generate designs that are robust with respect of the full model being either the Scheffé quadratic model or the special cubic mixture model. The number of terms in the Scheffé quadratic and special cubic mixture

models are $\frac{q(q+1)}{2}$ and $\frac{q(q^2+5)}{6}$, respectively.

3. If the full model is the Scheffé quadratic model, the following cases will be considered: three component experiments having seven to twelve points and four component experiments having eleven to sixteen points. While, if the full model is a Scheffé special cubic model, the following cases will be considered: three component experiments having eight to thirteen points and four component experiments having fifteen to twenty points. The minimum number of design points for each case were selected to provide sufficient degrees of freedom to test the adequacy of the fit of the full model. Thus, the minimum number of design points should be the number of term in the full model plus 1.

4. Consider reduced models to assess model robustness. Two specific classes of reduced models based on heredity principles (Chipman, 1996) are considered where model terms are removed from the full model based on hierarchical structures. In this dissertation, we additionally assume that all single component effects (main effects) must occur in each possible reduced model. The two heredity principles for constructing reduced models for mixture experiments are defined as :

4.1 *Strong heredity (SH)* requires that (1) if a model contains the quadratic term ($x_i x_j$), then it must contain both corresponding active main effects (x_i and x_j) and (2) if a model contains the cubic term ($x_i x_j x_k$), then it must contain all corresponding active interaction effects ($x_i x_j$ and $x_i x_k$ and $x_j x_k$).

4.2 *Weak heredity (WH)* requires that (1) if a model contains the quadratic term ($x_i x_j$), then it must contain one or both of the corresponding active main effects (x_i or x_j) and (2) if a model contains the cubic term ($x_i x_j x_k$), then it must contain one or more of the corresponding active interaction effects ($x_i x_j$ or $x_i x_k$ or $x_j x_k$).

In this dissertation, the SH and WH principles are applied to construct the set of all possible reduced models when the full model is either the Scheffé quadratic model or the special cubic model. For SH with $q=3$ and 4 components, there are,

respectively, 8 and 64 SH models of the full quadratic model. The set of WH reduced models of the full quadratic model with $q=3$ and 4 components are identical with the set of SH reduced models because of the additional condition that all single component (main) effects must be included in each reduced model. Therefore the WH condition is modified by replacing ‘one or both of the corresponding main effects’ with ‘both corresponding main effects’. Tables 4 and 5 contain the set of reduced models of the full quadratic model for $q=3$ and 4 components, respectively. For SH, there are, respectively, 9 and 113 SH models of the full special cubic model for $q=3$ and 4 components. For WH, there are, respectively, 15 and 809 WH models of the full special cubic model for $q=3$ and 4 components. The set of SH and WH reduced models for 3 components mixture experiments for the full special cubic model are shown in Tables 6 and 7, respectively. Tables 8 and 9 show the set of SH and WH reduced models for 4 component mixture experiments for the full special cubic model, respectively. In Tables 4 to 9, the 1’s and 0’s in the ‘Terms in model’ columns represent the presence or absence of the terms in the reduced model, respectively. The column p , cp , and cb indicates the number of model parameters, quadratic terms and cubic terms, respectively. Note that model 1 represents the full model in each table.

Table 4 SH and WH models for the full quadratic mixture model with $q = 3$.

model	Terms in model						p	cp
	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3		
1	1	1	1	1	1	1	6	3
2	1	1	1	0	1	1	5	2
3	1	1	1	1	0	1	5	2
4	1	1	1	1	1	0	5	2
5	1	1	1	0	0	1	4	1
6	1	1	1	0	1	0	4	1
7	1	1	1	1	0	0	4	1
8	1	1	1	0	0	0	3	0

Table 5 SH and WH models for the full quadratic mixture model with $q = 4$.

model	Terms in model										p	cp
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4		
1	1	1	1	1	1	1	1	1	1	1	10	6
2	1	1	1	1	0	1	1	1	1	1	9	5
3	1	1	1	1	1	0	1	1	1	1	9	5
4	1	1	1	1	1	1	0	1	1	1	9	5
5	1	1	1	1	1	1	1	0	1	1	9	5
6	1	1	1	1	1	1	1	1	0	1	9	5
7	1	1	1	1	1	1	1	1	1	0	9	5
8	1	1	1	1	0	0	1	1	1	1	8	4
9	1	1	1	1	0	1	0	1	1	1	8	4
10	1	1	1	1	0	1	1	0	1	1	8	4
11	1	1	1	1	0	1	1	1	0	1	8	4
12	1	1	1	1	0	1	1	1	1	0	8	4
13	1	1	1	1	1	0	0	1	1	1	8	4
14	1	1	1	1	1	0	1	0	1	1	8	4
15	1	1	1	1	1	0	1	1	0	1	8	4
16	1	1	1	1	1	0	1	1	1	0	8	4
17	1	1	1	1	1	1	0	0	1	1	8	4
18	1	1	1	1	1	1	0	1	0	1	8	4
19	1	1	1	1	1	1	0	1	1	0	8	4
20	1	1	1	1	1	1	1	0	0	1	8	4
21	1	1	1	1	1	1	1	0	1	0	8	4
22	1	1	1	1	1	1	1	1	0	0	8	4
23	1	1	1	1	0	0	0	1	1	1	7	3
24	1	1	1	1	0	0	1	0	1	1	7	3
25	1	1	1	1	0	0	1	1	0	1	7	3
26	1	1	1	1	0	0	1	1	1	0	7	3
27	1	1	1	1	0	1	0	0	1	1	7	3
28	1	1	1	1	0	1	0	1	0	1	7	3
29	1	1	1	1	0	1	0	1	1	0	7	3
30	1	1	1	1	0	1	1	0	0	1	7	3
31	1	1	1	1	0	1	1	0	1	0	7	3
32	1	1	1	1	0	1	1	1	0	0	7	3
33	1	1	1	1	1	0	0	0	1	1	7	3
34	1	1	1	1	1	0	0	1	0	1	7	3
35	1	1	1	1	1	0	0	1	1	0	7	3
36	1	1	1	1	1	0	1	0	0	1	7	3
37	1	1	1	1	1	0	1	0	1	0	7	3
38	1	1	1	1	1	0	1	1	0	0	7	3
39	1	1	1	1	1	1	0	0	0	1	7	3
40	1	1	1	1	1	1	0	0	1	0	7	3

Table 5 (Continued)

model	Terms in model										p	cp
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4		
41	1	1	1	1	1	1	0	1	0	0	7	3
42	1	1	1	1	1	1	1	0	0	0	7	3
43	1	1	1	1	0	0	0	0	1	1	6	2
44	1	1	1	1	0	0	0	1	0	1	6	2
45	1	1	1	1	0	0	0	1	1	0	6	2
46	1	1	1	1	0	0	1	0	0	1	6	2
47	1	1	1	1	0	0	1	0	1	0	6	2
48	1	1	1	1	0	0	1	1	0	0	6	2
49	1	1	1	1	0	1	0	0	0	1	6	2
50	1	1	1	1	0	1	0	0	1	0	6	2
51	1	1	1	1	0	1	0	1	0	0	6	2
52	1	1	1	1	0	1	1	0	0	0	6	2
53	1	1	1	1	1	0	0	0	0	1	6	2
54	1	1	1	1	1	0	0	0	1	0	6	2
55	1	1	1	1	1	0	0	1	0	0	6	2
56	1	1	1	1	1	0	1	0	0	0	6	2
57	1	1	1	1	1	1	0	0	0	0	6	2
58	1	1	1	1	0	0	0	0	0	1	5	1
59	1	1	1	1	0	0	0	0	1	0	5	1
60	1	1	1	1	0	0	0	1	0	0	5	1
61	1	1	1	1	0	0	1	0	0	0	5	1
62	1	1	1	1	0	1	0	0	0	0	5	1
63	1	1	1	1	1	0	0	0	0	0	5	1
64	1	1	1	1	0	0	0	0	0	0	4	0

Table 6 SH models for the full special cubic mixture model with $q = 3$.

model	Terms in model							p	cp	cb
	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3	$x_1x_2x_3$			
1	1	1	1	1	1	1	1	7	3	1
2	1	1	1	1	1	1	0	6	3	0
3	1	1	1	0	1	1	0	5	2	0
4	1	1	1	1	0	1	0	5	2	0
5	1	1	1	1	1	0	0	5	2	0
6	1	1	1	0	0	1	0	4	1	0
7	1	1	1	0	1	0	0	4	1	0
8	1	1	1	1	0	0	0	4	1	0
9	1	1	1	0	0	0	0	3	0	0

Table 7 WH models for the full special cubic mixture model with $q = 3$.

model	Terms in model							p	cp	cb
	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3	$x_1x_2x_3$			
1	1	1	1	1	1	1	1	7	3	1
2	1	1	1	0	1	1	1	6	2	1
3	1	1	1	1	0	1	1	6	2	1
4	1	1	1	1	1	0	1	6	2	1
5	1	1	1	1	1	1	0	6	3	0
6	1	1	1	0	0	1	1	5	1	1
7	1	1	1	0	1	0	1	5	1	1
8	1	1	1	0	1	1	0	5	2	0
9	1	1	1	1	0	0	1	5	1	1
10	1	1	1	1	0	1	0	5	2	0
11	1	1	1	1	1	0	0	5	2	0
12	1	1	1	0	0	1	0	4	1	0
13	1	1	1	0	1	0	0	4	1	0
14	1	1	1	1	0	0	0	4	1	0
15	1	1	1	0	0	0	0	3	0	0

Table 8 SH models for the full special cubic mixture model with $q = 4$.

model	Terms in model															p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$				
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	14	6	4	
2	1	1	1	1	1	1	1	1	1	1	0	1	1	1	13	6	3	
3	1	1	1	1	1	1	1	1	1	1	1	0	1	1	13	6	3	
4	1	1	1	1	1	1	1	1	1	1	1	1	0	1	13	6	3	
5	1	1	1	1	1	1	1	1	1	1	1	1	1	0	13	6	3	
6	1	1	1	1	1	1	1	1	1	1	0	0	1	1	12	6	2	
7	1	1	1	1	1	1	1	1	1	1	0	1	0	1	12	6	2	
8	1	1	1	1	1	1	1	1	1	1	0	1	1	0	12	6	2	
9	1	1	1	1	1	1	1	1	1	1	1	0	0	1	12	6	2	
10	1	1	1	1	1	1	1	1	1	1	1	0	1	0	12	6	2	
11	1	1	1	1	1	1	1	1	1	1	1	1	0	0	12	6	2	
12	1	1	1	1	0	1	1	1	1	1	0	0	1	1	11	5	2	
13	1	1	1	1	1	0	1	1	1	1	0	1	0	1	11	5	2	
14	1	1	1	1	1	1	0	1	1	1	1	0	0	1	11	5	2	
15	1	1	1	1	1	1	1	0	1	1	0	1	1	0	11	5	2	
16	1	1	1	1	1	1	1	1	0	1	1	0	1	0	11	5	2	

Table 8 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
17	1	1	1	1	1	1	1	1	1	0	1	1	0	0	11	5	2
18	1	1	1	1	1	1	1	1	1	1	0	0	0	1	11	6	1
19	1	1	1	1	1	1	1	1	1	1	0	0	1	0	11	6	1
20	1	1	1	1	1	1	1	1	1	1	0	1	0	0	11	6	1
21	1	1	1	1	1	1	1	1	1	1	1	0	0	0	11	6	1
22	1	1	1	1	0	1	1	1	1	1	0	0	0	1	10	5	1
23	1	1	1	1	0	1	1	1	1	1	0	0	1	0	10	5	1
24	1	1	1	1	1	0	1	1	1	1	0	0	0	1	10	5	1
25	1	1	1	1	1	0	1	1	1	1	0	1	0	0	10	5	1
26	1	1	1	1	1	1	0	1	1	1	0	0	0	1	10	5	1
27	1	1	1	1	1	1	0	1	1	1	1	0	0	0	10	5	1
28	1	1	1	1	1	1	1	0	1	1	0	0	1	0	10	5	1
29	1	1	1	1	1	1	1	0	1	1	0	1	0	0	10	5	1
30	1	1	1	1	1	1	1	1	0	1	0	0	1	0	10	5	1
31	1	1	1	1	1	1	1	1	0	1	1	0	0	0	10	5	1
32	1	1	1	1	1	1	1	1	1	0	0	1	0	0	10	5	1
33	1	1	1	1	1	1	1	1	1	0	1	0	0	0	10	5	1
34	1	1	1	1	1	1	1	1	1	1	0	0	0	0	10	6	0
35	1	1	1	1	0	0	1	1	1	1	0	0	0	1	9	4	1
36	1	1	1	1	0	1	0	1	1	1	0	0	0	1	9	4	1
37	1	1	1	1	0	1	1	0	1	1	0	0	1	0	9	4	1
38	1	1	1	1	0	1	1	1	0	1	0	0	1	0	9	4	1
39	1	1	1	1	0	1	1	1	1	1	0	0	0	0	9	5	0
40	1	1	1	1	1	0	0	1	1	1	0	0	0	1	9	4	1
41	1	1	1	1	1	0	1	0	1	1	0	1	0	0	9	4	1
42	1	1	1	1	1	0	1	1	1	0	0	1	0	0	9	4	1
43	1	1	1	1	1	0	1	1	1	1	0	0	0	0	9	5	0
44	1	1	1	1	1	1	0	1	0	1	1	0	0	0	9	4	1
45	1	1	1	1	1	1	0	1	1	0	1	0	0	0	9	4	1
46	1	1	1	1	1	1	0	1	1	1	0	0	0	0	9	5	0
47	1	1	1	1	1	1	1	0	0	1	0	0	1	0	9	4	1
48	1	1	1	1	1	1	1	0	1	0	0	1	0	0	9	4	1
49	1	1	1	1	1	1	1	0	1	1	0	0	0	0	9	5	0
50	1	1	1	1	1	1	1	1	0	0	1	0	0	0	9	4	1
51	1	1	1	1	1	1	1	1	0	1	0	0	0	0	9	5	0
52	1	1	1	1	1	1	1	1	1	0	0	0	0	0	9	5	0
53	1	1	1	1	0	0	0	1	1	1	0	0	0	1	8	3	1
54	1	1	1	1	0	0	1	1	1	1	0	0	0	0	8	4	0
55	1	1	1	1	0	1	0	1	1	1	0	0	0	0	8	4	0
56	1	1	1	1	0	1	1	0	0	1	0	0	1	0	8	3	1
57	1	1	1	1	0	1	1	0	1	1	0	0	0	0	8	4	0
58	1	1	1	1	0	1	1	1	0	1	0	0	0	0	8	4	0

Table 8 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
59	1	1	1	1	0	1	1	1	1	0	0	0	0	0	8	4	0
60	1	1	1	1	1	0	0	1	1	1	0	0	0	0	8	4	0
61	1	1	1	1	1	0	1	0	1	0	0	1	0	0	8	3	1
62	1	1	1	1	1	0	1	0	1	1	0	0	0	0	8	4	0
63	1	1	1	1	1	0	1	1	0	1	0	0	0	0	8	4	0
64	1	1	1	1	1	0	1	1	1	0	0	0	0	0	8	4	0
65	1	1	1	1	1	1	0	0	1	1	0	0	0	0	8	4	0
66	1	1	1	1	1	1	0	1	0	0	1	0	0	0	8	3	1
67	1	1	1	1	1	1	0	1	0	1	0	0	0	0	8	4	0
68	1	1	1	1	1	1	0	1	1	0	0	0	0	0	8	4	0
69	1	1	1	1	1	1	1	0	0	1	0	0	0	0	8	4	0
70	1	1	1	1	1	1	1	0	1	0	0	0	0	0	8	4	0
71	1	1	1	1	1	1	1	1	0	0	0	0	0	0	8	4	0
72	1	1	1	1	0	0	0	1	1	1	0	0	0	0	7	3	0
73	1	1	1	1	0	0	1	0	1	1	0	0	0	0	7	3	0
74	1	1	1	1	0	0	1	1	0	1	0	0	0	0	7	3	0
75	1	1	1	1	0	0	1	1	1	0	0	0	0	0	7	3	0
76	1	1	1	1	0	1	0	0	1	1	0	0	0	0	7	3	0
77	1	1	1	1	0	1	0	1	0	1	0	0	0	0	7	3	0
78	1	1	1	1	0	1	0	1	1	0	0	0	0	0	7	3	0
79	1	1	1	1	0	1	1	0	0	1	0	0	0	0	7	3	0
80	1	1	1	1	0	1	1	0	1	0	0	0	0	0	7	3	0
81	1	1	1	1	0	1	1	1	0	0	0	0	0	0	7	3	0
82	1	1	1	1	1	0	0	0	1	1	0	0	0	0	7	3	0
83	1	1	1	1	1	0	0	1	0	1	0	0	0	0	7	3	0
84	1	1	1	1	1	0	0	1	1	0	0	0	0	0	7	3	0
85	1	1	1	1	1	0	1	0	0	1	0	0	0	0	7	3	0
86	1	1	1	1	1	0	1	0	1	0	0	0	0	0	7	3	0
87	1	1	1	1	1	0	1	1	0	0	0	0	0	0	7	3	0
88	1	1	1	1	1	1	0	0	0	1	0	0	0	0	7	3	0
89	1	1	1	1	1	1	0	0	1	0	0	0	0	0	7	3	0
90	1	1	1	1	1	1	0	1	0	0	0	0	0	0	7	3	0
91	1	1	1	1	1	1	1	0	0	0	0	0	0	0	7	3	0
92	1	1	1	1	0	0	0	0	1	1	0	0	0	0	6	2	0
93	1	1	1	1	0	0	0	1	0	1	0	0	0	0	6	2	0
94	1	1	1	1	0	0	0	1	1	0	0	0	0	0	6	2	0
95	1	1	1	1	0	0	1	0	0	1	0	0	0	0	6	2	0
96	1	1	1	1	0	0	1	0	1	0	0	0	0	0	6	2	0
97	1	1	1	1	0	0	1	1	0	0	0	0	0	0	6	2	0
98	1	1	1	1	0	1	0	0	0	1	0	0	0	0	6	2	0
99	1	1	1	1	0	1	0	0	1	0	0	0	0	0	6	2	0
100	1	1	1	1	0	1	0	1	0	0	0	0	0	0	6	2	0

Table 8 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
101	1	1	1	1	0	1	1	0	0	0	0	0	0	0	6	2	0
102	1	1	1	1	1	0	0	0	0	1	0	0	0	0	6	2	0
103	1	1	1	1	1	0	0	0	1	0	0	0	0	0	6	2	0
104	1	1	1	1	1	0	0	1	0	0	0	0	0	0	6	2	0
105	1	1	1	1	1	0	1	0	0	0	0	0	0	0	6	2	0
106	1	1	1	1	1	1	0	0	0	0	0	0	0	0	6	2	0
107	1	1	1	1	0	0	0	0	0	1	0	0	0	0	5	1	0
108	1	1	1	1	0	0	0	0	1	0	0	0	0	0	5	1	0
109	1	1	1	1	0	0	0	1	0	0	0	0	0	0	5	1	0
110	1	1	1	1	0	0	1	0	0	0	0	0	0	0	5	1	0
111	1	1	1	1	0	1	0	0	0	0	0	0	0	0	5	1	0
112	1	1	1	1	1	0	0	0	0	0	0	0	0	0	5	1	0
113	1	1	1	1	0	0	0	0	0	0	0	0	0	0	4	0	0

Table 9 WH models for the full special cubic mixture model with $q = 4$.

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	14	6	4
2	1	1	1	1	0	1	1	1	1	1	1	1	1	1	13	5	4
3	1	1	1	1	1	0	1	1	1	1	1	1	1	1	13	5	4
4	1	1	1	1	1	1	0	1	1	1	1	1	1	1	13	5	4
5	1	1	1	1	1	1	1	0	1	1	1	1	1	1	13	5	4
6	1	1	1	1	1	1	1	1	0	1	1	1	1	1	13	5	4
7	1	1	1	1	1	1	1	1	1	0	1	1	1	1	13	5	4
8	1	1	1	1	1	1	1	1	1	1	0	1	1	1	13	6	3
9	1	1	1	1	1	1	1	1	1	1	1	0	1	1	13	6	3
10	1	1	1	1	1	1	1	1	1	1	1	1	0	1	13	6	3
11	1	1	1	1	1	1	1	1	1	1	1	1	1	0	13	6	3
12	1	1	1	1	0	0	1	1	1	1	1	1	1	1	12	4	4
13	1	1	1	1	0	1	0	1	1	1	1	1	1	1	12	4	4
14	1	1	1	1	0	1	1	0	1	1	1	1	1	1	12	4	4
15	1	1	1	1	0	1	1	1	0	1	1	1	1	1	12	4	4
16	1	1	1	1	0	1	1	1	1	0	1	1	1	1	12	4	4
17	1	1	1	1	0	1	1	1	1	1	0	1	1	1	12	5	3
18	1	1	1	1	0	1	1	1	1	1	1	0	1	1	12	5	3
19	1	1	1	1	0	1	1	1	1	1	1	1	0	1	12	5	3

Table 9 (Continued)

model	Terms in model															p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$				
20	1	1	1	1	0	1	1	1	1	1	1	1	1	0	12	5	3	
21	1	1	1	1	1	0	0	1	1	1	1	1	1	1	12	4	4	
22	1	1	1	1	1	0	1	0	1	1	1	1	1	1	12	4	4	
23	1	1	1	1	1	0	1	1	0	1	1	1	1	1	12	4	4	
24	1	1	1	1	1	0	1	1	1	0	1	1	1	1	12	4	4	
25	1	1	1	1	1	0	1	1	1	1	0	1	1	1	12	5	3	
26	1	1	1	1	1	0	1	1	1	1	1	0	1	1	12	5	3	
27	1	1	1	1	1	0	1	1	1	1	1	1	0	1	12	5	3	
28	1	1	1	1	1	0	1	1	1	1	1	1	1	0	12	5	3	
29	1	1	1	1	1	1	0	0	1	1	1	1	1	1	12	4	4	
30	1	1	1	1	1	1	0	1	0	1	1	1	1	1	12	4	4	
31	1	1	1	1	1	1	0	1	1	0	1	1	1	1	12	4	4	
32	1	1	1	1	1	1	0	1	1	1	0	1	1	1	12	5	3	
33	1	1	1	1	1	1	0	1	1	1	1	0	1	1	12	5	3	
34	1	1	1	1	1	1	0	1	1	1	1	1	0	1	12	5	3	
35	1	1	1	1	1	1	0	1	1	1	1	1	1	0	12	5	3	
36	1	1	1	1	1	1	1	0	0	1	1	1	1	1	12	4	4	
37	1	1	1	1	1	1	1	0	1	0	1	1	1	1	12	4	4	
38	1	1	1	1	1	1	1	0	1	1	0	1	1	1	12	5	3	
39	1	1	1	1	1	1	1	0	1	1	1	0	1	1	12	5	3	
40	1	1	1	1	1	1	1	0	1	1	1	1	0	1	12	5	3	
41	1	1	1	1	1	1	1	0	1	1	1	1	1	0	12	5	3	
42	1	1	1	1	1	1	1	1	0	0	1	1	1	1	12	4	4	
43	1	1	1	1	1	1	1	1	0	1	0	1	1	1	12	5	3	
44	1	1	1	1	1	1	1	1	0	1	1	0	1	1	12	5	3	
45	1	1	1	1	1	1	1	1	0	1	1	1	0	1	12	5	3	
46	1	1	1	1	1	1	1	1	0	1	1	1	1	0	12	5	3	
47	1	1	1	1	1	1	1	1	1	0	0	1	1	1	12	5	3	
48	1	1	1	1	1	1	1	1	1	0	1	0	1	1	12	5	3	
49	1	1	1	1	1	1	1	1	1	0	1	1	0	1	12	5	3	
50	1	1	1	1	1	1	1	1	1	0	1	1	1	0	12	5	3	
51	1	1	1	1	1	1	1	1	1	1	0	0	1	1	12	6	2	
52	1	1	1	1	1	1	1	1	1	1	0	1	0	1	12	6	2	
53	1	1	1	1	1	1	1	1	1	1	0	1	1	0	12	6	2	
54	1	1	1	1	1	1	1	1	1	1	1	0	0	1	12	6	2	
55	1	1	1	1	1	1	1	1	1	1	1	0	1	0	12	6	2	
56	1	1	1	1	1	1	1	1	1	1	1	1	0	0	12	6	2	
57	1	1	1	1	0	0	0	1	1	1	1	1	1	1	11	3	4	
58	1	1	1	1	0	0	1	1	0	1	1	1	1	1	11	3	4	
59	1	1	1	1	0	0	1	1	1	0	1	1	1	1	11	3	4	
60	1	1	1	1	0	0	1	1	1	1	0	1	1	1	11	4	3	
61	1	1	1	1	0	0	1	1	1	1	1	0	1	1	11	4	3	

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
62	1	1	1	1	0	0	1	1	1	1	1	1	0	1	11	4	3
63	1	1	1	1	0	0	1	1	1	1	1	1	1	0	11	4	3
64	1	1	1	1	0	1	0	0	1	1	1	1	1	1	11	3	4
65	1	1	1	1	0	1	0	1	1	0	1	1	1	1	11	3	4
66	1	1	1	1	0	1	0	1	1	1	0	1	1	1	11	4	3
67	1	1	1	1	0	1	0	1	1	1	1	0	1	1	11	4	3
68	1	1	1	1	0	1	0	1	1	1	1	1	0	1	11	4	3
69	1	1	1	1	0	1	0	1	1	1	1	1	1	0	11	4	3
70	1	1	1	1	0	1	1	0	0	1	1	1	1	1	11	3	4
71	1	1	1	1	0	1	1	0	1	0	1	1	1	1	11	3	4
72	1	1	1	1	0	1	1	0	1	1	0	1	1	1	11	4	3
73	1	1	1	1	0	1	1	0	1	1	1	0	1	1	11	4	3
74	1	1	1	1	0	1	1	0	1	1	1	1	0	1	11	4	3
75	1	1	1	1	0	1	1	0	1	1	1	1	1	0	11	4	3
76	1	1	1	1	0	1	1	1	0	0	1	1	1	1	11	3	4
77	1	1	1	1	0	1	1	1	0	1	0	1	1	1	11	4	3
78	1	1	1	1	0	1	1	1	0	1	1	0	1	1	11	4	3
79	1	1	1	1	0	1	1	1	0	1	1	1	0	1	11	4	3
80	1	1	1	1	0	1	1	1	0	1	1	1	1	0	11	4	3
81	1	1	1	1	0	1	1	1	1	0	0	1	1	1	11	4	3
82	1	1	1	1	0	1	1	1	1	0	1	0	1	1	11	4	3
83	1	1	1	1	0	1	1	1	1	0	1	1	0	1	11	4	3
84	1	1	1	1	0	1	1	1	1	0	1	1	1	0	11	4	3
85	1	1	1	1	0	1	1	1	1	1	0	0	1	1	11	5	2
86	1	1	1	1	0	1	1	1	1	1	0	1	0	1	11	5	2
87	1	1	1	1	0	1	1	1	1	1	0	1	1	0	11	5	2
88	1	1	1	1	0	1	1	1	1	1	1	0	0	1	11	5	2
89	1	1	1	1	0	1	1	1	1	1	1	0	1	0	11	5	2
90	1	1	1	1	0	1	1	1	1	1	1	1	0	0	11	5	2
91	1	1	1	1	1	0	0	0	1	1	1	1	1	1	11	3	4
92	1	1	1	1	1	0	0	1	0	1	1	1	1	1	11	3	4
93	1	1	1	1	1	0	0	1	1	1	0	1	1	1	11	4	3
94	1	1	1	1	1	0	0	1	1	1	1	0	1	1	11	4	3
95	1	1	1	1	1	0	0	1	1	1	1	1	0	1	11	4	3
96	1	1	1	1	1	0	0	1	1	1	1	1	1	0	11	4	3
97	1	1	1	1	1	0	1	0	0	1	1	1	1	1	11	3	4
98	1	1	1	1	1	0	1	0	1	0	1	1	1	1	11	3	4
99	1	1	1	1	1	0	1	0	1	1	0	1	1	1	11	4	3
100	1	1	1	1	1	0	1	0	1	1	1	0	1	1	11	4	3
101	1	1	1	1	1	0	1	0	1	1	1	1	0	1	11	4	3
102	1	1	1	1	1	0	1	0	1	1	1	1	1	0	11	4	3
103	1	1	1	1	1	0	1	1	0	0	1	1	1	1	11	3	4

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
104	1	1	1	1	1	0	1	1	0	1	0	1	1	1	11	4	3
105	1	1	1	1	1	0	1	1	0	1	1	0	1	1	11	4	3
106	1	1	1	1	1	0	1	1	0	1	1	1	0	1	11	4	3
107	1	1	1	1	1	0	1	1	0	1	1	1	1	0	11	4	3
108	1	1	1	1	1	0	1	1	1	0	0	1	1	1	11	4	3
109	1	1	1	1	1	0	1	1	1	0	1	0	1	1	11	4	3
110	1	1	1	1	1	0	1	1	1	0	1	1	0	1	11	4	3
111	1	1	1	1	1	0	1	1	1	0	1	1	1	0	11	4	3
112	1	1	1	1	1	0	1	1	1	1	0	0	1	1	11	5	2
113	1	1	1	1	1	0	1	1	1	1	0	1	0	1	11	5	2
114	1	1	1	1	1	0	1	1	1	1	0	1	1	0	11	5	2
115	1	1	1	1	1	0	1	1	1	1	1	0	0	1	11	5	2
116	1	1	1	1	1	0	1	1	1	1	1	0	1	0	11	5	2
117	1	1	1	1	1	0	1	1	1	1	1	1	0	0	11	5	2
118	1	1	1	1	1	1	0	0	0	1	1	1	1	1	11	3	4
119	1	1	1	1	1	1	0	0	1	0	1	1	1	1	11	3	4
120	1	1	1	1	1	1	0	0	1	1	0	1	1	1	11	4	3
121	1	1	1	1	1	1	0	0	1	1	1	0	1	1	11	4	3
122	1	1	1	1	1	1	0	0	1	1	1	1	0	1	11	4	3
123	1	1	1	1	1	1	0	0	1	1	1	1	1	0	11	4	3
124	1	1	1	1	1	1	0	1	0	0	1	1	1	1	11	3	4
125	1	1	1	1	1	1	0	1	0	1	0	1	1	1	11	4	3
126	1	1	1	1	1	1	0	1	0	1	1	0	1	1	11	4	3
127	1	1	1	1	1	1	0	1	0	1	1	1	0	1	11	4	3
128	1	1	1	1	1	1	0	1	0	1	1	1	1	0	11	4	3
129	1	1	1	1	1	1	0	1	1	0	0	1	1	1	11	4	3
130	1	1	1	1	1	1	0	1	1	0	1	0	1	1	11	4	3
131	1	1	1	1	1	1	0	1	1	0	1	1	0	1	11	4	3
132	1	1	1	1	1	1	0	1	1	0	1	1	1	0	11	4	3
133	1	1	1	1	1	1	0	1	1	1	0	0	1	1	11	5	2
134	1	1	1	1	1	1	0	1	1	1	0	1	0	1	11	5	2
135	1	1	1	1	1	1	0	1	1	1	0	1	1	0	11	5	2
136	1	1	1	1	1	1	0	1	1	1	1	0	0	1	11	5	2
137	1	1	1	1	1	1	0	1	1	1	1	0	1	0	11	5	2
138	1	1	1	1	1	1	0	1	1	1	1	1	0	0	11	5	2
139	1	1	1	1	1	1	1	0	0	1	0	1	1	1	11	4	3
140	1	1	1	1	1	1	1	0	0	1	1	0	1	1	11	4	3
141	1	1	1	1	1	1	1	0	0	1	1	1	0	1	11	4	3
142	1	1	1	1	1	1	1	0	0	1	1	1	1	0	11	4	3
143	1	1	1	1	1	1	1	0	1	0	0	1	1	1	11	4	3
144	1	1	1	1	1	1	1	0	1	0	1	0	1	1	11	4	3
145	1	1	1	1	1	1	1	0	1	0	1	1	0	1	11	4	3

Table 9 (Continued)

model	Terms in model															p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$				
146	1	1	1	1	1	1	1	0	1	0	1	1	1	0	11	4	3	
147	1	1	1	1	1	1	1	0	1	1	0	0	1	1	11	5	2	
148	1	1	1	1	1	1	1	0	1	1	0	1	0	1	11	5	2	
149	1	1	1	1	1	1	1	0	1	1	0	1	1	0	11	5	2	
150	1	1	1	1	1	1	1	0	1	1	1	0	0	1	11	5	2	
151	1	1	1	1	1	1	1	0	1	1	1	0	1	0	11	5	2	
152	1	1	1	1	1	1	1	0	1	1	1	1	0	0	11	5	2	
153	1	1	1	1	1	1	1	1	0	0	0	1	1	1	11	4	3	
154	1	1	1	1	1	1	1	1	0	0	1	0	1	1	11	4	3	
155	1	1	1	1	1	1	1	1	0	0	1	1	0	1	11	4	3	
156	1	1	1	1	1	1	1	1	0	0	1	1	1	0	11	4	3	
157	1	1	1	1	1	1	1	1	0	1	0	0	1	1	11	5	2	
158	1	1	1	1	1	1	1	1	0	1	0	1	0	1	11	5	2	
159	1	1	1	1	1	1	1	1	0	1	0	1	1	0	11	5	2	
160	1	1	1	1	1	1	1	1	0	1	1	0	0	1	11	5	2	
161	1	1	1	1	1	1	1	1	0	1	1	0	1	0	11	5	2	
162	1	1	1	1	1	1	1	1	0	1	1	1	0	0	11	5	2	
163	1	1	1	1	1	1	1	1	1	0	0	0	1	1	11	5	2	
164	1	1	1	1	1	1	1	1	1	0	0	1	0	1	11	5	2	
165	1	1	1	1	1	1	1	1	1	0	0	1	1	0	11	5	2	
166	1	1	1	1	1	1	1	1	1	0	1	0	0	1	11	5	2	
167	1	1	1	1	1	1	1	1	1	0	1	0	1	0	11	5	2	
168	1	1	1	1	1	1	1	1	1	0	1	1	0	0	11	5	2	
169	1	1	1	1	1	1	1	1	1	1	0	0	0	1	11	6	1	
170	1	1	1	1	1	1	1	1	1	1	0	0	1	0	11	6	1	
171	1	1	1	1	1	1	1	1	1	1	0	1	0	0	11	6	1	
172	1	1	1	1	1	1	1	1	1	1	1	0	0	0	11	6	1	
173	1	1	1	1	0	0	0	1	1	1	0	1	1	1	10	3	3	
174	1	1	1	1	0	0	0	1	1	1	1	0	1	1	10	3	3	
175	1	1	1	1	0	0	0	1	1	1	1	1	0	1	10	3	3	
176	1	1	1	1	0	0	0	1	1	1	1	1	1	0	10	3	3	
177	1	1	1	1	0	0	1	0	1	1	0	1	1	1	10	3	3	
178	1	1	1	1	0	0	1	1	0	0	1	1	1	1	10	2	4	
179	1	1	1	1	0	0	1	1	0	1	0	1	1	1	10	3	3	
180	1	1	1	1	0	0	1	1	0	1	1	0	1	1	10	3	3	
181	1	1	1	1	0	0	1	1	0	1	1	1	0	1	10	3	3	
182	1	1	1	1	0	0	1	1	0	1	1	1	1	0	10	3	3	
183	1	1	1	1	0	0	1	1	1	0	0	1	1	1	10	3	3	
184	1	1	1	1	0	0	1	1	1	0	1	0	1	1	10	3	3	
185	1	1	1	1	0	0	1	1	1	0	1	1	0	1	10	3	3	
186	1	1	1	1	0	0	1	1	1	0	1	1	1	0	10	3	3	
187	1	1	1	1	0	0	1	1	1	1	0	0	1	1	10	4	2	

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
188	1	1	1	1	0	0	1	1	1	1	0	1	0	1	10	4	2
189	1	1	1	1	0	0	1	1	1	1	0	1	1	0	10	4	2
190	1	1	1	1	0	0	1	1	1	1	1	0	0	1	10	4	2
191	1	1	1	1	0	0	1	1	1	1	1	0	1	0	10	4	2
192	1	1	1	1	0	0	1	1	1	1	1	1	0	0	10	4	2
193	1	1	1	1	0	1	0	0	1	0	1	1	1	1	10	2	4
194	1	1	1	1	0	1	0	0	1	1	0	1	1	1	10	3	3
195	1	1	1	1	0	1	0	0	1	1	1	0	1	1	10	3	3
196	1	1	1	1	0	1	0	0	1	1	1	1	0	1	10	3	3
197	1	1	1	1	0	1	0	0	1	1	1	1	1	0	10	3	3
198	1	1	1	1	0	1	0	1	0	1	1	0	1	1	10	3	3
199	1	1	1	1	0	1	0	1	1	0	0	1	1	1	10	3	3
200	1	1	1	1	0	1	0	1	1	0	1	0	1	1	10	3	3
201	1	1	1	1	0	1	0	1	1	0	1	1	0	1	10	3	3
202	1	1	1	1	0	1	0	1	1	0	1	1	1	0	10	3	3
203	1	1	1	1	0	1	0	1	1	1	0	0	1	1	10	4	2
204	1	1	1	1	0	1	0	1	1	1	0	1	0	1	10	4	2
205	1	1	1	1	0	1	0	1	1	1	0	1	1	0	10	4	2
206	1	1	1	1	0	1	0	1	1	1	1	0	0	1	10	4	2
207	1	1	1	1	0	1	0	1	1	1	1	0	1	0	10	4	2
208	1	1	1	1	0	1	0	1	1	1	1	1	0	0	10	4	2
209	1	1	1	1	0	1	1	0	0	1	0	1	1	1	10	3	3
210	1	1	1	1	0	1	1	0	0	1	1	0	1	1	10	3	3
211	1	1	1	1	0	1	1	0	0	1	1	1	0	1	10	3	3
212	1	1	1	1	0	1	1	0	0	1	1	1	1	0	10	3	3
213	1	1	1	1	0	1	1	0	1	0	0	1	1	1	10	3	3
214	1	1	1	1	0	1	1	0	1	0	1	0	1	1	10	3	3
215	1	1	1	1	0	1	1	0	1	0	1	1	0	1	10	3	3
216	1	1	1	1	0	1	1	0	1	0	1	1	1	0	10	3	3
217	1	1	1	1	0	1	1	0	1	1	0	0	1	1	10	4	2
218	1	1	1	1	0	1	1	0	1	1	0	1	0	1	10	4	2
219	1	1	1	1	0	1	1	0	1	1	0	1	1	0	10	4	2
220	1	1	1	1	0	1	1	0	1	1	1	0	0	1	10	4	2
221	1	1	1	1	0	1	1	0	1	1	1	0	1	0	10	4	2
222	1	1	1	1	0	1	1	0	1	1	1	1	0	0	10	4	2
223	1	1	1	1	0	1	1	1	0	0	0	1	1	1	10	3	3
224	1	1	1	1	0	1	1	1	0	0	1	0	1	1	10	3	3
225	1	1	1	1	0	1	1	1	0	0	1	1	0	1	10	3	3
226	1	1	1	1	0	1	1	1	0	0	1	1	1	0	10	3	3
227	1	1	1	1	0	1	1	1	0	1	0	0	1	1	10	4	2
228	1	1	1	1	0	1	1	1	0	1	0	1	0	1	10	4	2
229	1	1	1	1	0	1	1	1	0	1	0	1	1	0	10	4	2

Table 9 (Continued)

model	Terms in model															p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$				
230	1	1	1	1	0	1	1	1	0	1	1	0	0	1	10	4	2	
231	1	1	1	1	0	1	1	1	0	1	1	0	1	0	10	4	2	
232	1	1	1	1	0	1	1	1	0	1	1	1	0	0	10	4	2	
233	1	1	1	1	0	1	1	1	1	0	0	0	1	1	10	4	2	
234	1	1	1	1	0	1	1	1	1	0	0	1	0	1	10	4	2	
235	1	1	1	1	0	1	1	1	1	0	0	1	1	0	10	4	2	
236	1	1	1	1	0	1	1	1	1	0	1	0	0	1	10	4	2	
237	1	1	1	1	0	1	1	1	1	0	1	0	1	0	10	4	2	
238	1	1	1	1	0	1	1	1	1	0	1	1	0	0	10	4	2	
239	1	1	1	1	0	1	1	1	1	1	0	0	0	1	10	5	1	
240	1	1	1	1	0	1	1	1	1	1	0	0	1	0	10	5	1	
241	1	1	1	1	0	1	1	1	1	1	0	1	0	0	10	5	1	
242	1	1	1	1	0	1	1	1	1	1	1	0	0	0	10	5	1	
243	1	1	1	1	1	0	0	0	0	1	1	1	1	1	10	2	4	
244	1	1	1	1	1	0	0	0	1	1	0	1	1	1	10	3	3	
245	1	1	1	1	1	0	0	0	1	1	1	0	1	1	10	3	3	
246	1	1	1	1	1	0	0	0	1	1	1	1	0	1	10	3	3	
247	1	1	1	1	1	0	0	0	1	1	1	1	1	0	10	3	3	
248	1	1	1	1	1	0	0	1	0	1	0	1	1	1	10	3	3	
249	1	1	1	1	1	0	0	1	0	1	1	0	1	1	10	3	3	
250	1	1	1	1	1	0	0	1	0	1	1	1	0	1	10	3	3	
251	1	1	1	1	1	0	0	1	0	1	1	1	1	0	10	3	3	
252	1	1	1	1	1	0	0	1	1	0	1	1	0	1	10	3	3	
253	1	1	1	1	1	0	0	1	1	1	0	0	1	1	10	4	2	
254	1	1	1	1	1	0	0	1	1	1	0	1	0	1	10	4	2	
255	1	1	1	1	1	0	0	1	1	1	0	1	1	0	10	4	2	
256	1	1	1	1	1	0	0	1	1	1	1	0	0	1	10	4	2	
257	1	1	1	1	1	0	0	1	1	1	1	0	1	0	10	4	2	
258	1	1	1	1	1	0	0	1	1	1	1	1	0	0	10	4	2	
259	1	1	1	1	1	0	1	0	0	1	0	1	1	1	10	3	3	
260	1	1	1	1	1	0	1	0	0	1	1	0	1	1	10	3	3	
261	1	1	1	1	1	0	1	0	0	1	1	1	0	1	10	3	3	
262	1	1	1	1	1	0	1	0	0	1	1	1	1	0	10	3	3	
263	1	1	1	1	1	0	1	0	1	0	0	1	1	1	10	3	3	
264	1	1	1	1	1	0	1	0	1	0	1	0	1	1	10	3	3	
265	1	1	1	1	1	0	1	0	1	0	1	1	0	1	10	3	3	
266	1	1	1	1	1	0	1	0	1	0	1	1	1	0	10	3	3	
267	1	1	1	1	1	0	1	0	1	1	0	0	1	1	10	4	2	
268	1	1	1	1	1	0	1	0	1	1	0	1	0	1	10	4	2	
269	1	1	1	1	1	0	1	0	1	1	0	1	1	0	10	4	2	
270	1	1	1	1	1	0	1	0	1	1	1	0	0	1	10	4	2	
271	1	1	1	1	1	0	1	0	1	1	1	0	1	0	10	4	2	

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
272	1	1	1	1	1	0	1	0	1	1	1	1	0	0	10	4	2
273	1	1	1	1	1	0	1	1	0	0	0	1	1	1	10	3	3
274	1	1	1	1	1	0	1	1	0	0	1	0	1	1	10	3	3
275	1	1	1	1	1	0	1	1	0	0	1	1	0	1	10	3	3
276	1	1	1	1	1	0	1	1	0	0	1	1	1	0	10	3	3
277	1	1	1	1	1	0	1	1	0	1	0	0	1	1	10	4	2
278	1	1	1	1	1	0	1	1	0	1	0	1	0	1	10	4	2
279	1	1	1	1	1	0	1	1	0	1	0	1	1	0	10	4	2
280	1	1	1	1	1	0	1	1	0	1	1	0	0	1	10	4	2
281	1	1	1	1	1	0	1	1	0	1	1	0	1	0	10	4	2
282	1	1	1	1	1	0	1	1	0	1	1	1	0	0	10	4	2
283	1	1	1	1	1	0	1	1	1	0	0	0	1	1	10	4	2
284	1	1	1	1	1	0	1	1	1	0	0	1	0	1	10	4	2
285	1	1	1	1	1	0	1	1	1	0	0	1	1	0	10	4	2
286	1	1	1	1	1	0	1	1	1	0	1	0	0	1	10	4	2
287	1	1	1	1	1	0	1	1	1	0	1	0	1	0	10	4	2
288	1	1	1	1	1	0	1	1	1	0	1	1	0	0	10	4	2
289	1	1	1	1	1	0	1	1	1	1	0	0	0	1	10	5	1
290	1	1	1	1	1	0	1	1	1	1	0	0	1	0	10	5	1
291	1	1	1	1	1	0	1	1	1	1	0	1	0	0	10	5	1
292	1	1	1	1	1	0	1	1	1	1	1	0	0	0	10	5	1
293	1	1	1	1	1	1	0	0	0	1	0	1	1	1	10	3	3
294	1	1	1	1	1	1	0	0	0	1	1	0	1	1	10	3	3
295	1	1	1	1	1	1	0	0	0	1	1	1	0	1	10	3	3
296	1	1	1	1	1	1	0	0	0	1	1	1	1	0	10	3	3
297	1	1	1	1	1	1	0	0	1	0	0	1	1	1	10	3	3
298	1	1	1	1	1	1	0	0	1	0	1	0	1	1	10	3	3
299	1	1	1	1	1	1	0	0	1	0	1	1	0	1	10	3	3
300	1	1	1	1	1	1	0	0	1	0	1	1	1	0	10	3	3
301	1	1	1	1	1	1	0	0	1	1	0	0	1	1	10	4	2
302	1	1	1	1	1	1	0	0	1	1	0	1	0	1	10	4	2
303	1	1	1	1	1	1	0	0	1	1	0	1	1	0	10	4	2
304	1	1	1	1	1	1	0	0	1	1	1	0	0	1	10	4	2
305	1	1	1	1	1	1	0	0	1	1	1	0	1	0	10	4	2
306	1	1	1	1	1	1	0	0	1	1	1	1	0	0	10	4	2
307	1	1	1	1	1	1	0	1	0	0	0	1	1	1	10	3	3
308	1	1	1	1	1	1	0	1	0	0	1	0	1	1	10	3	3
309	1	1	1	1	1	1	0	1	0	0	1	1	0	1	10	3	3
310	1	1	1	1	1	1	0	1	0	0	1	1	1	0	10	3	3
311	1	1	1	1	1	1	0	1	0	1	0	0	1	1	10	4	2
312	1	1	1	1	1	1	0	1	0	1	0	1	0	1	10	4	2
313	1	1	1	1	1	1	0	1	0	1	0	1	1	0	10	4	2

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
314	1	1	1	1	1	1	0	1	0	1	1	0	0	1	10	4	2
315	1	1	1	1	1	1	0	1	0	1	1	0	1	0	10	4	2
316	1	1	1	1	1	1	0	1	0	1	1	1	0	0	10	4	2
317	1	1	1	1	1	1	0	1	1	0	0	0	1	1	10	4	2
318	1	1	1	1	1	1	0	1	1	0	0	1	0	1	10	4	2
319	1	1	1	1	1	1	0	1	1	0	0	1	1	0	10	4	2
320	1	1	1	1	1	1	0	1	1	0	1	0	0	1	10	4	2
321	1	1	1	1	1	1	0	1	1	0	1	0	1	0	10	4	2
322	1	1	1	1	1	1	0	1	1	0	1	1	0	0	10	4	2
323	1	1	1	1	1	1	0	1	1	1	0	0	0	1	10	5	1
324	1	1	1	1	1	1	0	1	1	1	0	0	1	0	10	5	1
325	1	1	1	1	1	1	0	1	1	1	0	1	0	0	10	5	1
326	1	1	1	1	1	1	0	1	1	1	1	0	0	0	10	5	1
327	1	1	1	1	1	1	1	0	0	0	1	1	1	0	10	3	3
328	1	1	1	1	1	1	1	0	0	1	0	0	1	1	10	4	2
329	1	1	1	1	1	1	1	0	0	1	0	1	0	1	10	4	2
330	1	1	1	1	1	1	1	0	0	1	0	1	1	0	10	4	2
331	1	1	1	1	1	1	1	0	0	1	1	0	0	1	10	4	2
332	1	1	1	1	1	1	1	0	0	1	1	0	1	0	10	4	2
333	1	1	1	1	1	1	1	0	0	1	1	1	0	0	10	4	2
334	1	1	1	1	1	1	1	0	1	0	0	0	1	1	10	4	2
335	1	1	1	1	1	1	1	0	1	0	0	1	0	1	10	4	2
336	1	1	1	1	1	1	1	0	1	0	0	1	1	0	10	4	2
337	1	1	1	1	1	1	1	0	1	0	1	0	0	1	10	4	2
338	1	1	1	1	1	1	1	0	1	0	1	0	1	0	10	4	2
339	1	1	1	1	1	1	1	0	1	0	1	1	0	0	10	4	2
340	1	1	1	1	1	1	1	0	1	1	0	0	0	1	10	5	1
341	1	1	1	1	1	1	1	0	1	1	0	0	1	0	10	5	1
342	1	1	1	1	1	1	1	0	1	1	0	1	0	0	10	5	1
343	1	1	1	1	1	1	1	0	1	1	1	0	0	0	10	5	1
344	1	1	1	1	1	1	1	1	0	0	0	0	1	1	10	4	2
345	1	1	1	1	1	1	1	1	0	0	0	1	0	1	10	4	2
346	1	1	1	1	1	1	1	1	0	0	0	1	1	0	10	4	2
347	1	1	1	1	1	1	1	1	0	0	1	0	0	1	10	4	2
348	1	1	1	1	1	1	1	1	0	0	1	0	1	0	10	4	2
349	1	1	1	1	1	1	1	1	0	0	1	1	0	0	10	4	2
350	1	1	1	1	1	1	1	1	0	1	0	0	0	1	10	5	1
351	1	1	1	1	1	1	1	1	0	1	0	0	1	0	10	5	1
352	1	1	1	1	1	1	1	1	0	1	0	1	0	0	10	5	1
353	1	1	1	1	1	1	1	1	0	1	1	0	0	0	10	5	1
354	1	1	1	1	1	1	1	1	1	0	0	0	0	1	10	5	1
355	1	1	1	1	1	1	1	1	1	0	0	0	1	0	10	5	1

Table 9 (Continued)

model	Terms in model															p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$				
356	1	1	1	1	1	1	1	1	1	0	0	1	0	0	10	5	1	
357	1	1	1	1	1	1	1	1	1	0	1	0	0	0	10	5	1	
358	1	1	1	1	1	1	1	1	1	1	0	0	0	0	10	6	0	
359	1	1	1	1	0	0	0	0	1	1	0	1	1	1	9	2	3	
360	1	1	1	1	0	0	0	1	0	1	1	0	1	1	9	2	3	
361	1	1	1	1	0	0	0	1	1	0	1	1	0	1	9	2	3	
362	1	1	1	1	0	0	0	1	1	1	0	0	1	1	9	3	2	
363	1	1	1	1	0	0	0	1	1	1	0	1	0	1	9	3	2	
364	1	1	1	1	0	0	0	1	1	1	0	1	1	0	9	3	2	
365	1	1	1	1	0	0	0	1	1	1	1	0	0	1	9	3	2	
366	1	1	1	1	0	0	0	1	1	1	1	0	1	0	9	3	2	
367	1	1	1	1	0	0	0	1	1	1	1	1	0	0	9	3	2	
368	1	1	1	1	0	0	1	0	0	1	0	1	1	1	9	2	3	
369	1	1	1	1	0	0	1	0	1	0	0	1	1	1	9	2	3	
370	1	1	1	1	0	0	1	0	1	1	0	0	1	1	9	3	2	
371	1	1	1	1	0	0	1	0	1	1	0	1	0	1	9	3	2	
372	1	1	1	1	0	0	1	0	1	1	0	1	1	0	9	3	2	
373	1	1	1	1	0	0	1	1	0	0	0	1	1	1	9	2	3	
374	1	1	1	1	0	0	1	1	0	0	1	0	1	1	9	2	3	
375	1	1	1	1	0	0	1	1	0	0	1	1	0	1	9	2	3	
376	1	1	1	1	0	0	1	1	0	0	1	1	1	0	9	2	3	
377	1	1	1	1	0	0	1	1	0	1	0	0	1	1	9	3	2	
378	1	1	1	1	0	0	1	1	0	1	0	1	0	1	9	3	2	
379	1	1	1	1	0	0	1	1	0	1	0	1	1	0	9	3	2	
380	1	1	1	1	0	0	1	1	0	1	1	0	0	1	9	3	2	
381	1	1	1	1	0	0	1	1	0	1	1	0	1	0	9	3	2	
382	1	1	1	1	0	0	1	1	0	1	1	1	0	0	9	3	2	
383	1	1	1	1	0	0	1	1	1	0	0	0	1	1	9	3	2	
384	1	1	1	1	0	0	1	1	1	0	0	1	0	1	9	3	2	
385	1	1	1	1	0	0	1	1	1	0	0	1	1	0	9	3	2	
386	1	1	1	1	0	0	1	1	1	0	1	0	0	1	9	3	2	
387	1	1	1	1	0	0	1	1	1	0	1	0	1	0	9	3	2	
388	1	1	1	1	0	0	1	1	1	0	1	1	0	0	9	3	2	
389	1	1	1	1	0	0	1	1	1	1	0	0	0	1	9	4	1	
390	1	1	1	1	0	0	1	1	1	1	0	0	1	0	9	4	1	
391	1	1	1	1	0	0	1	1	1	1	0	1	0	0	9	4	1	
392	1	1	1	1	0	0	1	1	1	1	1	0	0	0	9	4	1	
393	1	1	1	1	0	1	0	0	0	1	1	0	1	1	9	2	3	
394	1	1	1	1	0	1	0	0	1	0	0	1	1	1	9	2	3	
395	1	1	1	1	0	1	0	0	1	0	1	0	1	1	9	2	3	
396	1	1	1	1	0	1	0	0	1	0	1	1	0	1	9	2	3	
397	1	1	1	1	0	1	0	0	1	0	1	1	1	0	9	2	3	

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
398	1	1	1	1	0	1	0	0	1	1	0	0	1	1	9	3	2
399	1	1	1	1	0	1	0	0	1	1	0	1	0	1	9	3	2
400	1	1	1	1	0	1	0	0	1	1	0	1	1	0	9	3	2
401	1	1	1	1	0	1	0	0	1	1	1	0	0	1	9	3	2
402	1	1	1	1	0	1	0	0	1	1	1	0	1	0	9	3	2
403	1	1	1	1	0	1	0	0	1	1	1	1	0	0	9	3	2
404	1	1	1	1	0	1	0	1	0	0	1	0	1	1	9	2	3
405	1	1	1	1	0	1	0	1	0	1	0	0	1	1	9	3	2
406	1	1	1	1	0	1	0	1	0	1	1	0	0	1	9	3	2
407	1	1	1	1	0	1	0	1	0	1	1	0	1	0	9	3	2
408	1	1	1	1	0	1	0	1	1	0	0	0	1	1	9	3	2
409	1	1	1	1	0	1	0	1	1	0	0	1	0	1	9	3	2
410	1	1	1	1	0	1	0	1	1	0	0	1	1	0	9	3	2
411	1	1	1	1	0	1	0	1	1	0	1	0	0	1	9	3	2
412	1	1	1	1	0	1	0	1	1	0	1	0	1	0	9	3	2
413	1	1	1	1	0	1	0	1	1	0	1	1	0	0	9	3	2
414	1	1	1	1	0	1	0	1	1	1	0	0	0	1	9	4	1
415	1	1	1	1	0	1	0	1	1	1	0	0	1	0	9	4	1
416	1	1	1	1	0	1	0	1	1	1	0	1	0	0	9	4	1
417	1	1	1	1	0	1	0	1	1	1	1	0	0	0	9	4	1
418	1	1	1	1	0	1	1	0	0	0	1	1	1	0	9	2	3
419	1	1	1	1	0	1	1	0	0	1	0	0	1	1	9	3	2
420	1	1	1	1	0	1	1	0	0	1	0	1	0	1	9	3	2
421	1	1	1	1	0	1	1	0	0	1	0	1	1	0	9	3	2
422	1	1	1	1	0	1	1	0	0	1	1	0	0	1	9	3	2
423	1	1	1	1	0	1	1	0	0	1	1	0	1	0	9	3	2
424	1	1	1	1	0	1	1	0	0	1	1	1	0	0	9	3	2
425	1	1	1	1	0	1	1	0	1	0	0	0	1	1	9	3	2
426	1	1	1	1	0	1	1	0	1	0	0	1	0	1	9	3	2
427	1	1	1	1	0	1	1	0	1	0	0	1	1	0	9	3	2
428	1	1	1	1	0	1	1	0	1	0	1	0	0	1	9	3	2
429	1	1	1	1	0	1	1	0	1	0	1	0	1	0	9	3	2
430	1	1	1	1	0	1	1	0	1	0	1	1	0	0	9	3	2
431	1	1	1	1	0	1	1	0	1	1	0	0	0	1	9	4	1
432	1	1	1	1	0	1	1	0	1	1	0	0	1	0	9	4	1
433	1	1	1	1	0	1	1	0	1	1	0	1	0	0	9	4	1
434	1	1	1	1	0	1	1	0	1	1	1	0	0	0	9	4	1
435	1	1	1	1	0	1	1	1	0	0	0	0	1	1	9	3	2
436	1	1	1	1	0	1	1	1	0	0	0	1	0	1	9	3	2
437	1	1	1	1	0	1	1	1	0	0	0	1	1	0	9	3	2
438	1	1	1	1	0	1	1	1	0	0	1	0	0	1	9	3	2
439	1	1	1	1	0	1	1	1	0	0	1	0	1	0	9	3	2

Table 9 (Continued)

model	Terms in model															p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$				
440	1	1	1	1	0	1	1	1	0	0	1	1	0	0	9	3	2	
441	1	1	1	1	0	1	1	1	0	1	0	0	0	1	9	4	1	
442	1	1	1	1	0	1	1	1	0	1	0	0	1	0	9	4	1	
443	1	1	1	1	0	1	1	1	0	1	0	1	0	0	9	4	1	
444	1	1	1	1	0	1	1	1	0	1	1	0	0	0	9	4	1	
445	1	1	1	1	0	1	1	1	1	0	0	0	0	1	9	4	1	
446	1	1	1	1	0	1	1	1	1	0	0	0	1	0	9	4	1	
447	1	1	1	1	0	1	1	1	1	0	0	1	0	0	9	4	1	
448	1	1	1	1	0	1	1	1	1	0	1	0	0	0	9	4	1	
449	1	1	1	1	0	1	1	1	1	1	0	0	0	0	9	5	0	
450	1	1	1	1	1	0	0	0	0	1	0	1	1	1	9	2	3	
451	1	1	1	1	1	0	0	0	0	1	1	0	1	1	9	2	3	
452	1	1	1	1	1	0	0	0	0	1	1	1	0	1	9	2	3	
453	1	1	1	1	1	0	0	0	0	1	1	1	1	0	9	2	3	
454	1	1	1	1	1	0	0	0	1	0	1	1	0	1	9	2	3	
455	1	1	1	1	1	0	0	0	1	1	0	0	1	1	9	3	2	
456	1	1	1	1	1	0	0	0	1	1	0	1	0	1	9	3	2	
457	1	1	1	1	1	0	0	0	1	1	0	1	1	0	9	3	2	
458	1	1	1	1	1	0	0	0	1	1	1	0	0	1	9	3	2	
459	1	1	1	1	1	0	0	0	1	1	1	0	1	0	9	3	2	
460	1	1	1	1	1	0	0	0	1	1	1	1	0	0	9	3	2	
461	1	1	1	1	1	0	0	1	0	0	1	1	0	1	9	2	3	
462	1	1	1	1	1	0	0	1	0	1	0	0	1	1	9	3	2	
463	1	1	1	1	1	0	0	1	0	1	0	1	0	1	9	3	2	
464	1	1	1	1	1	0	0	1	0	1	0	1	1	0	9	3	2	
465	1	1	1	1	1	0	0	1	0	1	1	0	0	1	9	3	2	
466	1	1	1	1	1	0	0	1	0	1	1	0	1	0	9	3	2	
467	1	1	1	1	1	0	0	1	0	1	1	1	0	0	9	3	2	
468	1	1	1	1	1	0	0	1	1	0	0	1	0	1	9	3	2	
469	1	1	1	1	1	0	0	1	1	0	1	0	0	1	9	3	2	
470	1	1	1	1	1	0	0	1	1	0	1	1	0	0	9	3	2	
471	1	1	1	1	1	0	0	1	1	1	0	0	0	1	9	4	1	
472	1	1	1	1	1	0	0	1	1	1	0	0	1	0	9	4	1	
473	1	1	1	1	1	0	0	1	1	1	0	1	0	0	9	4	1	
474	1	1	1	1	1	0	0	1	1	1	1	0	0	0	9	4	1	
475	1	1	1	1	1	0	1	0	0	0	1	1	1	0	9	2	3	
476	1	1	1	1	1	0	1	0	0	1	0	0	1	1	9	3	2	
477	1	1	1	1	1	0	1	0	0	1	0	1	0	1	9	3	2	
478	1	1	1	1	1	0	1	0	0	1	0	1	1	0	9	3	2	
479	1	1	1	1	1	0	1	0	0	1	1	0	0	1	9	3	2	
480	1	1	1	1	1	0	1	0	0	1	1	0	1	0	9	3	2	
481	1	1	1	1	1	0	1	0	0	1	1	1	0	0	9	3	2	

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
482	1	1	1	1	1	0	1	0	1	0	0	0	1	1	9	3	2
483	1	1	1	1	1	0	1	0	1	0	0	1	0	1	9	3	2
484	1	1	1	1	1	0	1	0	1	0	0	1	1	0	9	3	2
485	1	1	1	1	1	0	1	0	1	0	1	0	0	1	9	3	2
486	1	1	1	1	1	0	1	0	1	0	1	0	1	0	9	3	2
487	1	1	1	1	1	0	1	0	1	0	1	1	0	0	9	3	2
488	1	1	1	1	1	0	1	0	1	1	0	0	0	1	9	4	1
489	1	1	1	1	1	0	1	0	1	1	0	0	1	0	9	4	1
490	1	1	1	1	1	0	1	0	1	1	0	1	0	0	9	4	1
491	1	1	1	1	1	0	1	0	1	1	1	0	0	0	9	4	1
492	1	1	1	1	1	0	1	1	0	0	0	0	1	1	9	3	2
493	1	1	1	1	1	0	1	1	0	0	0	1	0	1	9	3	2
494	1	1	1	1	1	0	1	1	0	0	0	1	1	0	9	3	2
495	1	1	1	1	1	0	1	1	0	0	1	0	0	1	9	3	2
496	1	1	1	1	1	0	1	1	0	0	1	0	1	0	9	3	2
497	1	1	1	1	1	0	1	1	0	0	1	1	0	0	9	3	2
498	1	1	1	1	1	0	1	1	0	1	0	0	0	1	9	4	1
499	1	1	1	1	1	0	1	1	0	1	0	0	1	0	9	4	1
500	1	1	1	1	1	0	1	1	0	1	0	1	0	0	9	4	1
501	1	1	1	1	1	0	1	1	0	1	1	0	0	0	9	4	1
502	1	1	1	1	1	0	1	1	1	0	0	0	0	1	9	4	1
503	1	1	1	1	1	0	1	1	1	0	0	0	1	0	9	4	1
504	1	1	1	1	1	0	1	1	1	0	0	1	0	0	9	4	1
505	1	1	1	1	1	0	1	1	1	0	1	0	0	0	9	4	1
506	1	1	1	1	1	0	1	1	1	1	0	0	0	0	9	5	0
507	1	1	1	1	1	1	0	0	0	0	1	1	1	0	9	2	3
508	1	1	1	1	1	1	0	0	0	1	0	0	1	1	9	3	2
509	1	1	1	1	1	1	0	0	0	1	0	1	0	1	9	3	2
510	1	1	1	1	1	1	0	0	0	1	0	1	1	0	9	3	2
511	1	1	1	1	1	1	0	0	0	1	1	0	0	1	9	3	2
512	1	1	1	1	1	1	0	0	0	1	1	0	1	0	9	3	2
513	1	1	1	1	1	1	0	0	0	1	1	1	0	0	9	3	2
514	1	1	1	1	1	1	0	0	1	0	0	0	1	1	9	3	2
515	1	1	1	1	1	1	0	0	1	0	0	1	0	1	9	3	2
516	1	1	1	1	1	1	0	0	1	0	0	1	1	0	9	3	2
517	1	1	1	1	1	1	0	0	1	0	1	0	0	1	9	3	2
518	1	1	1	1	1	1	0	0	1	0	1	0	1	0	9	3	2
519	1	1	1	1	1	1	0	0	1	0	1	1	0	0	9	3	2
520	1	1	1	1	1	1	0	0	1	1	0	0	0	1	9	4	1
521	1	1	1	1	1	1	0	0	1	1	0	0	1	0	9	4	1
522	1	1	1	1	1	1	0	0	1	1	0	1	0	0	9	4	1
523	1	1	1	1	1	1	0	0	1	1	1	0	0	0	9	4	1

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
524	1	1	1	1	1	1	0	1	0	0	0	0	1	1	9	3	2
525	1	1	1	1	1	1	0	1	0	0	0	1	0	1	9	3	2
526	1	1	1	1	1	1	0	1	0	0	0	1	1	0	9	3	2
527	1	1	1	1	1	1	0	1	0	0	1	0	0	1	9	3	2
528	1	1	1	1	1	1	0	1	0	0	1	0	1	0	9	3	2
529	1	1	1	1	1	1	0	1	0	0	1	1	0	0	9	3	2
530	1	1	1	1	1	1	0	1	0	1	0	0	0	1	9	4	1
531	1	1	1	1	1	1	0	1	0	1	0	0	1	0	9	4	1
532	1	1	1	1	1	1	0	1	0	1	0	1	0	0	9	4	1
533	1	1	1	1	1	1	0	1	0	1	1	0	0	0	9	4	1
534	1	1	1	1	1	1	0	1	1	0	0	0	0	1	9	4	1
535	1	1	1	1	1	1	0	1	1	0	0	0	1	0	9	4	1
536	1	1	1	1	1	1	0	1	1	0	0	1	0	0	9	4	1
537	1	1	1	1	1	1	0	1	1	0	1	0	0	0	9	4	1
538	1	1	1	1	1	1	0	1	1	1	0	0	0	0	9	5	0
539	1	1	1	1	1	1	1	0	0	0	0	1	1	0	9	3	2
540	1	1	1	1	1	1	1	0	0	0	1	0	1	0	9	3	2
541	1	1	1	1	1	1	1	0	0	0	1	1	0	0	9	3	2
542	1	1	1	1	1	1	1	0	0	1	0	0	0	1	9	4	1
543	1	1	1	1	1	1	1	0	0	1	0	0	1	0	9	4	1
544	1	1	1	1	1	1	1	0	0	1	0	1	0	0	9	4	1
545	1	1	1	1	1	1	1	0	0	1	1	0	0	0	9	4	1
546	1	1	1	1	1	1	1	0	1	0	0	0	0	1	9	4	1
547	1	1	1	1	1	1	1	0	1	0	0	0	1	0	9	4	1
548	1	1	1	1	1	1	1	0	1	0	0	1	0	0	9	4	1
549	1	1	1	1	1	1	1	0	1	0	1	0	0	0	9	4	1
550	1	1	1	1	1	1	1	0	1	1	0	0	0	0	9	5	0
551	1	1	1	1	1	1	1	1	0	0	0	0	0	1	9	4	1
552	1	1	1	1	1	1	1	1	0	0	0	0	1	0	9	4	1
553	1	1	1	1	1	1	1	1	0	0	0	1	0	0	9	4	1
554	1	1	1	1	1	1	1	1	0	0	1	0	0	0	9	4	1
555	1	1	1	1	1	1	1	1	0	1	0	0	0	0	9	5	0
556	1	1	1	1	1	1	1	1	1	0	0	0	0	0	9	5	0
557	1	1	1	1	0	0	0	0	1	1	0	0	1	1	8	2	2
558	1	1	1	1	0	0	0	0	1	1	0	1	0	1	8	2	2
559	1	1	1	1	0	0	0	0	1	1	0	1	1	0	8	2	2
560	1	1	1	1	0	0	0	1	0	1	0	0	1	1	8	2	2
561	1	1	1	1	0	0	0	1	0	1	1	0	0	1	8	2	2
562	1	1	1	1	0	0	0	1	0	1	1	0	1	0	8	2	2
563	1	1	1	1	0	0	0	1	1	0	0	1	0	1	8	2	2
564	1	1	1	1	0	0	0	1	1	0	1	0	0	1	8	2	2
565	1	1	1	1	0	0	0	1	1	0	1	1	0	0	8	2	2

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
566	1	1	1	1	0	0	0	1	1	1	0	0	0	1	8	3	1
567	1	1	1	1	0	0	0	1	1	1	0	0	1	0	8	3	1
568	1	1	1	1	0	0	0	1	1	1	0	1	0	0	8	3	1
569	1	1	1	1	0	0	0	1	1	1	1	0	0	0	8	3	1
570	1	1	1	1	0	0	1	0	0	1	0	0	1	1	8	2	2
571	1	1	1	1	0	0	1	0	0	1	0	1	0	1	8	2	2
572	1	1	1	1	0	0	1	0	0	1	0	1	1	0	8	2	2
573	1	1	1	1	0	0	1	0	1	0	0	0	1	1	8	2	2
574	1	1	1	1	0	0	1	0	1	0	0	1	0	1	8	2	2
575	1	1	1	1	0	0	1	0	1	0	0	1	1	0	8	2	2
576	1	1	1	1	0	0	1	0	1	1	0	0	0	1	8	3	1
577	1	1	1	1	0	0	1	0	1	1	0	0	1	0	8	3	1
578	1	1	1	1	0	0	1	0	1	1	0	1	0	0	8	3	1
579	1	1	1	1	0	0	1	1	0	0	0	0	1	1	8	2	2
580	1	1	1	1	0	0	1	1	0	0	0	1	0	1	8	2	2
581	1	1	1	1	0	0	1	1	0	0	0	1	1	0	8	2	2
582	1	1	1	1	0	0	1	1	0	0	1	0	0	1	8	2	2
583	1	1	1	1	0	0	1	1	0	0	1	0	1	0	8	2	2
584	1	1	1	1	0	0	1	1	0	0	1	1	0	0	8	2	2
585	1	1	1	1	0	0	1	1	0	1	0	0	0	1	8	3	1
586	1	1	1	1	0	0	1	1	0	1	0	0	1	0	8	3	1
587	1	1	1	1	0	0	1	1	0	1	0	1	0	0	8	3	1
588	1	1	1	1	0	0	1	1	0	1	1	0	0	0	8	3	1
589	1	1	1	1	0	0	1	1	1	0	0	0	0	1	8	3	1
590	1	1	1	1	0	0	1	1	1	0	0	0	1	0	8	3	1
591	1	1	1	1	0	0	1	1	1	0	0	1	0	0	8	3	1
592	1	1	1	1	0	0	1	1	1	0	1	0	0	0	8	3	1
593	1	1	1	1	0	0	1	1	1	1	0	0	0	0	8	4	0
594	1	1	1	1	0	1	0	0	0	1	0	0	1	1	8	2	2
595	1	1	1	1	0	1	0	0	0	1	1	0	0	1	8	2	2
596	1	1	1	1	0	1	0	0	0	1	1	0	1	0	8	2	2
597	1	1	1	1	0	1	0	0	1	0	0	0	1	1	8	2	2
598	1	1	1	1	0	1	0	0	1	0	0	1	0	1	8	2	2
599	1	1	1	1	0	1	0	0	1	0	0	1	1	0	8	2	2
600	1	1	1	1	0	1	0	0	1	0	1	0	0	1	8	2	2
601	1	1	1	1	0	1	0	0	1	0	1	0	1	0	8	2	2
602	1	1	1	1	0	1	0	0	1	0	1	1	0	0	8	2	2
603	1	1	1	1	0	1	0	0	1	1	0	0	0	1	8	3	1
604	1	1	1	1	0	1	0	0	1	1	0	0	1	0	8	3	1
605	1	1	1	1	0	1	0	0	1	1	0	1	0	0	8	3	1
606	1	1	1	1	0	1	0	0	1	1	1	0	0	0	8	3	1
607	1	1	1	1	0	1	0	1	0	0	0	0	1	1	8	2	2

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
608	1	1	1	1	0	1	0	1	0	0	1	0	0	1	8	2	2
609	1	1	1	1	0	1	0	1	0	0	1	0	1	0	8	2	2
610	1	1	1	1	0	1	0	1	0	1	0	0	0	1	8	3	1
611	1	1	1	1	0	1	0	1	0	1	0	0	1	0	8	3	1
612	1	1	1	1	0	1	0	1	0	1	1	0	0	0	8	3	1
613	1	1	1	1	0	1	0	1	1	0	0	0	0	1	8	3	1
614	1	1	1	1	0	1	0	1	1	0	0	0	1	0	8	3	1
615	1	1	1	1	0	1	0	1	1	0	0	1	0	0	8	3	1
616	1	1	1	1	0	1	0	1	1	0	1	0	0	0	8	3	1
617	1	1	1	1	0	1	0	1	1	1	0	0	0	0	8	4	0
618	1	1	1	1	0	1	1	0	0	0	0	1	1	0	8	2	2
619	1	1	1	1	0	1	1	0	0	0	1	0	1	0	8	2	2
620	1	1	1	1	0	1	1	0	0	0	1	1	0	0	8	2	2
621	1	1	1	1	0	1	1	0	0	1	0	0	0	1	8	3	1
622	1	1	1	1	0	1	1	0	0	1	0	0	1	0	8	3	1
623	1	1	1	1	0	1	1	0	0	1	0	1	0	0	8	3	1
624	1	1	1	1	0	1	1	0	0	1	1	0	0	0	8	3	1
625	1	1	1	1	0	1	1	0	1	0	0	0	0	1	8	3	1
626	1	1	1	1	0	1	1	0	1	0	0	0	1	0	8	3	1
627	1	1	1	1	0	1	1	0	1	0	0	1	0	0	8	3	1
628	1	1	1	1	0	1	1	0	1	0	1	0	0	0	8	3	1
629	1	1	1	1	0	1	1	0	1	1	0	0	0	0	8	4	0
630	1	1	1	1	0	1	1	1	0	0	0	0	0	1	8	3	1
631	1	1	1	1	0	1	1	1	0	0	0	0	1	0	8	3	1
632	1	1	1	1	0	1	1	1	0	0	0	1	0	0	8	3	1
633	1	1	1	1	0	1	1	1	0	0	1	0	0	0	8	3	1
634	1	1	1	1	0	1	1	1	0	1	0	0	0	0	8	4	0
635	1	1	1	1	0	1	1	1	1	0	0	0	0	0	8	4	0
636	1	1	1	1	1	0	0	0	0	1	0	0	1	1	8	2	2
637	1	1	1	1	1	0	0	0	0	1	0	1	0	1	8	2	2
638	1	1	1	1	1	0	0	0	0	1	0	1	1	0	8	2	2
639	1	1	1	1	1	0	0	0	0	1	1	0	0	1	8	2	2
640	1	1	1	1	1	0	0	0	0	1	1	0	1	0	8	2	2
641	1	1	1	1	1	0	0	0	0	1	1	1	0	0	8	2	2
642	1	1	1	1	1	0	0	0	1	0	0	1	0	1	8	2	2
643	1	1	1	1	1	0	0	0	1	0	1	0	0	1	8	2	2
644	1	1	1	1	1	0	0	0	1	0	1	1	0	0	8	2	2
645	1	1	1	1	1	0	0	0	1	1	0	0	0	1	8	3	1
646	1	1	1	1	1	0	0	0	1	1	0	0	1	0	8	3	1
647	1	1	1	1	1	0	0	0	1	1	0	1	0	0	8	3	1
648	1	1	1	1	1	0	0	0	1	1	1	0	0	0	8	3	1
649	1	1	1	1	1	0	0	1	0	0	0	1	0	1	8	2	2

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
650	1	1	1	1	1	0	0	1	0	0	1	0	0	1	8	2	2
651	1	1	1	1	1	0	0	1	0	0	1	1	0	0	8	2	2
652	1	1	1	1	1	0	0	1	0	1	0	0	0	1	8	3	1
653	1	1	1	1	1	0	0	1	0	1	0	0	1	0	8	3	1
654	1	1	1	1	1	0	0	1	0	1	0	1	0	0	8	3	1
655	1	1	1	1	1	0	0	1	0	1	1	0	0	0	8	3	1
656	1	1	1	1	1	0	0	1	1	0	0	0	0	1	8	3	1
657	1	1	1	1	1	0	0	1	1	0	0	1	0	0	8	3	1
658	1	1	1	1	1	0	0	1	1	0	1	0	0	0	8	3	1
659	1	1	1	1	1	0	0	1	1	1	0	0	0	0	8	4	0
660	1	1	1	1	1	0	1	0	0	0	0	1	1	0	8	2	2
661	1	1	1	1	1	0	1	0	0	0	1	0	1	0	8	2	2
662	1	1	1	1	1	0	1	0	0	0	1	1	0	0	8	2	2
663	1	1	1	1	1	0	1	0	0	1	0	0	0	1	8	3	1
664	1	1	1	1	1	0	1	0	0	1	0	0	1	0	8	3	1
665	1	1	1	1	1	0	1	0	0	1	0	1	0	0	8	3	1
666	1	1	1	1	1	0	1	0	0	1	1	0	0	0	8	3	1
667	1	1	1	1	1	0	1	0	1	0	0	0	0	1	8	3	1
668	1	1	1	1	1	0	1	0	1	0	0	0	1	0	8	3	1
669	1	1	1	1	1	0	1	0	1	0	0	1	0	0	8	3	1
670	1	1	1	1	1	0	1	0	1	0	1	0	0	0	8	3	1
671	1	1	1	1	1	0	1	0	1	1	0	0	0	0	8	4	0
672	1	1	1	1	1	0	1	1	0	0	0	0	0	1	8	3	1
673	1	1	1	1	1	0	1	1	0	0	0	0	1	0	8	3	1
674	1	1	1	1	1	0	1	1	0	0	0	1	0	0	8	3	1
675	1	1	1	1	1	0	1	1	0	0	1	0	0	0	8	3	1
676	1	1	1	1	1	0	1	1	0	1	0	0	0	0	8	4	0
677	1	1	1	1	1	0	1	1	1	0	0	0	0	0	8	4	0
678	1	1	1	1	1	1	0	0	0	0	0	1	1	0	8	2	2
679	1	1	1	1	1	1	0	0	0	0	1	0	1	0	8	2	2
680	1	1	1	1	1	1	0	0	0	0	1	1	0	0	8	2	2
681	1	1	1	1	1	1	0	0	0	1	0	0	0	1	8	3	1
682	1	1	1	1	1	1	0	0	0	1	0	0	1	0	8	3	1
683	1	1	1	1	1	1	0	0	0	1	0	1	0	0	8	3	1
684	1	1	1	1	1	1	0	0	0	1	1	0	0	0	8	3	1
685	1	1	1	1	1	1	0	0	1	0	0	0	0	1	8	3	1
686	1	1	1	1	1	1	0	0	1	0	0	0	1	0	8	3	1
687	1	1	1	1	1	1	0	0	1	0	0	1	0	0	8	3	1
688	1	1	1	1	1	1	0	0	1	0	1	0	0	0	8	3	1
689	1	1	1	1	1	1	0	0	1	1	0	0	0	0	8	4	0
690	1	1	1	1	1	1	0	1	0	0	0	0	0	1	8	3	1
691	1	1	1	1	1	1	0	1	0	0	0	0	1	0	8	3	1

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
692	1	1	1	1	1	1	0	1	0	0	0	1	0	0	8	3	1
693	1	1	1	1	1	1	0	1	0	0	1	0	0	0	8	3	1
694	1	1	1	1	1	1	0	1	0	1	0	0	0	0	8	4	0
695	1	1	1	1	1	1	0	1	1	0	0	0	0	0	8	4	0
696	1	1	1	1	1	1	1	0	0	0	0	0	1	0	8	3	1
697	1	1	1	1	1	1	1	0	0	0	0	1	0	0	8	3	1
698	1	1	1	1	1	1	1	0	0	0	1	0	0	0	8	3	1
699	1	1	1	1	1	1	1	0	0	1	0	0	0	0	8	4	0
700	1	1	1	1	1	1	1	0	1	0	0	0	0	0	8	4	0
701	1	1	1	1	1	1	1	1	0	0	0	0	0	0	8	4	0
702	1	1	1	1	0	0	0	0	0	1	0	0	1	1	7	1	2
703	1	1	1	1	0	0	0	0	1	0	0	1	0	1	7	1	2
704	1	1	1	1	0	0	0	0	1	1	0	0	0	1	7	2	1
705	1	1	1	1	0	0	0	0	1	1	0	0	1	0	7	2	1
706	1	1	1	1	0	0	0	0	1	1	0	1	0	0	7	2	1
707	1	1	1	1	0	0	0	1	0	0	1	0	0	1	7	1	2
708	1	1	1	1	0	0	0	1	0	1	0	0	0	1	7	2	1
709	1	1	1	1	0	0	0	1	0	1	0	0	1	0	7	2	1
710	1	1	1	1	0	0	0	1	0	1	1	0	0	0	7	2	1
711	1	1	1	1	0	0	0	1	1	0	0	0	0	1	7	2	1
712	1	1	1	1	0	0	0	1	1	0	0	1	0	0	7	2	1
713	1	1	1	1	0	0	0	1	1	0	1	0	0	0	7	2	1
714	1	1	1	1	0	0	0	1	1	1	0	0	0	0	7	3	0
715	1	1	1	1	0	0	1	0	0	0	0	1	1	0	7	1	2
716	1	1	1	1	0	0	1	0	0	1	0	0	0	1	7	2	1
717	1	1	1	1	0	0	1	0	0	1	0	0	1	0	7	2	1
718	1	1	1	1	0	0	1	0	0	1	0	1	0	0	7	2	1
719	1	1	1	1	0	0	1	0	1	0	0	0	0	1	7	2	1
720	1	1	1	1	0	0	1	0	1	0	0	0	1	0	7	2	1
721	1	1	1	1	0	0	1	0	1	0	0	1	0	0	7	2	1
722	1	1	1	1	0	0	1	0	1	1	0	0	0	0	7	3	0
723	1	1	1	1	0	0	1	1	0	0	0	0	0	1	7	2	1
724	1	1	1	1	0	0	1	1	0	0	0	0	1	0	7	2	1
725	1	1	1	1	0	0	1	1	0	0	0	1	0	0	7	2	1
726	1	1	1	1	0	0	1	1	0	0	1	0	0	0	7	2	1
727	1	1	1	1	0	0	1	1	0	1	0	0	0	0	7	3	0
728	1	1	1	1	0	0	1	1	1	0	0	0	0	0	7	3	0
729	1	1	1	1	0	1	0	0	0	0	1	0	1	0	7	1	2
730	1	1	1	1	0	1	0	0	0	1	0	0	0	1	7	2	1
731	1	1	1	1	0	1	0	0	0	1	0	0	1	0	7	2	1
732	1	1	1	1	0	1	0	0	0	1	1	0	0	0	7	2	1
733	1	1	1	1	0	1	0	0	1	0	0	0	0	1	7	2	1

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
734	1	1	1	1	0	1	0	0	1	0	0	0	1	0	7	2	1
735	1	1	1	1	0	1	0	0	1	0	0	1	0	0	7	2	1
736	1	1	1	1	0	1	0	0	1	0	1	0	0	0	7	2	1
737	1	1	1	1	0	1	0	0	1	1	0	0	0	0	7	3	0
738	1	1	1	1	0	1	0	1	0	0	0	0	0	1	7	2	1
739	1	1	1	1	0	1	0	1	0	0	0	0	1	0	7	2	1
740	1	1	1	1	0	1	0	1	0	0	1	0	0	0	7	2	1
741	1	1	1	1	0	1	0	1	0	1	0	0	0	0	7	3	0
742	1	1	1	1	0	1	0	1	1	0	0	0	0	0	7	3	0
743	1	1	1	1	0	1	1	0	0	0	0	0	1	0	7	2	1
744	1	1	1	1	0	1	1	0	0	0	0	1	0	0	7	2	1
745	1	1	1	1	0	1	1	0	0	0	1	0	0	0	7	2	1
746	1	1	1	1	0	1	1	0	0	1	0	0	0	0	7	3	0
747	1	1	1	1	0	1	1	0	1	0	0	0	0	0	7	3	0
748	1	1	1	1	0	1	1	1	0	0	0	0	0	0	7	3	0
749	1	1	1	1	1	0	0	0	0	0	1	1	0	0	7	1	2
750	1	1	1	1	1	0	0	0	0	1	0	0	0	1	7	2	1
751	1	1	1	1	1	0	0	0	0	1	0	0	1	0	7	2	1
752	1	1	1	1	1	0	0	0	0	1	0	1	0	0	7	2	1
753	1	1	1	1	1	0	0	0	0	1	1	0	0	0	7	2	1
754	1	1	1	1	1	0	0	0	1	0	0	0	0	1	7	2	1
755	1	1	1	1	1	0	0	0	1	0	0	1	0	0	7	2	1
756	1	1	1	1	1	0	0	0	1	0	1	0	0	0	7	2	1
757	1	1	1	1	1	0	0	0	1	1	0	0	0	0	7	3	0
758	1	1	1	1	1	0	0	1	0	0	0	0	0	1	7	2	1
759	1	1	1	1	1	0	0	1	0	0	0	1	0	0	7	2	1
760	1	1	1	1	1	0	0	1	0	0	1	0	0	0	7	2	1
761	1	1	1	1	1	0	0	1	0	1	0	0	0	0	7	3	0
762	1	1	1	1	1	0	0	1	1	0	0	0	0	0	7	3	0
763	1	1	1	1	1	0	1	0	0	0	0	0	1	0	7	2	1
764	1	1	1	1	1	0	1	0	0	0	0	1	0	0	7	2	1
765	1	1	1	1	1	0	1	0	0	0	1	0	0	0	7	2	1
766	1	1	1	1	1	0	1	0	0	1	0	0	0	0	7	3	0
767	1	1	1	1	1	0	1	0	1	0	0	0	0	0	7	3	0
768	1	1	1	1	1	0	1	1	0	0	0	0	0	0	7	3	0
769	1	1	1	1	1	1	0	0	0	0	0	0	1	0	7	2	1
770	1	1	1	1	1	1	0	0	0	0	0	1	0	0	7	2	1
771	1	1	1	1	1	1	0	0	0	0	1	0	0	0	7	2	1
772	1	1	1	1	1	1	0	0	0	1	0	0	0	0	7	3	0
773	1	1	1	1	1	1	0	0	1	0	0	0	0	0	7	3	0
774	1	1	1	1	1	1	0	1	0	0	0	0	0	0	7	3	0
775	1	1	1	1	1	1	1	0	0	0	0	0	0	0	7	3	0

Table 9 (Continued)

model	Terms in model														p	cp	cb
	x_1	x_2	x_3	x_4	x_1x_2	x_1x_3	x_1x_4	x_2x_3	x_2x_4	x_3x_4	$x_1x_2x_3$	$x_1x_2x_4$	$x_1x_3x_4$	$x_2x_3x_4$			
776	1	1	1	1	0	0	0	0	0	1	0	0	0	1	6	1	1
777	1	1	1	1	0	0	0	0	0	1	0	0	1	0	6	1	1
778	1	1	1	1	0	0	0	0	1	0	0	0	0	1	6	1	1
779	1	1	1	1	0	0	0	0	1	0	0	1	0	0	6	1	1
780	1	1	1	1	0	0	0	0	1	1	0	0	0	0	6	2	0
781	1	1	1	1	0	0	0	1	0	0	0	0	0	1	6	1	1
782	1	1	1	1	0	0	0	1	0	0	1	0	0	0	6	1	1
783	1	1	1	1	0	0	0	1	0	1	0	0	0	0	6	2	0
784	1	1	1	1	0	0	0	1	1	0	0	0	0	0	6	2	0
785	1	1	1	1	0	0	1	0	0	0	0	0	1	0	6	1	1
786	1	1	1	1	0	0	1	0	0	0	0	1	0	0	6	1	1
787	1	1	1	1	0	0	1	0	0	1	0	0	0	0	6	2	0
788	1	1	1	1	0	0	1	0	1	0	0	0	0	0	6	2	0
789	1	1	1	1	0	0	1	1	0	0	0	0	0	0	6	2	0
790	1	1	1	1	0	1	0	0	0	0	0	0	1	0	6	1	1
791	1	1	1	1	0	1	0	0	0	0	1	0	0	0	6	1	1
792	1	1	1	1	0	1	0	0	0	1	0	0	0	0	6	2	0
793	1	1	1	1	0	1	0	0	1	0	0	0	0	0	6	2	0
794	1	1	1	1	0	1	0	1	0	0	0	0	0	0	6	2	0
795	1	1	1	1	0	1	1	0	0	0	0	0	0	0	6	2	0
796	1	1	1	1	1	0	0	0	0	0	0	1	0	0	6	1	1
797	1	1	1	1	1	0	0	0	0	0	1	0	0	0	6	1	1
798	1	1	1	1	1	0	0	0	0	1	0	0	0	0	6	2	0
799	1	1	1	1	1	0	0	0	1	0	0	0	0	0	6	2	0
800	1	1	1	1	1	0	0	1	0	0	0	0	0	0	6	2	0
801	1	1	1	1	1	0	1	0	0	0	0	0	0	0	6	2	0
802	1	1	1	1	1	1	0	0	0	0	0	0	0	0	6	2	0
803	1	1	1	1	0	0	0	0	0	1	0	0	0	0	5	1	0
804	1	1	1	1	0	0	0	0	1	0	0	0	0	0	5	1	0
805	1	1	1	1	0	0	0	1	0	0	0	0	0	0	5	1	0
806	1	1	1	1	0	0	1	0	0	0	0	0	0	0	5	1	0
807	1	1	1	1	0	1	0	0	0	0	0	0	0	0	5	1	0
808	1	1	1	1	1	0	0	0	0	0	0	0	0	0	5	1	0
809	1	1	1	1	0	0	0	0	0	0	0	0	0	0	4	0	0

5. Use the genetic algorithm to construct model-robust mixture designs in the mixture region of interest. The steps of the genetic algorithm used for constructing a mixture experiment over an irregularly-shaped mixture region are as follows:

5.1 Use real-value encoding to encode each chromosome. This encoding is flexible enough to allow a unique representation for every variable, compatible with other optimization algorithms, easy to interpret, and can be modified to adjust for many applications.

5.2 Create the initial population that consists of an odd number (M) chromosomes (designs) which also equals the number of chromosomes at the beginning of every generation. In this dissertation, we chose $M = 7$ chromosomes as the size of the initial population. A **chromosome** is a potential design that can be encoded as an $n \times q$ matrix where n is the number of the design points and q is the number of components in the mixture experiment. A **gene** $\mathbf{x}_i$ is a row in a chromosome matrix. Thus, $\mathbf{x}_i$ is the coded setting of the i th experiment mixture ($i = 1, 2, \dots, n$) in the design using a level of precision appropriate for the problem of interest. For example, if $n = 5$, a chromosome $C = (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5)$ where $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4$ and $\mathbf{x}_5$ are five genes (experimental mixtures). In this dissertation, all mixtures in the initial population of chromosomes are randomly generated satisfying all SCCs and MCCs such that $\sum_{j=1}^q x_{ij} = 1$ where x_{ij} is the coded setting of component j in gene $\mathbf{x}_i$. Although a large M is desirable, the choice of M is based on practical computing time considerations.

5.3 Use the objective function (F) to evaluate the fitness of each of the M chromosomes (designs). That is, F takes a chromosome as input and outputs an objective function value. The design is evaluated by using a weighted D or G

criterion. Therefore, two objective functions are considered. An objective function F_i selected for the genetic algorithm is either

$$F_D = \sum_{i=1}^r w_i D(i) \quad \text{or} \quad F_G = \sum_{i=1}^r w_i G(i) \quad (89)$$

where $D(i) = \frac{100|\mathbf{X}'\mathbf{X}|^{1/p(i)}}{n}$ is the D -efficiency for model i and

$$G(i) = \frac{100p(i)}{\max_{\mathbf{x} \in \mathcal{X}} \left[n\mathbf{x}'_{\mathbf{m}} (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_{\mathbf{m}} \right]}$$
 is the G -efficiency for model i

r is the number of WH or SH reduced models for each of full model

w_i is the weight for model i

$p(i)$ is the number of parameters for model i

$\mathbf{x}'_{\mathbf{m}}$ is a vector associated with the terms in model i

$\mathbf{X}$ is a mixture model matrix for model i

$\mathcal{X}$ is the design space.

For the quadratic mixture model,

$$\mathbf{x}'_{\mathbf{m}} = \left[x_1, x_2, \dots, x_q, x_1x_2, x_1x_3, \dots, x_{q-1}x_q \right].$$

For the special cubic mixture model,

$$\mathbf{x}'_{\mathbf{m}} = \left[x_1, x_2, \dots, x_q, x_1x_2, x_1x_3, \dots, x_{q-1}x_q, x_1x_2x_3, x_1x_2x_4, \dots, x_{q-2}x_{q-1}x_q \right].$$

For any reduced model of the full model, $\mathbf{x}'_{\mathbf{m}}$ contains a subset of terms from the full model. The research goal is to find an $n \times q$ chromosome (design) matrix that optimizes the weighted D or G criterion.

In this dissertation, an objective function is calculated using the actual experimental mixture proportions. That is, $\mathbf{X}$ contains the unscaled component proportions that are used for fitting models after experimental data are collected. The D -optimality criterion is focused on parameter estimation and the minimization of $|\mathbf{X}'\mathbf{X}|$ while the G -optimality criterion is focused on prediction variance and the minimization of $\max_{\mathbf{x} \in \mathcal{X}} \left[n\mathbf{x}'_m (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_m \right]$. G -efficiencies are approximated over the set of points from an extreme vertices (EV) design because the maximum scaled prediction variance typically occurs at a boundary point such as a vertex, face centroid or edge centroid. For D and G efficiencies, larger values imply a better design.

The two objective functions will be referred to as *weighted design optimality criteria*. Although the concept of weighted optimality criteria is not new, the additional generalizations that (1) not all models should be weighted equally and (2) only models having an equal number of model parameters receive equal weight are new and are adopted in this dissertation. Given the above criteria, we now define the weight associated with each reduced model. The weight for model i is defined as

$$w_i = \frac{W_j}{m(j)} \quad (90)$$

where W_j is the j th weighting factor, $j = P_{SMALL}, P_{SMALL+1}, \dots, P_{FULL}$

P_{SMALL} is the number of parameters of the Scheffé linear mixture model

P_{FULL} is the number of parameter of the full quadratic or special cubic model

$m(j)$ is the number of reduced models equivalent to a j -parameter model.

The weighting factors $W_{P_{SMALL}}, W_{P_{SMALL+1}}, \dots, W_{P_{FULL}}$ are positive subject to the restriction $\sum_{j=P_{SMALL}}^{P_{FULL}} W_j = 1$. To compute the weighting factors, suppose the *relative weighting factor* (supplied by the experimenter) is defined as

$$R = \frac{W_{P_{FULL}}}{W_{P_{SMALL}}} . \quad (91)$$

The number of levels of the weighting factor is

$$P_{RANGE} = P_{FULL} - P_{SMALL} + 1 . \quad (92)$$

The range of the weighting factor is

$$\begin{aligned} W_{P_{RANGE}} &= W_{P_{FULL}} - W_{P_{SMALL}} \\ &= RW_{P_{SMALL}} - W_{P_{SMALL}} \\ &= (R-1)W_{P_{SMALL}} . \end{aligned} \quad (93)$$

The incremental value of the weighting factor is given by

$$INCR = \frac{W_{P_{RANGE}}}{P_{RANGE}} = \frac{(R-1)W_{P_{SMALL}}}{P_{RANGE}} . \quad (94)$$

Again, the weighting factor must satisfy the following constraint:

$$W_{P_{SMALL}} + W_{P_{SMALL+1}} + \dots + W_{P_{FULL-1}} + W_{P_{FULL}} = 1 . \quad (95)$$

Given that there are P_{RANGE} equispaced levels of the weighting factor, the values of the weighting factor can be represented as follows:

$$\begin{aligned} W_{P_{SMALL}} &= W_{P_{SMALL}} \\ W_{P_{SMALL+1}} &= W_{P_{SMALL}} + INCR \\ W_{P_{SMALL+2}} &= W_{P_{SMALL}} + 2INCR \\ &\vdots \\ W_{P_{FULL-1}} &= W_{P_{SMALL}} + (P_{RANGE} - 2) INCR \\ W_{P_{FULL}} &= W_{P_{SMALL}} + (P_{RANGE} - 1) INCR . \end{aligned} \quad (96)$$

Then Eq. (95) can be rewritten in the form

$$W_{P_{SMALL}} + (W_{P_{SMALL}} + INCR) + (W_{P_{SMALL}} + 2INCR) + \dots + (W_{P_{SMALL}} + (P_{RANGE} - 1)INCR) = 1$$

which reduces to

$$P_{RANGE} W_{P_{SMALL}} + INCR \sum_{i=0}^{P_{RANGE}-1} i = 1. \quad (97)$$

It is not hard to verify that Eq. (97) can be written as

$$P_{RANGE} W_{P_{SMALL}} + INCR \left[\frac{(P_{RANGE} - 1)(P_{RANGE} - 1 + 1)}{2} \right] = 1. \quad (98)$$

Thus, the minimum weighting factor is

$$W_{P_{SMALL}} = \frac{1}{P_{RANGE}} - \frac{INCR(P_{RANGE} - 1)}{2}. \quad (99)$$

For instance, suppose SH or WH holds and the full model is the quadratic mixture model with four mixture components ($q = 4$). Suppose also that the experimenter sets $R=100$. Hence, the number of levels of the weighting factor is $P_{RANGE} = 10 - 4 + 1 = 7$ with $W_{P_{SMALL}} = W_4$, $W_{P_{FULL}} = W_{10}$, and the incremental value of weighting factor is therefore defined as

$$INCR = \frac{99 \left(\frac{1}{7} - 3 \times INCR \right)}{7} = 0.0465.$$

Table 10 shows the calculations for the weighting factors for 4 components. We now consider the 58th reduced model in Table 5,

$$E(y) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{34} x_3 x_4,$$

that has 5-parameters. There are 6 reduced models having 5-parameters as shown in Table 5. Thus, the weight of the 58th model is

$$w_{58} = \frac{W_5}{6} = \frac{0.0498}{6} = 0.0083.$$

Table 10 The weighting factor values of the 4-component quadratic mixture model.

Parameter	Weighting factor calculations			
4	$W_4 = \frac{1}{P_{RANGE}} - \frac{INCR(P_{RANGE}-1)}{2}$	$= \frac{1}{7} - 3INCR$	$= 0.0033$	
5	$W_5 = \frac{1}{P_{RANGE}} - \frac{INCR(P_{RANGE}-1)}{2} + INCR$	$= \frac{1}{7} - 2INCR$	$= 0.0498$	
6	$W_6 = \frac{1}{P_{RANGE}} - \frac{INCR(P_{RANGE}-1)}{2} + 2INCR$	$= \frac{1}{7} - 1INCR$	$= 0.0963$	
7	$W_7 = \frac{1}{P_{RANGE}} - \frac{INCR(P_{RANGE}-1)}{2} + 3INCR$	$= \frac{1}{7} - 0INCR$	$= 0.1429$	
8	$W_8 = \frac{1}{P_{RANGE}} - \frac{INCR(P_{RANGE}-1)}{2} + 4INCR$	$= \frac{1}{7} + 1INCR$	$= 0.1894$	
9	$W_9 = \frac{1}{P_{RANGE}} - \frac{INCR(P_{RANGE}-1)}{2} + 5INCR$	$= \frac{1}{7} + 2INCR$	$= 0.2359$	
10	$W_{10} = \frac{1}{P_{RANGE}} - \frac{INCR(P_{RANGE}-1)}{2} + 6INCR$	$= \frac{1}{7} + 3INCR$	$= 0.2824$	
TOTAL				1

5.4 Use selection with *elitism*. That is, at the beginning of each generation, the chromosome having the largest objective function F value is left unchanged for that generation which guarantees that the best chromosome is retained from one generation to the next generation. The best chromosome will be the elite chromosome. The remaining $M-1$ chromosomes are randomly partitioned into $\frac{M-1}{2}$ pairs of ‘parent’ chromosomes, and the reproduction operators described in

steps (v), (vi) and (vii) are then applied to the parental pairs with each parent creating an ‘offspring’ chromosome. Therefore, at the end of each generation, the 1 elite chromosome and $M - 1$ future parent chromosomes survive to the next generation. Note that a new elite chromosome may result at the end of any generation.

5.5 Use *blending* to alter the $\frac{M-1}{2}$ parental design pairs to produce $\frac{M-1}{2}$ offspring design (chromosome) pairs. Suppose A and B are two parents paired in this process. Let A_a be the a^{th} row of A and B_b be the b^{th} row of B. If a probability test is passed (PTIP) for A_a and B_b , then A_a and B_b are to be blended. By definition, a PTIP for any reproduction operation if $0 \leq u \leq \alpha$ where u is a random deviate from a uniform $U[0,1]$ distribution and α is the probability of success for a Bernoulli trial (with the choice of α set by the experimenter). That is, if a PTIP then a gene or set of genes will change. If, however, $\alpha < u \leq 1$ then the probability test is failed (PTIF) and the chromosome is unchanged. For blending, if a PTIP then the resulting rows in offspring A_a^* and B_b^* are defined as

$$A_a^* = \beta A_a + (1 - \beta) B_b \quad \text{and} \quad B_b^* = (1 - \beta) A_a + \beta B_b, \quad (100)$$

respectively, where $\beta \sim U[0,1]$ is a random blending factor.

5.6 Use a single-crossover point (CP). A CP is defined to occur at the maximum number of decimal places appearing in the lower (L_i) and upper (U_i) bound in the SCCs and MCCs. The crossover operator swaps the tail fraction of one or more mixture components beyond the CP decimal places between genes in parent chromosomes creating offspring chromosomes. If a PTIP, then a gene or set of genes will change. Although the crossover concept is not new, the following two crossover operators were developed and are new with respect to handling the constraints associated with mixture experiments. Specifically:

5.6.1 For the *Between-Parent Crossover (BPC)*, offspring are obtained by swapping the tail fractions of two genes of two paired parents if a PTIP. For example, suppose we crossover genes (0.4710, 0.4289, 0.1001) and (0.4352, 0.4521, 0.1127) and the crossover point is the second decimal place. Then, the offspring genes are (0.4752, 0.4221, 0.1027) and (0.4310, 0.4589, 0.1101).

5.6.2 For the *Within-Parent Crossover (WPC)*, an offspring is obtained by swapping the tail fractions within a gene if a PTIP. Before swapping, the crossover pattern of components within the genes corresponds to a random permutation of $(1, 2, \dots, q)$. For example, suppose the crossover is within gene (0.4710, 0.4289, 0.1001). If the random permutation of (1,2,3) is (3,1,2) and using a second-decimal place crossover point, then the offspring gene is (0.4701, 0.4210, 0.1089).

Suppose that $C_r = (x_{r1}, x_{r2}, \dots, x_{rq})$ is the r^{th} row (gene) of an offspring (chromosome) for each type of crossover operator for which a PTIP. If $\sum_{i=1}^q x_{ri} \neq 1$, then the j^{th} component of C_r which is randomly selected for adjustment in C_r is defined to be

$$x_{rj}^* = x_{rj} - \Delta_r; j = 1, 2, \dots, q, \quad (101)$$

where $\Delta_r = \sum_{i=1}^q x_{ri} - 1$ be the difference between $\sum_{i=1}^q x_{ri}$ and unity. This adjustment is to ensure that sum of component proportions is equal to 1. However, after adjustment, if C_r does not satisfy the lower and upper bounds, then C_r will be reset to the parent (chromosome).

5.7 Use *mutation* to alter subsets of genes of the $M - 1$ non-elite designs pairs for generating $M - 1$ offspring designs. If a PTIP, then a gene will change. Let R be a parent (chromosome) in this process and $R_r = (x_{r1}, x_{r2}, \dots, x_{rq})$ be the r^{th} row (gene) of R . If a PTIP, then one of the q components (say h) is randomly chosen.

The mutation operator begins by generating $\varepsilon \sim N(0, \sigma^2)$ which is added to x_{rh} to a form $x_{rh}^* = x_{rh} + \varepsilon_h$. If $x_{rh}^* > U_h$ then x_{rh}^* will be reset to the upper bound U_h . Similarly, if $x_{rh}^* < L_h$ then x_{rh}^* will be reset to the lower bound L_h . The remaining component proportions in gene R_r must be adjusted to ensure that sum of the component proportions equals 1. Let ε_{rj} be the adjustment to x_{rj} ($j \neq h$). If ε_h is positive, then the adjustment to component j is defined to be

$$\varepsilon_{rj} = \frac{x_{rj} - L_j}{\sum_{\substack{j=1 \\ j \neq h}}^q (x_{rj} - L_j) - (x_{rh} - L_h)} (-\varepsilon_h) ; j = 1, \dots, h-1, h+1, \dots, q. \quad (102)$$

If ε_h is negative, then the adjustment to component j is defined to be

$$\varepsilon_{rj} = \frac{U_j - x_{rj}}{\sum_{\substack{j=1 \\ j \neq h}}^q (U_j - x_{rj}) - (U_h - x_{rh})} (-\varepsilon_h) ; j = 1, \dots, h-1, h+1, \dots, q. \quad (103)$$

For example, suppose a PTIP and gene (0.6164, 0.1488, 0.2348) is to be mutated. Suppose the third component is randomly selected. A random $\varepsilon_3 = 0.2114$ is added to x_{r3} yielding 0.4462. After calculating the values of ε_{r1} and ε_{r2} , the offspring gene is (0.4726, 0.0812, 0.4462).

5.8 If MCCs are present, some genes may not satisfy any/all of the MCCs after the reproduction process is performed across chromosomes. If a gene does not satisfy any/all of the MCCs, this gene must be adjusted to ensure that it does satisfy all of the MCCs. Let R be a potential ‘offspring’ chromosome after the reproduction process. Suppose $\mathbf{A}_m = (x_{m1}^a, x_{m2}^a, \dots, x_{mq}^a)$ is the m^{th} row of R and it violates any/all of the MCCs as a result of the reproduction process. Let $\mathbf{B}_m = (x_{m1}^b, x_{m2}^b, \dots, x_{mq}^b)$ be the m^{th} row of the parent chromosome of R before the reproduction process. Thus, $\mathbf{B}_m$

does not violate any of the MCCs. If $\alpha_j = (A_{1j}, A_{2j}, \dots, A_{qj})'$ is a vector of the scalar constants defining the j th MCC and C_j is the upper or lower bound of the j th MCC that is violated by $\mathbf{A}_m$, then the adjustment to $\mathbf{A}_m$ is defined as

$$\mathbf{A}_m^* = \beta \mathbf{A}_m + (1 - \beta) \mathbf{B}_m \quad (104)$$

where β is an adjustment factor that pulls $\mathbf{A}_m$ onto the boundary of the design region. To find the adjustment factor β , consider the linear combination:

$$\beta \mathbf{B}_m \alpha_j + (1 - \beta) \mathbf{A}_m \alpha_j = C_j \quad (105)$$

which simplifies to

$$\beta = \frac{C_j - \mathbf{A}_m \alpha_j}{(\mathbf{B}_m - \mathbf{A}_m) \alpha_j}. \quad (106)$$

This Step is not necessary to consider when there are no MCCs.

5.9 Calculate the objective function F for each ‘parent’ and ‘offspring’ chromosome resulting from the reproduction process. For each parent and offspring pair, the chromosome with the larger F value survives to be a future parent while the other is removed from the population. Therefore, at the end of every generation, the 1 elite chromosome and $M - 1$ future parent chromosomes survive to the next generation. Note that a new elite chromosome may result at the end of any generation if one of the $M - 1$ future parent chromosomes now has a larger F value than the elite chromosome from the previous generation.

5.10 Iterate Steps iv) to ix) for a large number of generations (B).

5.11 After the last iteration, a local grid search is applied to the points of the design with the largest value of objective function F . The local grid search will increase the objective function value slightly until no further improvement can be

found. This is discussed in Borkowski (2003). That is, the optimal exact mixture design is found.

The values assigned to genetic algorithm parameters are very important for the performance of the genetic algorithm (GA) and affects the speed of convergence to the optimal design. The genetic algorithm parameters that may affect the performance of a GA consist of the population size (M), the number of iterations B , the success probabilities for the blending operator (α_b), the success probabilities for the between-parent crossover (α_{bc}), the success probabilities for the within-parent crossover (α_{wc}), the success probabilities for the mutation operator (α_m) and the standard deviation of a random variate for mutation (σ). There are no rules for selecting the optimal success probabilities and the choice of α_i for $i = b, bc, wc$ and m remains an open research area. The choice of the each α_i is often problem-specific and based on subjective judgments through examination of convergence rates. Therefore, the value of α_i, σ, M , and the number of iteration should be carefully considered. The values of α_i and σ are considered by creating 8 sets of these values as seen in Table 11. The number of iterations is considered by plotting the objective function values of the elite chromosome for each generation over the large number of iterations. To assign the number of iterations (B) to use in the GA, we select the iteration indicating stability (i.e., there is minimal or no increase in the plot). These are discussed in results and discussion chapter.

6. Use (i) graphical approaches (such as variance dispersion graphs (VDGs), fraction of design space (FDS) plots and componentwise variance dispersion graphs (CVDGs)) and (ii) the alphabetic optimality criteria approach (such as the weighted D- and G-optimality criteria) for examining model robustness.

Table 11 The values of α_i for $i = b, bc, wc$ and m with 8 sets.

Set	Value
Set1	$0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.2; 0.05 \leq \alpha_m \leq 0.1; 0.1 \leq \sigma \leq 0.2$
Set2	$0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.2; 0.05 \leq \alpha_m \leq 0.1; 0.1 \leq \sigma \leq 0.3$
Set3	$0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.2; 0.05 \leq \alpha_m \leq 0.2; 0.1 \leq \sigma \leq 0.2$
Set4	$0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.2; 0.05 \leq \alpha_m \leq 0.2; 0.1 \leq \sigma \leq 0.3$
Set5	$0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.1; 0.05 \leq \alpha_m \leq 0.1; 0.1 \leq \sigma \leq 0.2$
Set6	$0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.1; 0.05 \leq \alpha_m \leq 0.1; 0.1 \leq \sigma \leq 0.3$
Set7	$0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.1; 0.05 \leq \alpha_m \leq 0.2; 0.1 \leq \sigma \leq 0.2$
Set8	$0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.1; 0.05 \leq \alpha_m \leq 0.2; 0.1 \leq \sigma \leq 0.3$

Location and Duration of the Research

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RESULTS AND DISCUSSION

Results

In this chapter a GA-generated mixture design for model robustness is presented where the experimental region is an irregularly-shaped polyhedron. The design points are greatly dependent on the shape of the constrained experimental region and the form of the model to be fitted. The resulting designs are evaluated based on alphabetical optimal criteria and graphical methods. Specifically, the following mixture experiment problems and results are presented:

- *Case 1* : SCCs in a three-component mixture experiment.
- *Case 2* : SCCs in a four-component mixture experiment.
- *Case 3* : SCCs and MCCs in a three-component mixture experiment.

For the designs generated in this dissertation, objective functions based on weighted D and G optimality criteria are considered, and are denoted simply as D_w and G_w .

Case 1: Only Single Component Constraints with Three Component Mixtures

A poultry feed blend experiment with three mixture components taken from Snee and Raynor (1982) serves as an initial example illustrating our method. There are three ingredients in the mixture process, maize(x_1), fish(x_2), and soybean(x_3). These ingredients have the following lower and upper proportion constraints:

$$\begin{aligned} 0.3 &\leq x_1 \leq 0.8 \\ 0.0 &\leq x_2 \leq 0.3 \\ 0.0 &\leq x_3 \leq 0.5. \end{aligned} \tag{107}$$

The objective of the experiment is to evaluate the effects of the component proportions on the weight gain of chicks consuming the feed. In Figure 22, the boundary formed by the SCCs is indicated by the dashed line inside the simplex

bounded by six vertices with points labeled 1 to 6. The six extreme vertices are listed in Table 12.

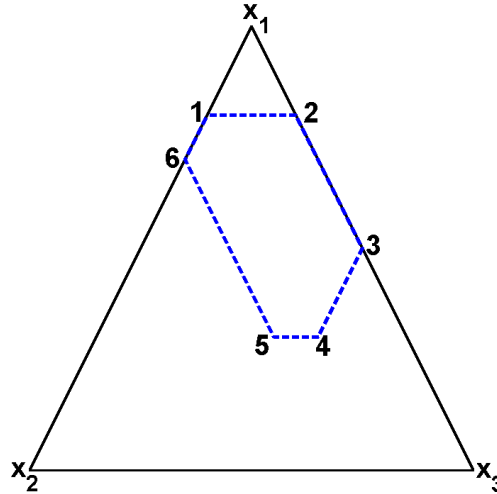


Figure 22 The six extreme vertices of the region defined by SCCs $0.3 \leq x_1 \leq 0.8$, $0.0 \leq x_2 \leq 0.3$, and $0.0 \leq x_3 \leq 0.5$.

Table 12 Coordinates of six vertices for the Snee and Raynor poultry experiment.

Vertex	x_1	x_2	x_3
1	0.8000	0.2000	0.0000
2	0.8000	0.0000	0.2000
3	0.5000	0.0000	0.5000
4	0.3000	0.2000	0.5000
5	0.3000	0.3000	0.4000
6	0.7000	0.3000	0.0000

The two full models under consideration are the Scheffé quadratic and special cubic mixture models:

$$E(y) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$

and

$$E(y) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3,$$

having six and seven unknown parameters, respectively.

1. Appropriate genetic algorithm (GA) parameters for Case 1

In this section, the genetic algorithm parameters for Case 1 are presented. The goal is to find appropriate values of α_i and σ as described in Table 11. We consider 5,000 as a large number of iterations, 7 as the size of the population (M) and 12 runs as the number of mixture design points to be created assuming a Scheffé quadratic model. However, when mixture designs are created assuming a Scheffé special cubic model, 13-runs is the number of mixture design points to consider under WH models.

Figure 23 shows the behavior of D_w for each α_i and σ value when the model being fit is the Scheffé quadratic model. The results show that the best set of the α_i and σ values is set 8 corresponding to $0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.1$; $0.05 \leq \alpha_m \leq 0.2$; $0.1 \leq \sigma \leq 0.3$. It is best because it quickly generates the highest D_w values and then becomes very stable and is superior to the other sets throughout the later iterations. Next, if population size M is increased from 7 to 9 for set 8, the chance of reporting a local optimum is decreased.

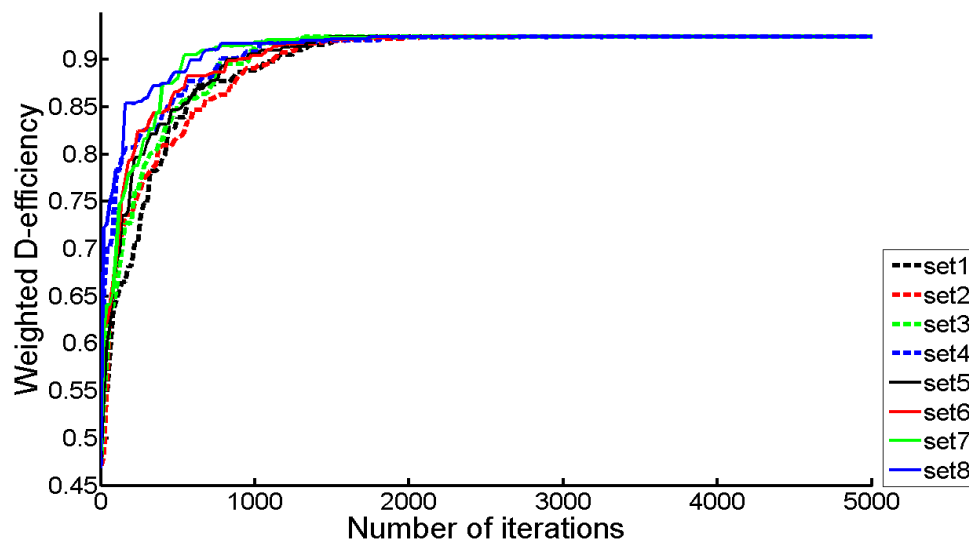


Figure 23 Progression of the D_w values for 8 sets of α_i and σ values assuming the Scheffé quadratic model for the poultry experiment.

As seen in Figure 24, in the early iterations, the improvement in D_w when $M = 7$ is superior to that when $M = 9$. After that, both cases have similar D_w values. In Figure 24, we also observe that there are no improvements for D_w after 2,500 iterations. On the other hand, Figure 25 indicates the progression of G_w values with set 8 and $M = 7$ when the model being fit is the quadratic model, and that there are no improvements for G_w after 4,500 iterations.

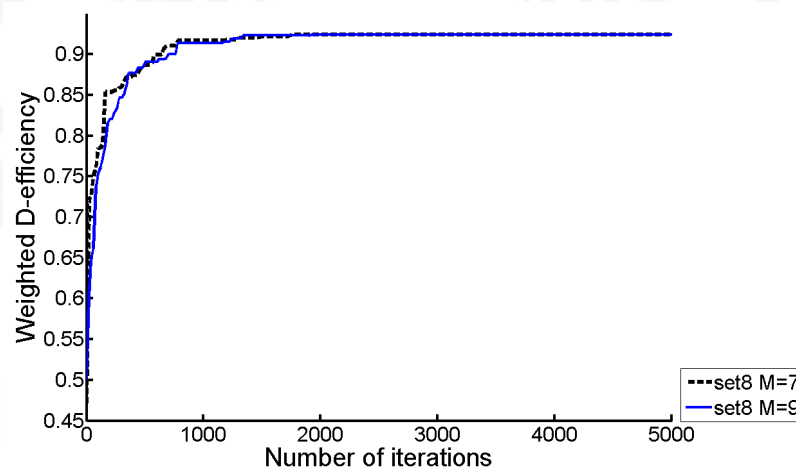


Figure 24 Behavior of the D_w values for the best set of the α_i and σ , with $M = 7$ and 9, assuming the Scheffé quadratic model for the poultry experiment.

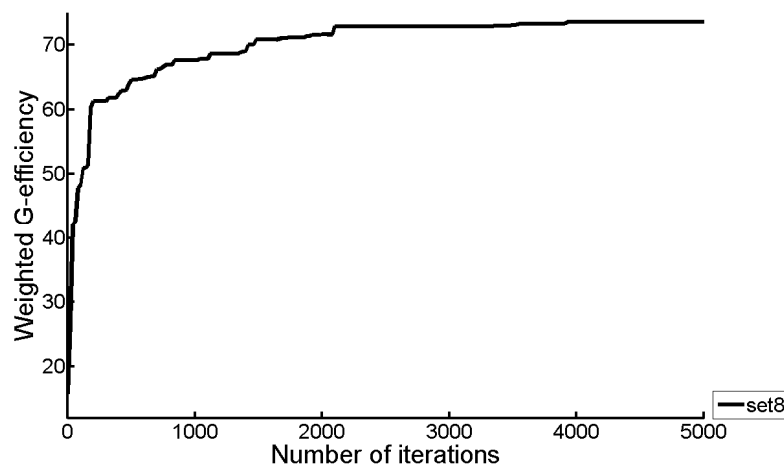


Figure 25 Progression of the G_w values for the best set of the α_i and σ , with $M = 7$, assuming the Scheffé quadratic model for the poultry experiment.

When the model being fit is the Scheffé quadratic model, we chose $M = 7$ as the size of the population, set 8 as the value of α_i and σ , and 2,500 and 4,500 as the number of iterations where D_w and G_w are the objective functions, respectively. The values of α_i and σ are reset to smaller values after 250 iterations.

We assume also that $M = 7$ as the population size and use the values of α_i and σ in set 8 to generate mixture designs. Assuming a Scheffé special cubic model, Figure 26 presents the behavior of D_w for the α_i and σ values in set 8. We also notice that there are slight improvements for D_w after 2,500 iterations. On the other hand, Figure 27 displays the progression for G_w values with set 8 and $M = 7$, assuming the special cubic model. We also observe that there are slight improvements for G_w after 4,500 iterations. Therefore, when assuming the special cubic model, we decided to use $M = 7$ for the population size, the values of α_i and σ for set 8, and 2,500 or 4500, respectively, as the number of iterations where D_w or G_w is the objective function. The values of α_i and σ are reset to smaller values after 250 iterations. Notice that the genetic algorithm parameters for the case of special cubic model are identical to the case of the quadratic model.

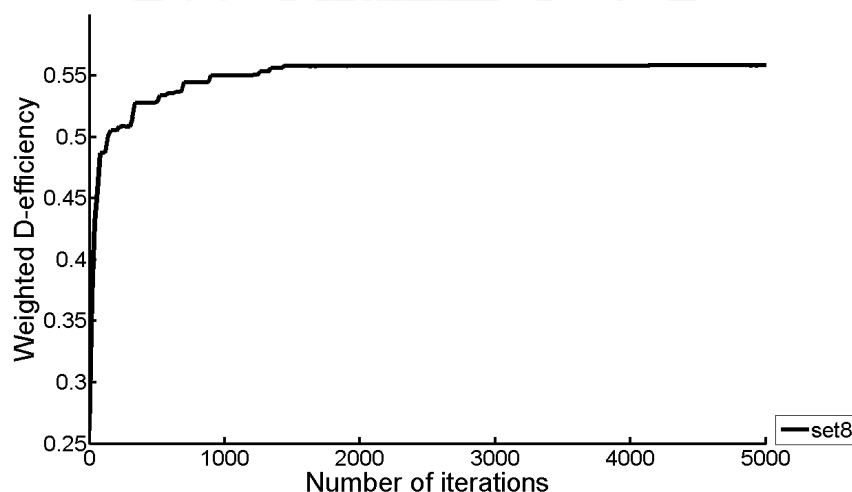


Figure 26 Behavior of D_w values with the best set of the α_i and σ and $M = 7$, assuming the Scheffé special cubic model for the poultry experiment.

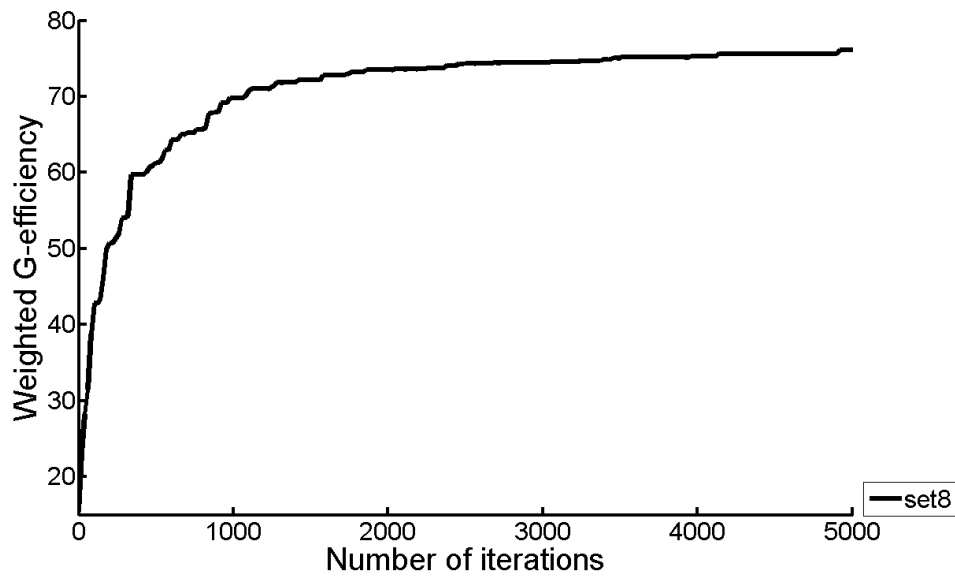


Figure 27 Progression of the G_w values for the best set of the α_i and σ , with $M = 7$, assuming the Scheffé special cubic model for the poultry experiment.

2. Generating optimal exact designs for Case 1

The best design generated by the GA is a near-optimal exact design, which then serves as the starting design for a local grid search to achieve the optimal exact design. We would like the design to be robust over classes of reduced models. We first consider the mixture design created by the GA when the model being fit is **the Scheffé quadratic model**. There are 8 reduced models under SH and WH as shown in Table 4. We focus on the following two cases that vary with respect to the choice of weighted design optimality criterion assuming the quadratic mixture model:

- For the D_w weighted optimality criterion, the GA generated designs and optimal exact designs having 7 to 12 points are shown in Appendix Tables A1 to A6.
- For the G_w weighted optimality criterion, the GA generated designs and optimal exact designs having 7 to 12 points are shown in Appendix Tables A7 to A12.

In addition to the Scheffé quadratic model, we consider **the Scheffé special cubic model** as the model to be fitted. Assuming the Scheffé special cubic model, there are 9 SH models and 15 WH models as shown in Table 6 and 7, respectively. We examine the following 4 cases that vary with respect to the choice of weighted design optimal criterion assuming the special cubic mixture model:

- For the D_w criterion with SH, the GA generated designs and optimal exact designs having 8 to 13 points are given in Appendix Tables A13 to A18.
- For the D_w criterion with WH, the GA generated designs and optimal exact design having 8 to 13 points are given in Appendix Tables A19 to A24.
- For the G_w criterion with SH, the GA generated designs and the optimal exact designs having 8 to 13 points are shown in Appendix Tables A25 to A30.
- For the G_w criterion with WH, the GA generated designs and the optimal exact designs having 8 to 13 points are shown in Appendix Tables A31 to A36.

After running a local grid search, most of the D_w values increase in the fifth decimal place. Thus, six decimal places are used to report the percentage increase in a D_w value. Otherwise, four decimal places are used. A local grid search leads to an increase in the D_w or G_w objective function value as seen at the bottom of Appendix Tables A1 to A36. Tables 13 and 14 highlight the percentage increase in the objective function value assuming a quadratic model and a special cubic model, respectively. The last column in both tables contains the percentage change in the objective function for the best GA design relative to the optimal exact design for that model. It is clear that the percentage change in D_w values is less than it is for the G_w values.

As shown in Table 13, there is no improvement in the D_w values for 7- and 8-point designs, while the maximum improvement in a D_w value occurs for the 9-point design. The highest percentage increase in a G_w value occurs for the 12-point design, while the lowest percentage increase in a G_w value occurs for the 7-point design.

Table 13 Comparison of objective function values and the percentage increase for the poultry experiment assuming the quadratic model.

Objective function	Run	Most fit designs via GA	Optimal exact design	Percentage increase (%)
D_w	7	0.910121	0.910121	0.0000
	8	0.908224	0.908224	0.0000
	9	0.917581	0.917644	0.0069
	10	0.918343	0.918352	0.0010
	11	0.919214	0.919218	0.0004
	12	0.924121	0.924131	0.0011
G_w	7	79.7656	80.2307	0.5831
	8	77.9279	81.0509	4.0076
	9	77.5300	80.4382	3.7511
	10	79.3559	80.9403	1.9966
	11	76.1713	78.4854	3.0380
	12	73.5764	76.9692	4.6113

When the model to be fitted is the quadratic model, the following twelve optimal exact designs were created:

(1) 7-point design with D_w (7Q-D)	(7) 7-point design with G_w (7Q-G)
(2) 8-point design with D_w (8Q-D)	(8) 8-point design with G_w (8Q-G)
(3) 9-point design with D_w (9Q-D)	(9) 9-point design with G_w (9Q-G)
(4) 10-point design with D_w (10Q-D)	(10) 10-point design with G_w (10Q-G)
(5) 11-point design with D_w (11Q-D)	(11) 11-point design with G_w (11Q-G)
(6) 12-point design with D_w (12Q-D)	(12) 12-point design with G_w (12Q-G)

As shown in Table 14 for D_w with SH, the lowest percentage increase occurs for the 10-point design, while the highest percentage increase occurs for the 13-point design. For D_w with WH, the lowest percentage increase occurs when the number of design points equals 8 and 10, while then 9-point design has the highest percentage increase. For G_w with SH, the lowest percentage increase occurs for the 10-point design, while the 9-point design has the highest percentage increase. For G_w with

WH, the 8-point design has the highest percentage increase, while the lowest percentage increase occurs for the 9-point design.

Table 14 Comparison of objective function values and the percentage increase for the poultry experiment assuming the special cubic model.

Objective function	Heredity	Run	Most fit designs via GA	Optimal exact design	Percentage increase (%)
D_w	SH	8	0.603485	0.603490	0.0008
		9	0.605693	0.605695	0.0003
		10	0.614326	0.614327	0.0002
		11	0.614187	0.614196	0.0015
		12	0.617569	0.617572	0.0005
		13	0.615383	0.61561	0.0369
	WH	8	0.545553	0.545554	0.0002
		9	0.548367	0.548413	0.0084
		10	0.556032	0.556033	0.0002
		11	0.557230	0.557233	0.0005
		12	0.560806	0.560818	0.0021
		13	0.557857	0.557868	0.0020
G_w	SH	8	70.6078	72.7775	3.0729
		9	81.1388	85.3896	5.2389
		10	79.6723	79.8722	0.2509
		11	76.2473	78.2705	2.6535
		12	77.4266	80.5527	4.0375
		13	75.9085	79.5852	4.8436
	WH	8	68.5531	76.4169	11.4711
		9	83.1989	83.4761	0.3332
		10	77.6776	78.0611	0.4937
		11	77.3873	77.9426	0.7176
		12	76.9225	78.8811	2.5462
		13	75.6435	78.3922	3.6338

When mixture designs are created, assuming the special cubic model, 24 optimal exact designs were generated. There were six designs for D_w with SH, six designs for D_w with WH, six designs for G_w with SH, and six designs for G_w with WH. For each group of six designs, the design sizes range from 8 to 13 points. The 24 designs with their abbreviated notations in parentheses are given below.

(1) 8-points / SH / D_w (8SC-S-D)	(13) 8-points / SH / G_w (8SC-S-G)
(2) 9-points / SH / D_w (9SC-S-D)	(14) 9-points / SH / G_w (9SC-S-G)
(3) 10-points / SH / D_w (10SC-S-D)	(15) 10-points / SH / G_w (10SC-S-G)
(4) 11-points / SH / D_w (11SC-S-D)	(16) 11-points / SH / G_w (11SC-S-G)
(5) 12-points / SH / D_w (12SC-S-D)	(17) 12-points / SH / G_w (12SC-S-G)
(6) 13-points / SH / D_w (13SC-S-D)	(18) 13-points / SH / G_w (13SC-S-G)
(7) 8-points / WH / D_w (8SC-W-D)	(19) 8-points / WH / G_w (8SC-W-G)
(8) 9-points / WH / D_w (9SC-W-D)	(20) 9-points / WH / G_w (9SC-W-G)
(9) 10-points / WH / D_w (10SC-W-D)	(21) 10-points / WH / G_w (10SC-W-G)
(10) 11-points / WH / D_w (11SC-W-D)	(22) 11-points / WH / G_w (11SC-W-G)
(11) 12-points / WH / D_w (12SC-W-D)	(23) 12-points / WH / G_w (12SC-W-G)
(12) 13-points / WH / D_w (13SC-W-D)	(24) 13-points / WH / G_w (13SC-W-G)

For the optimal exact designs, the set of points appearing in any one of the 36 optimal exact designs (12 for the quadratic model and 24 for the special cubic model) is given in Table 15. Table 16 summarizes which (and how many replicates) of the labeled points given in Table 15 are in each optimal exact design for both the quadratic model and special cubic model. In Figure 22, the boundary formed by the SCCs is indicated by the dashed line inside the simplex that has six vertices and six edge centroids. In Figure 28, the differences in the distributional patterns of the optimal exact designs for the quadratic model based on D_w and G_w are shown. Figures 29 and 30 display the distributional patterns of mixture points of the optimal exact designs for the special cubic model based on D_w and G_w , respectively.

For the quadratic model with D_w , there are obvious distribution patterns of points. For $n = 7$ to 9 (designs 7Q-D, 8Q-D, and 9Q-D), the points lie on all vertices with varying replication and an edge centroid. For $n = 10$ and 12 (designs 10Q-D and 12Q-D), the points contain all vertices with varying replication, an edge centroid, and a near overall centroid. For $n = 11$ (designs 11Q-D), the points include all vertices with varying replication, a near edge centroid, and a near overall centroid.

Table 15 List of points appearing in the set of 36 poultry example designs.

Label	x_1	x_2	x_3	Label	x_1	x_2	x_3
Vertices				Other points			
V ₁	0.8000	0.2000	0.0000	G ₂₆	0.5713	0.1573	0.2714
V ₂	0.8000	0.0000	0.2000	G ₂₇	0.6689	0.2586	0.0725
V ₃	0.3000	0.3000	0.4000	G ₂₈	0.4029	0.1734	0.4237
V ₄	0.7000	0.3000	0.0000	G ₂₉	0.8000	0.0360	0.1640
V ₅	0.5000	0.0000	0.5000	G ₃₀	0.5852	0.1493	0.2655
V ₆	0.3000	0.2000	0.5000	G ₃₁	0.4693	0.0307	0.5000
Edge centroid				G ₃₂	0.4208	0.3000	0.2792
E ₁	0.6500	0.0000	0.3500	G ₃₃	0.5911	0.1177	0.2912
E ₂	0.7500	0.2500	0.0000	G ₃₄	0.5873	0.1312	0.2815
E ₃	0.3000	0.2500	0.4500	G ₃₅	0.5538	0.1137	0.3325
E ₄	0.8000	0.1000	0.1000	G ₃₆	0.5470	0.3000	0.1530
E ₅	0.5000	0.3000	0.2000	G ₃₇	0.3408	0.1592	0.5000
E ₆	0.4000	0.1000	0.5000	G ₃₈	0.7571	0.0000	0.2429
Overall centroid				G ₃₉	0.5154	0.0000	0.4846
C	0.5667	0.1667	0.2666	G ₄₀	0.7260	0.2740	0.0000
Other Points				G ₄₁	0.7032	0.2968	0.0000
G ₁	0.3215	0.3000	0.3785	G ₄₂	0.3531	0.1469	0.5000
G ₂	0.3300	0.1700	0.5000	G ₄₃	0.7780	0.0000	0.2220
G ₃	0.5719	0.1611	0.2670	G ₄₄	0.6028	0.0928	0.3044
G ₄	0.6566	0.3000	0.0434	G ₄₅	0.5048	0.3000	0.1952
G ₅	0.6168	0.0664	0.3168	G ₄₆	0.8000	0.1444	0.0556
G ₆	0.3357	0.1643	0.5000	G ₄₇	0.5209	0.0000	0.4791
G ₇	0.5199	0.2602	0.2199	G ₄₈	0.5957	0.1329	0.2714
G ₈	0.8000	0.1643	0.0357	G ₄₉	0.5905	0.1456	0.2639
G ₉	0.8000	0.1766	0.0234	G ₅₀	0.5599	0.1786	0.2615
G ₁₀	0.5841	0.1464	0.2695	G ₅₁	0.3227	0.1773	0.5000
G ₁₁	0.3243	0.1757	0.5000	G ₅₂	0.8000	0.1772	0.0228
G ₁₂	0.5680	0.1641	0.2679	G ₅₃	0.5030	0.3000	0.1970
G ₁₃	0.4619	0.0567	0.4814	G ₅₄	0.5659	0.1657	0.2684
G ₁₄	0.5763	0.1596	0.2641	G ₅₅	0.3173	0.1827	0.5000
G ₁₅	0.4838	0.2894	0.2268	G ₅₆	0.8000	0.1826	0.0174
G ₁₆	0.7837	0.2163	0.0000	G ₅₇	0.5765	0.1470	0.2765
G ₁₇	0.8000	0.0642	0.1358	G ₅₈	0.5698	0.1608	0.2694
G ₁₈	0.5388	0.3000	0.1612	G ₅₉	0.4865	0.3000	0.2135
G ₁₉	0.5695	0.1614	0.2691	G ₆₀	0.7976	0.1124	0.0900
G ₂₀	0.6822	0.0000	0.3178	G ₆₁	0.6309	0.0000	0.3691
G ₂₁	0.7564	0.1079	0.1357	G ₆₂	0.5841	0.1732	0.2427
G ₂₂	0.5512	0.3000	0.1488	G ₆₃	0.3193	0.1807	0.5000
G ₂₃	0.4192	0.0808	0.5000	G ₆₄	0.5678	0.1637	0.2685
G ₂₄	0.3000	0.2349	0.4651	G ₆₅	0.8000	0.1089	0.0911
G ₂₅	0.5462	0.1659	0.2879	G ₆₆	0.3168	0.1832	0.5000

Table 15 (Continued)

Label	x_1	x_2	x_3	Label	x_1	x_2	x_3
Other points				Other points			
G ₆₇	0.4964	0.0036	0.5000	G ₉₅	0.4928	0.2544	0.2528
G ₆₈	0.6166	0.0000	0.3834	G ₉₆	0.6656	0.0000	0.3344
G ₆₉	0.5247	0.3000	0.1753	G ₉₇	0.4258	0.0742	0.5000
G ₇₀	0.5785	0.1445	0.2770	G ₉₈	0.7615	0.2385	0.0000
G ₇₁	0.4794	0.3000	0.2206	G ₉₉	0.5347	0.2642	0.2011
G ₇₂	0.5703	0.1585	0.2712	G ₁₀₀	0.4303	0.3000	0.2697
G ₇₃	0.4936	0.0593	0.4471	G ₁₀₁	0.5884	0.1087	0.3029
G ₇₄	0.5045	0.3000	0.1955	G ₁₀₂	0.5773	0.1400	0.2827
G ₇₅	0.3000	0.2034	0.4966	G ₁₀₃	0.5025	0.3000	0.1975
G ₇₆	0.6600	0.0000	0.3400	G ₁₀₄	0.5773	0.1542	0.2685
G ₇₇	0.5384	0.1946	0.2670	G ₁₀₅	0.4982	0.3000	0.2018
G ₇₈	0.8000	0.0738	0.1262	G ₁₀₆	0.4248	0.3000	0.2752
G ₇₉	0.6583	0.0000	0.3417	G ₁₀₇	0.4029	0.0971	0.5000
G ₈₀	0.4193	0.1000	0.4807	G ₁₀₈	0.5744	0.1666	0.2590
G ₈₁	0.6755	0.3000	0.0245	G ₁₀₉	0.6041	0.0000	0.3959
G ₈₂	0.5522	0.1828	0.2650	G ₁₁₀	0.6029	0.3000	0.0971
G ₈₃	0.7379	0.2621	0.0000	G ₁₁₁	0.6698	0.0550	0.2752
G ₈₄	0.3000	0.2220	0.4780	G ₁₁₂	0.8000	0.0627	0.1373
G ₈₅	0.8000	0.1384	0.0616	G ₁₁₃	0.3000	0.2237	0.4763
G ₈₆	0.5792	0.1416	0.2792	G ₁₁₄	0.5955	0.0450	0.3595
G ₈₇	0.5735	0.1550	0.2715	G ₁₁₅	0.5654	0.1587	0.2759
G ₈₈	0.3000	0.2319	0.4681	G ₁₁₆	0.4326	0.0674	0.5000
G ₈₉	0.5380	0.3000	0.1620	G ₁₁₇	0.4093	0.3000	0.2907
G ₉₀	0.6020	0.0980	0.3000	G ₁₁₈	0.8000	0.0784	0.1216
G ₉₁	0.4137	0.0863	0.5000	G ₁₁₉	0.6737	0.0000	0.3263
G ₉₂	0.6454	0.0000	0.3546	G ₁₂₀	0.5851	0.3000	0.1149
G ₉₃	0.8000	0.0800	0.1200	G ₁₂₁	0.3000	0.2137	0.4863
G ₉₄	0.7816	0.2184	0.0000	G ₁₂₂	0.7800	0.2200	0.0000

Table 16 Summary of points appearing in the poultry example designs.

Design	V ₁	V ₂	V ₃	V ₄	V ₅	V ₆	Edge centroid	Other points
7Q-D	1	1	1	1	1	1	E ₅	
7Q-G	1	1			1			G ₁ to G ₄
8Q-D	1	1	1	1	2	1	E ₅	
8Q-G		1	1	1	1			G ₅ to G ₈
9Q-D	1	2	1	1	2	1	E ₅	
9Q-G		1	1	1	1		E ₁ , E ₅	G ₉ to G ₁₁
10Q-D	1	2	1	1	2	1	E ₅	G ₁₂
10Q-G		1	1	1	1	1		G ₁₃ to G ₁₇
11Q-D	1	2	2	1	2	1		G ₁₈ , G ₁₉
11Q-G	1	1	1	1	1			G ₂₀ to G ₂₅
12Q-D	1	2	2	2	2	1	E ₅	G ₂₆
12Q-G	1	1	1	1	1	1		G ₂₇ to G ₃₂
8SC-S-D	1	1	1	1	1	1	E ₅	G ₃₃
8SC-W-D	1	1	1	1	1	1	E ₅	G ₃₄
8SC-S-G			1				E ₄	G ₃₅ to G ₄₀
8SC-W-G			1					G ₄₁ to G ₄₇
9SC-S-D	1	1	1	1	2	1	E ₅	G ₄₈
9SC-W-D	1	1	1	1	2	1	E ₅	G ₄₉
9SC-S-G		1	1	1	1		E ₁ , E ₅	G ₅₀ to G ₅₂
9SC-W-G		1	1	1	1		E ₁	G ₅₃ to G ₅₆
10SC-S-D	1	2	1	1	2	1	E ₅	G ₅₇
10SC-W-D	1	2	1	1	2	1	E ₅	G ₅₈
10SC-S-G	1	1	1	1	1			G ₅₉ to G ₆₃
10SC-W-G	1	1	1	1			E ₅	G ₆₄ to G ₆₈
11SC-S-D	1	2	2	1	2	1		G ₆₉ , G ₇₀
11SC-W-D	1	2	1	2	2	1		G ₇₁ , G ₇₂
11SC-S-G	1	1	1	1	1			G ₇₃ to G ₇₈
11SC-W-G		1	1		1		E ₅	G ₇₉ to G ₈₅
12SC-S-D	1	2	2	2	2	1	E ₅	G ₈₆
12SC-W-D	1	2	2	2	2	1	E ₅	G ₈₇
12SC-S-G		1	1	1	1			G ₈₈ to G ₉₅
12SC-W-G		1	1	1	1	1	E ₄	G ₉₆ to G ₁₀₁
13SC-S-D	2	2	2	2	2	1		G ₁₀₂ , G ₁₀₃
13SC-W-D	1	2	2	2	2	2		G ₁₀₄ , G ₁₀₅
13SC-S-G	1	1	1	1	1			G ₁₀₆ to G ₁₁₃
13SC-W-G		1	1	1	1			G ₁₁₄ to G ₁₂₂

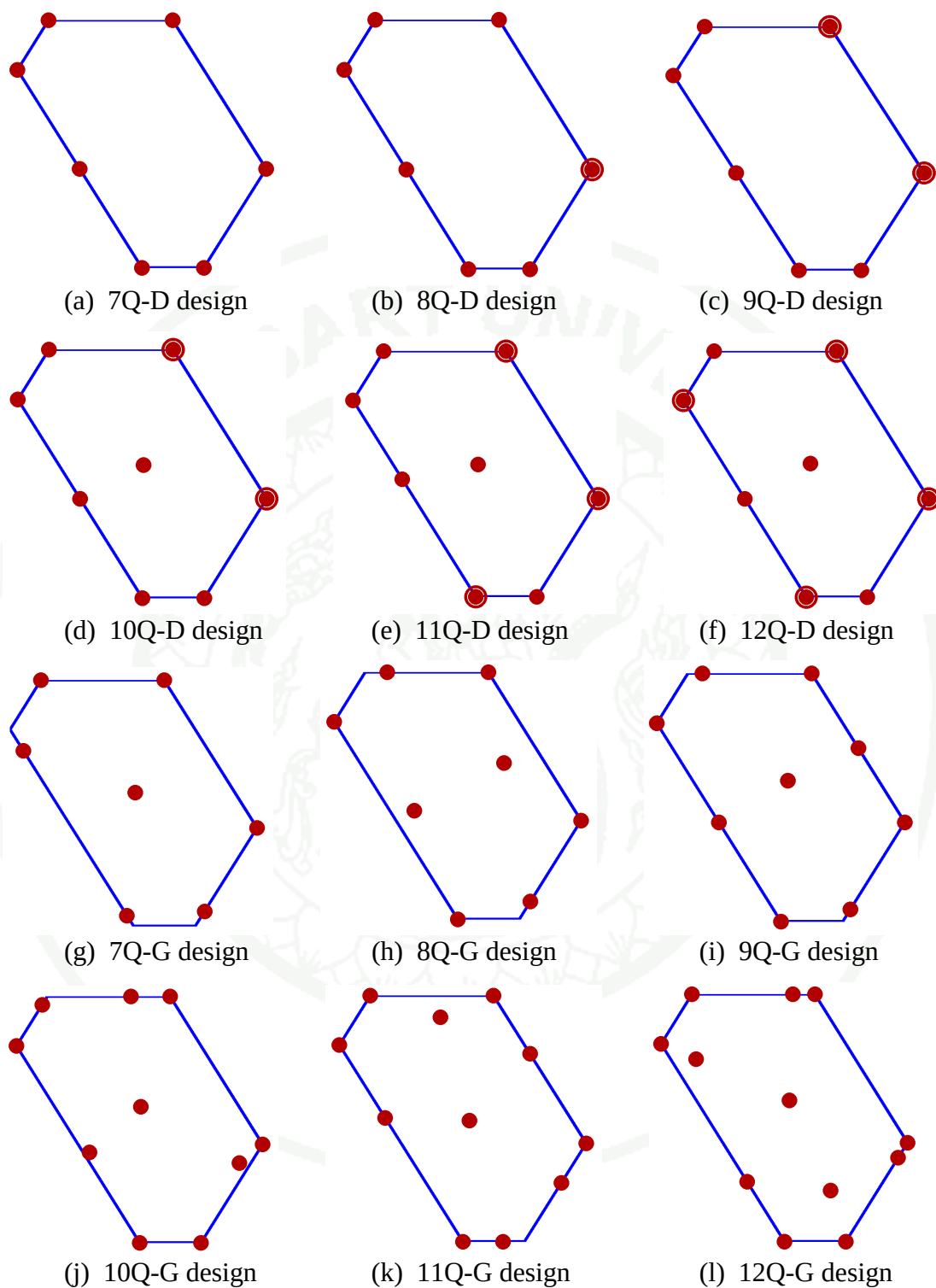


Figure 28 The optimal exact design points based on D_w and G_w when assuming the Scheffé quadratic model for the poultry experiment. ● and ⊙ represent 1 and 2 replicates of that design point, respectively.

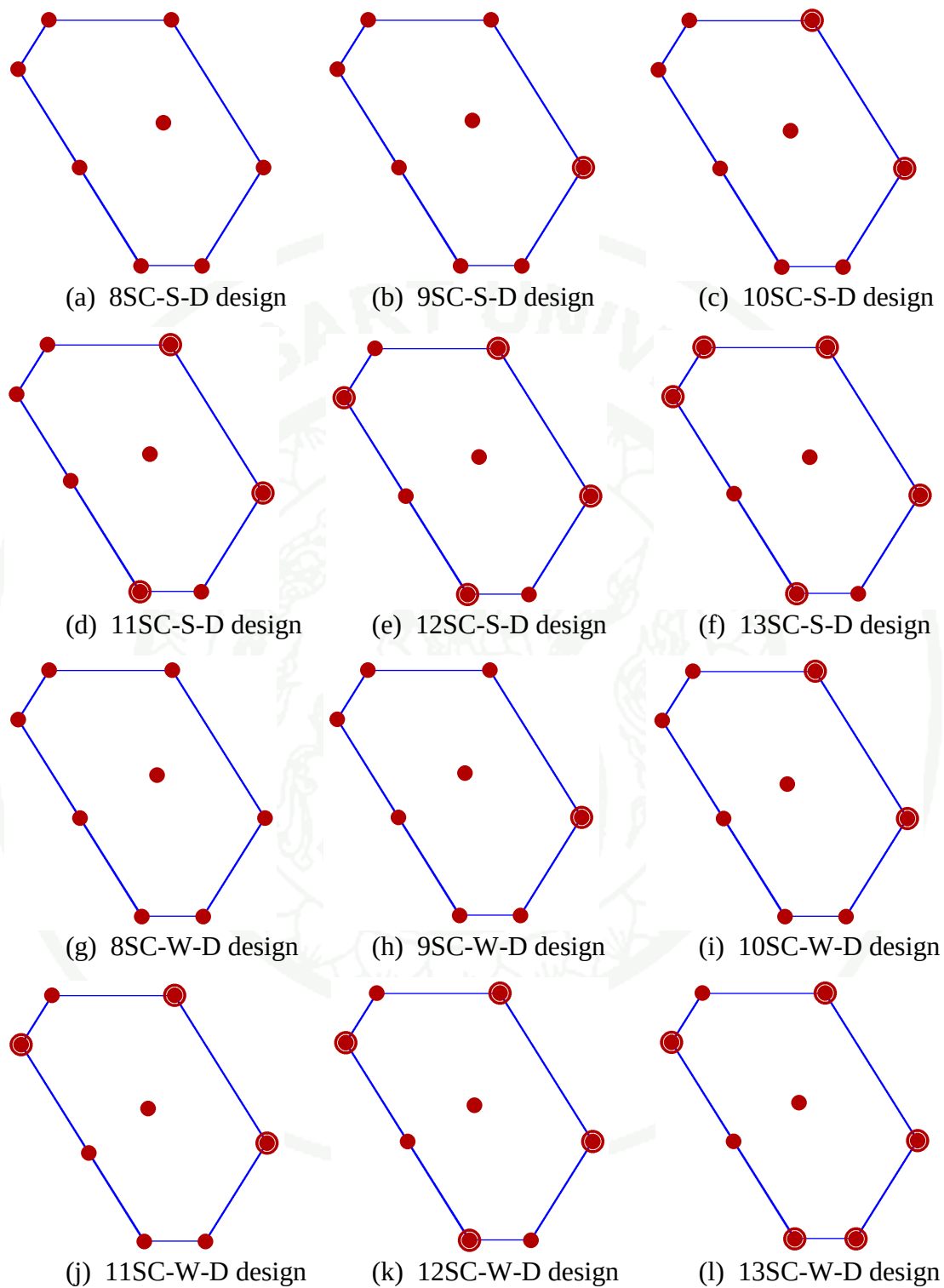


Figure 29 The optimal exact design points based on D_w when assuming the Scheffé special cubic model for the poultry experiment. ● and ⊙ represent 1 and 2 replicates of that design point, respectively.

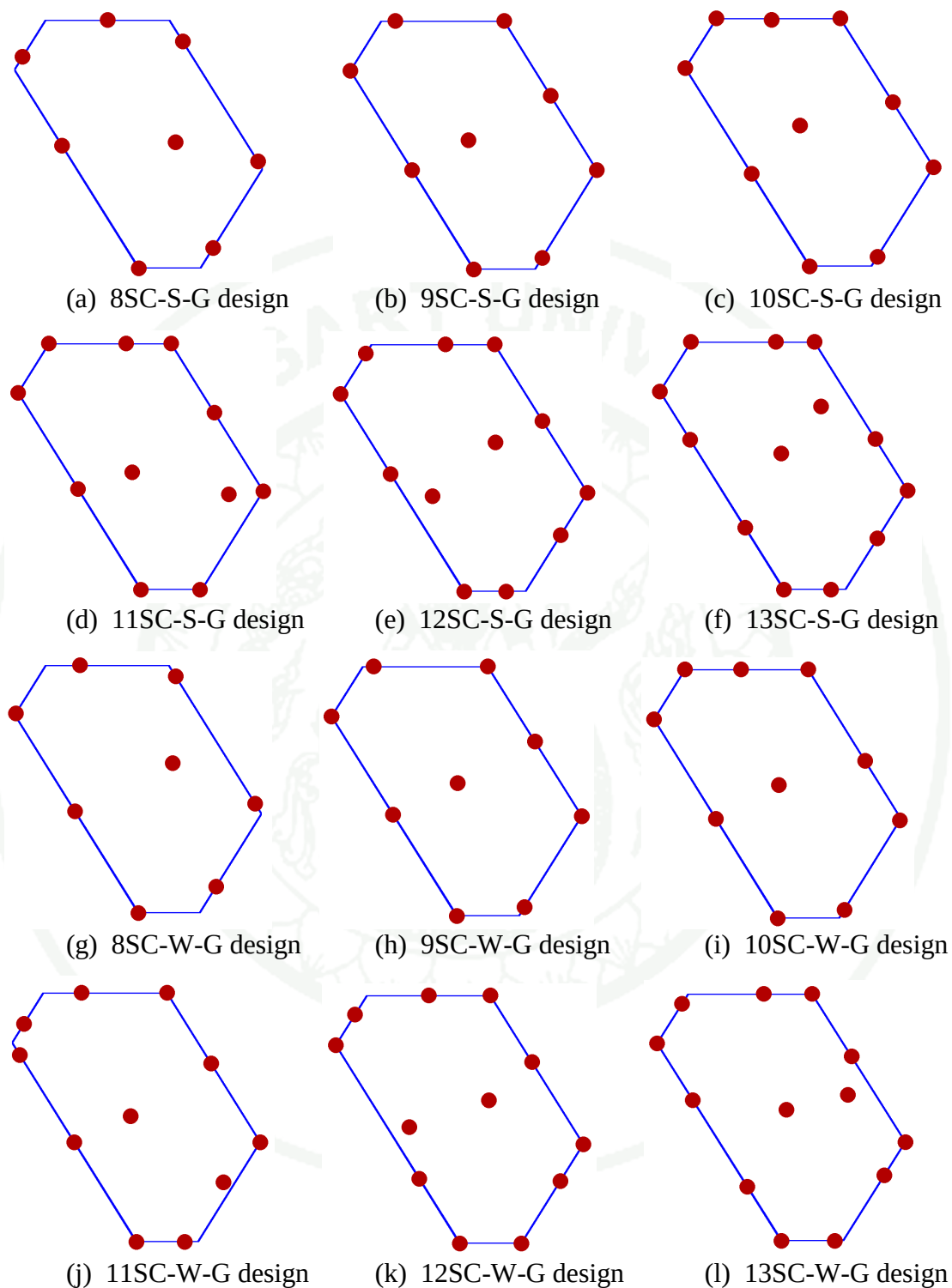


Figure 30 The optimal exact design points based on G_w when assuming the Scheffé special cubic model for the poultry experiment. ● represents 1 replicate of that design point.

When assuming the quadratic model with G_w , the designs (with the exception of the 8Q-G design) contain at least three of the six vertices plus a near overall centroid. For $n=7$ the 7Q-G design contains three vertices, near three vertices, and a near overall centroid. For $n=8$ and 9, the 8Q-G and 9Q-G designs both include the same four vertices and near two vertices. The remaining points of the 8Q-G design lie on faces which are close to an edge centroid, while the remaining points of the 9Q-G design contain near two edge centroids and a near overall centroid. For $n=10$ and 11, the 10Q-G and 11Q-G designs contain the same four vertices, one different vertex, and a near overall centroid. The remaining points of the 10Q-G design lie near two vertices and two edge centroids. The remaining points of the 11Q-G design lie near a vertex, three edge centroids, and an interior point which is close to an edge centroid. For $n=12$, the 12Q-G design includes all six vertices, near two vertices, near edge centroid and near overall centroid. The remaining points of 12Q-G lie on faces which are one point close to near edge centroid and another point close to vertices.

For the quadratic model, we notice that the patterns of points based on D_w are quite different than the patterns of points based on G_w in that they are all vertices with varying replication, either edge centroid or near edge centroid, and near overall centroid. Note that the 7Q-D, 8Q-D and 9-QD designs have no interior points, and thus, no near overall centroid.

For the special cubic model with D_w under SH and WH, there are obvious distributional patterns of the design points. For $n=8, 9, 10$, and 12, the designs (such as 8SC-S-D, 8SC-W-D, 9SC-S-D, 9SC-W-D, 10SC-S-D, 10SC-W-D, 12SC-S-D, 12SC-W-D) include all vertices with varying replications, an edge centroid, and a near overall centroid, while for $n=11$ and 13, the designs (such as 11SC-S-D, 11SC-W-D, 13SC-S-D, 13SC-W-D) include all vertices with varying replications, a near edge centroid, and a near overall centroid.

When assuming the special cubic model with G_w under SH and WH, the designs contain at least one of the six vertices plus a near overall centroid except for

the 12SC-S-G and 12SC-W-G designs. For $n=8$, the designs (such as 8SC-S-G, 8SC-W-G) are nearly identical containing a vertex, four near vertices, a near edge centroid and a near overall centroid. A remaining point of the 8SC-S-G and 8SC-W-G designs is an edge centroid and a near edge centroid, respectively. For $n=9$, the designs (such as 9SC-S-G, 9SC-W-G) are nearly identical containing four vertices, two near vertices, an edge centroid, a near edge centroid and a near overall centroid. The remaining point of the 9SC-S-G and 9SC-W-G designs is an edge centroid and a near edge centroid, respectively. For $n=10$, the designs (such as 10SC-S-G, 10SC-W-G) are nearly identical containing four vertices, a near vertex, three near edge centroids and a near overall centroid. A remaining point of the 10SC-S-G and 10SC-W-G designs is a vertex and a near vertex, respectively. For $n=11$, the designs (such as 11SC-S-G, 11SC-W-G) are nearly identical containing three vertices, a near vertex, three near edge centroids and a near overall centroid. The remaining points of the 11SC-S-G design contain two vertices and an interior point, while the remaining points of the 11SC-W-G design contain a near vertex and two near edge centroids. For $n=12$, the designs (such as 12SC-S-G, 12SC-W-G) are nearly identical containing four vertices, a near vertex, three near edge centroids and interior points which are close to an edge centroid. The remaining points of the 12SC-S-G design lie near a vertex and a near edge centroid, while the remaining points of the 12SC-W-G design contain a vertex and edge centroid.

For both SH and WH with the special cubic model as the model being fit, we observe that the distribution of points based on D_w are quite different than the distribution of points based on G_w in that they are all vertices with varying replications, either an edge centroid or near edge centroid, and a near overall centroid. Similar to the results for the quadratic model being fit, the geometries of the points based on D_w and G_w are different (see Figure 30). For both D_w and G_w and assuming the special cubic model, we see that the patterns of points under SH are quite similar to the patterns of points under WH. Note that all designs have interior points or a near overall centroid.

3. Evaluating designs for Case 1

When deciding which experimental design should be used, design optimality criteria are often used to evaluate proposed designs (in addition to considering the physical, time, cost, and design size constraints). However, the properties of a good design typically cannot be adequately summarized by single number criteria (such as an optimality criterion). That is, individual efficiency measures do not completely describe design performance. Graphical summaries such as a variance dispersion graph (VDG), a fraction of design space (FDS) plot, and a componentwise variance dispersion graph (CVDG) can provide additional information to aid the experimenter in design selection. The distribution of the scaled prediction variance (SPV) over the region of interest provides much more information than what can be obtained from a single number summary.

Relative design efficiencies are considered when the experimenter would like to assess how good his/her n -point designs are relative to all possible exact n -point designs based on an optimality criterion. Let D_w^{opt} and G_w^{opt} be the maxima of the D_w and G_w criteria when taken over all possible exact n -point designs. The relative design efficiencies can be expressed as

$$D_w^{eff} = \frac{D_w}{D_w^{opt}} \quad \text{and} \quad G_w^{eff} = \frac{G_w}{G_w^{opt}}. \quad (108)$$

The objective function values are used to calculate the relative design efficiencies for the optimal exact designs. The summary of the objective function values and the relative design efficiencies for the poultry experiment assuming the quadratic model and special cubic model are presented in Tables 17 and 19, respectively. The optimal exact designs have 100% relative efficiencies for their corresponding criterion. That is, the weighted D -optimal design is 100% D -efficient for the weighted D criterion, and the weighted G -optimal design is 100% G -efficient for the weighted G criterion. It is interesting to consider both criteria when evaluating a design.

Table 17 Performance comparison of the objective function and relative efficiencies of optimal exact designs when assuming the quadratic model for the poultry experiment.

Design points	Design	Objective function values		Relative efficiencies (%)	
		D_w	G_w	D_w^{eff}	G_w^{eff}
7	7Q-D	0.9101	46.3407	100	57.76
	7Q-G	0.8617	80.2307	94.68	100
8	8Q-D	0.9082	41.6180	100	51.35
	8Q-G	0.8449	81.0509	93.03	100
9	9Q-D	0.9176	44.8251	100	55.73
	9Q-G	0.8544	80.4382	93.11	100
10	10Q-D	0.9184	73.8626	100	91.26
	10Q-G	0.8523	80.9403	92.80	100
11	11Q-D	0.9192	68.9911	100	87.90
	11Q-G	0.8265	78.4854	89.92	100
12	12Q-D	0.9241	70.0024	100	90.95
	12Q-G	0.8243	76.9692	89.20	100

*Boldface indicates optimal exact value D_w^{opt} and G_w^{opt} .

In Table 17, assuming the quadratic model, the weighted D -optimal exact designs having $n \leq 9$ points have low G_w values, while the weighted G -optimal exact designs having $7 \leq n \leq 12$ points have high D_w values. For $10 \leq n \leq 12$, the weighted D - and G - optimal exact designs have efficiencies greater than 87% for both criteria. As the number of design points increase, the objective function values of the weighted optimal designs increase accordingly for the weighted D -optimal exact designs except when $n = 8$. As the number of design points increase, the objective function values of the weighted G -optimal designs do not yield a significant advantage.

In Figure 31, the VDGs of the minimum and maximum SPV values for shrinkage levels between 0 and 1 are plotted for the weighted D -optimal and weighted G -optimal exact designs assuming the quadratic model for the poultry experiment. Figure 32 contains the FDS plots for the weighted D -optimal and weighted G -optimal exact designs, assuming the quadratic model for the poultry experiment. For a given SPV value, a FDS plot shows the fraction of the design space with SPV values at or

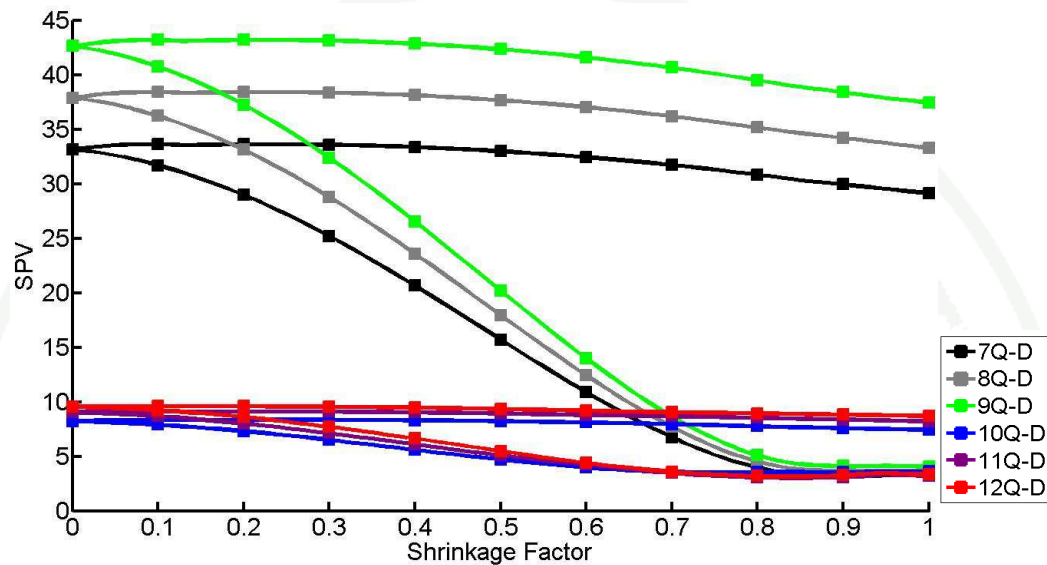
below the given SPV value. In Figure 33, the CVDGs of the maximum SPV for allowable mixtures with $x_i = a$ where $L_i \leq a \leq U_i$ are plotted for the weighted D -optimal and weighted G -optimal exact designs, assuming the quadratic model for the poultry experiment. The maximum SPV values for the weighted D -optimal and weighted G -optimal exact designs for the poultry experiment are presented in Table 18.

Table 18 Maximum SPV for the poultry experiment assuming the quadratic model.

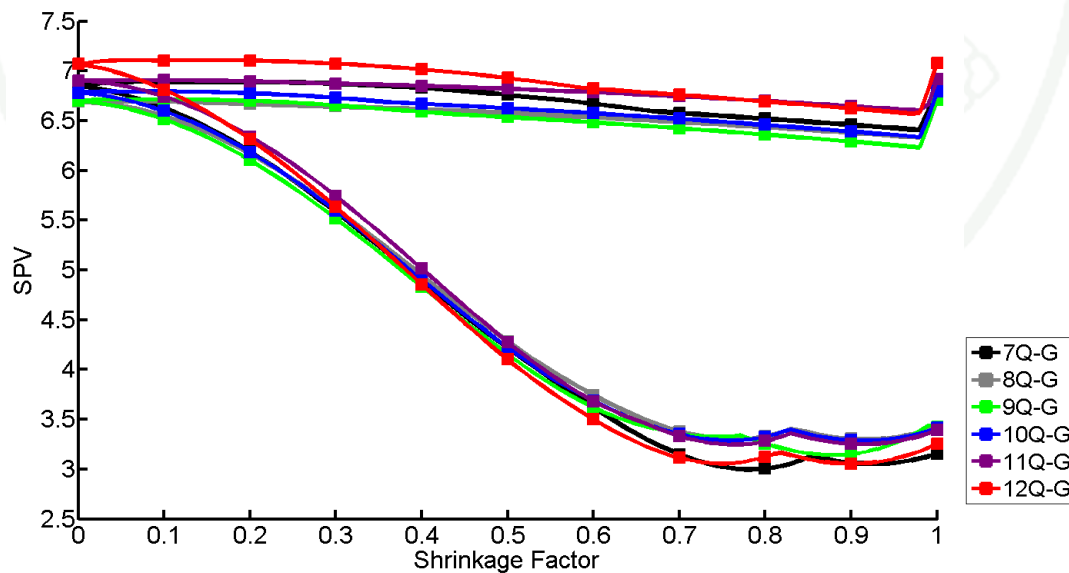
Design	Design points	Max SPV	Max SPV occurs that (x_1, x_2, x_3)
7Q-D	7	33.61	(0.575, 0.15, 0.275)
8Q-D	8	38.40	(0.575, 0.15, 0.275)
9Q-D	9	43.19	(0.575, 0.15, 0.275)
10Q-D	10	8.35	(0.575, 0.15, 0.275)
11Q-D	11	9.12	(0.57, 0.155, 0.275)
12Q-D	12	9.59	(0.575, 0.155, 0.27)
7Q-G	7	6.89	(0.575, 0.155, 0.27)
8Q-G	8	6.69	(0.7, 0.3, 0.0)
9Q-G	9	6.71	(0.57, 0.16, 0.27)
10Q-G	10	6.79	(0.57, 0.16, 0.27)
11Q-G	11	6.91	(0.8, 0, 0.2)
12Q-G	12	7.11	(0.58, 0.155, 0.265)

Figures 31 through 33 show that the SPVs for the 7Q-D, 8Q-D, and 9Q-D designs are not comparable with the other designs. The poor performance is likely due to having no design points in the interior or near the overall centroid (see Figure 28). In comparison to the weighted D -optimal exact designs, the 10Q-D design outperforms all of the weighted D -optimal designs with respect to the maximum SPV, although the 10Q-D, 11Q-D, and 12Q-D designs are quite comparable. The additional points near the overall centroid lower the maximum SPV. In comparison to the weighted G -optimal exact designs, the 8Q-G design outperforms all of the weighted

G-optimal designs with respect to the maximum SPV, although all of the weighted G-optimal designs are quite comparable. Figures 31 to 33 indicate that the additional design points, except for those near the overall centroid, do not significantly improve the SPV.



(a) The weighted *D*-optimal exact designs



(b) The weighted *G*-optimal exact designs

Figure 31 VDGs for the weighted optimal exact designs assuming the quadratic model for the poultry experiment.

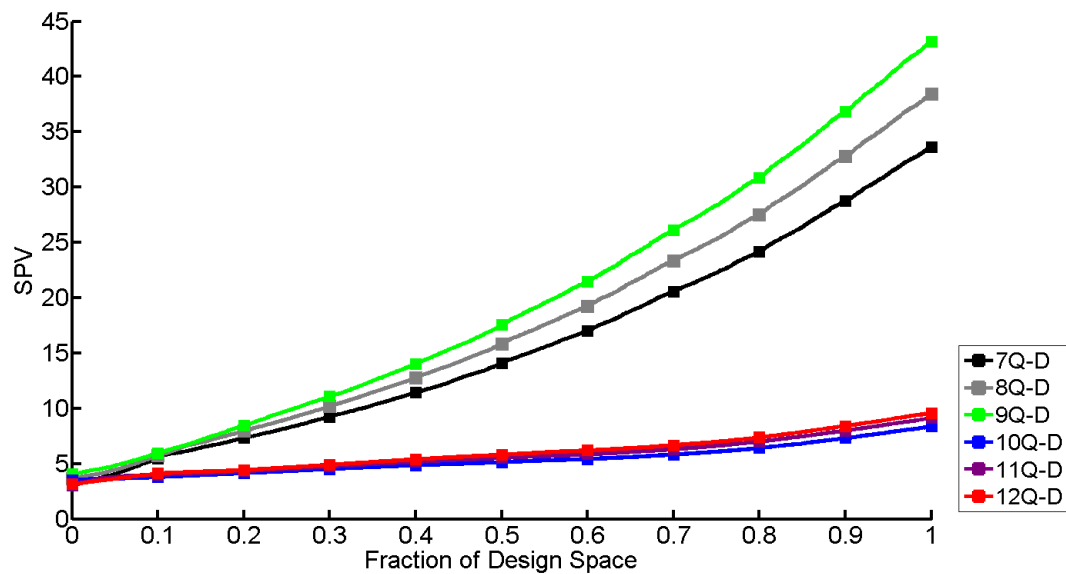
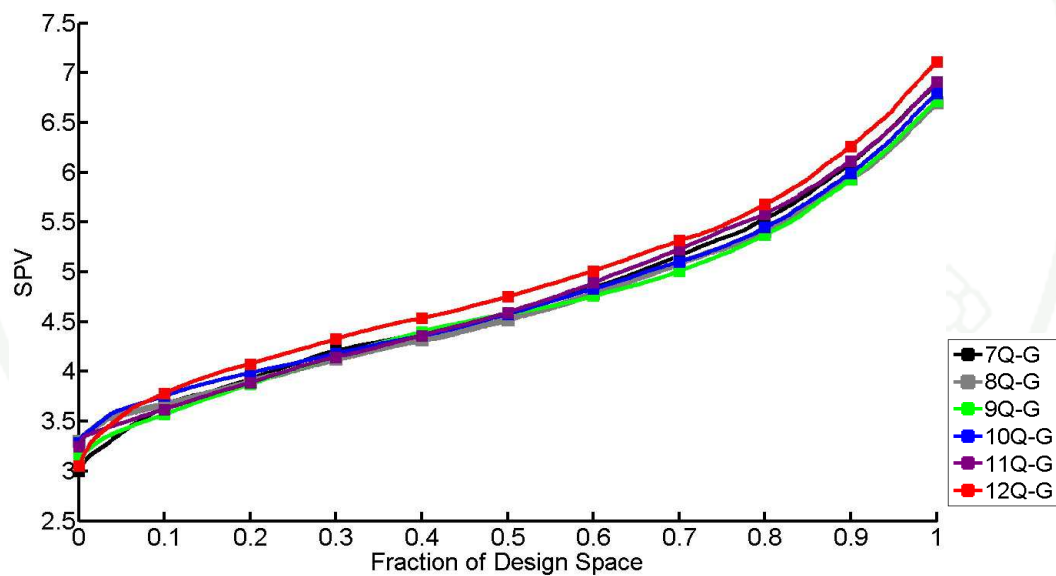
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 32 FDS plots for the weighted optimal exact designs assuming the quadratic model for the poultry experiment.

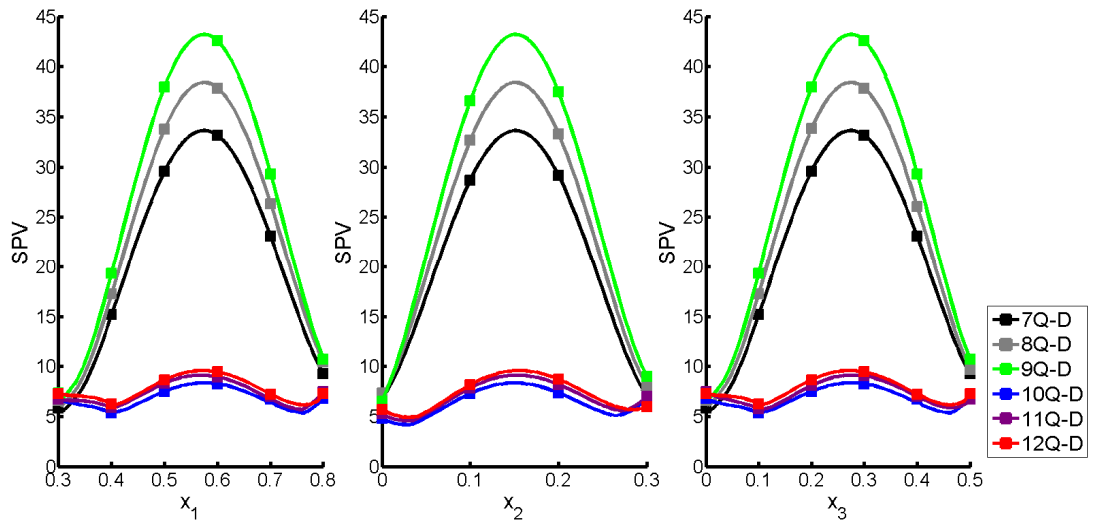
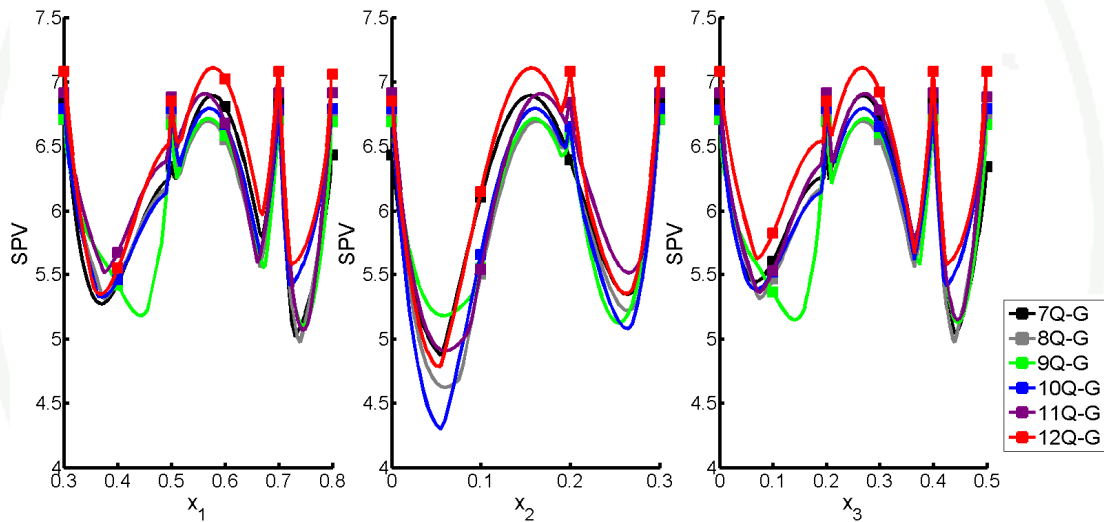
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 33 CVDGs of maximum SPV values for the weighted optimal exact designs assuming the quadratic model for the poultry experiment.

Figure 34 presents the VDG, FDS, and CVDG for the weighted D -optimal exact designs and weighted G -optimal exact designs for the poultry experiment. Solid lines are the weighted D -optimal exact designs and the dashed lines are the weighted G -optimal exact designs. We also see that the maximum SPV for 7Q-D, 8Q-D and 9Q-D design are significantly higher than that of the other designs. That is, 7Q-D, 8Q-D and 9Q-D designs have inferior prediction properties in comparison to other designs. Figure 35 is similar to Figure 34 without 7Q-D, 8Q-D, and 9Q-D design.

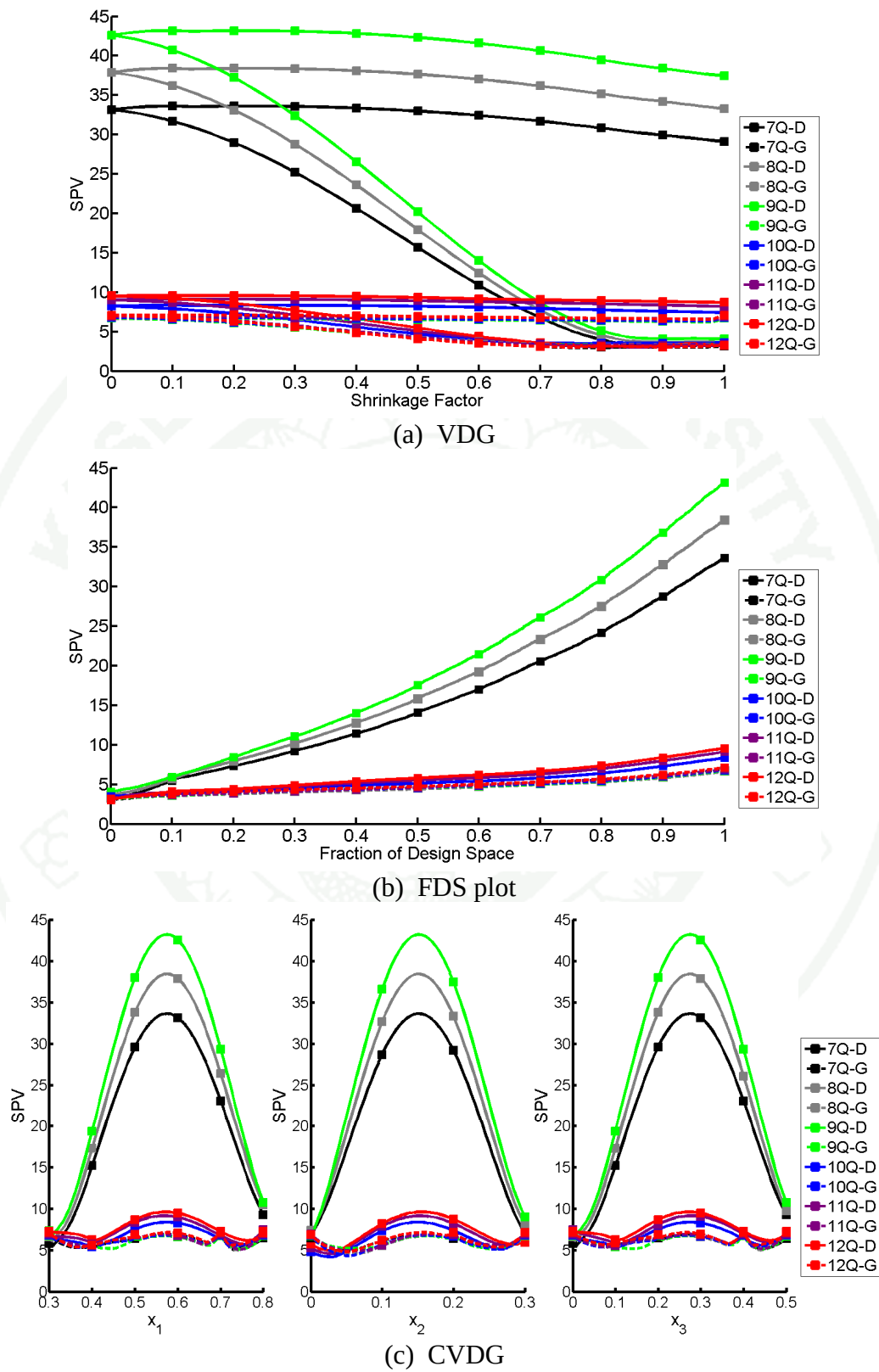


Figure 34 Graphical approaches for comparing 12 mixture designs for assuming the quadratic model for the poultry experiment.

In Figures 34(a) and 35(a), the VDGs are close for all weighted G -optimal exact designs, while the VDGs are quite different for the weighted D -optimal designs. An advantage of the weighted G -optimal exact designs is the smaller maximum across shrinkage levels between 0 and 1. In Figures 34(b) and 35(b), the FDS plot shows additional evidence of this advantage. For any chosen fraction of the design space, the corresponding SPV values for weighted D -optimal exact designs are larger than those of the weighted G -optimal exact designs. There is a clear separation of the weighted G -optimal exact designs from the weighted D -optimal exact designs when the fraction of the design space is $> 10\%$. The values of SPV for the weighted G -optimal designs are less than G -optimal bound (≈ 6) for approximately 85% of the design region. In Figures 34(c) and 35(c), the CVDGs describes the variability of the maximum SPV throughout the entire mixture design space. The weighted G -optimal exact designs are clearly superior to the weighted D -optimal designs.

From the VDGs on shrunken boundaries, the SPVs are larger for the weighted D -optimal exact designs than that for the weighted G -optimal exact designs. From the FDS plots, for over 95% of the design space, the weighted G -optimal exact designs are superior to the weighted D -optimal exact designs. It is clear that the weighted G -optimal exact designs have much flatter and lower FDS curves, indicating a more desirable SPV distribution. From the CVDGs, the mixture (x_1, x_2, x_3) yielding the maximum SPV value for the weighted D -optimal and weighted G -optimal exact design is given in the last column of Table 18. The SPVs near $(x_1, x_2, x_3) = (0.575, 0.15, 0.275)$ are inflated for 7Q-D, 8Q-D, and 9Q-D designs. These designs can be improved by adding the mixture at which the maximum SPV occurs.

Assuming the quadratic model, we conclude that (1) the weighted G -optimal exact designs have better prediction variance properties than the weighted D -optimal exact designs for nearly 95% of the design region, (2) the maximum SPVs for the weighted D -optimal exact designs are larger than those for the weighted G -optimal exact designs in all cases, and (3) the additional design points, except those near the overall centroid, do not produce better prediction properties.

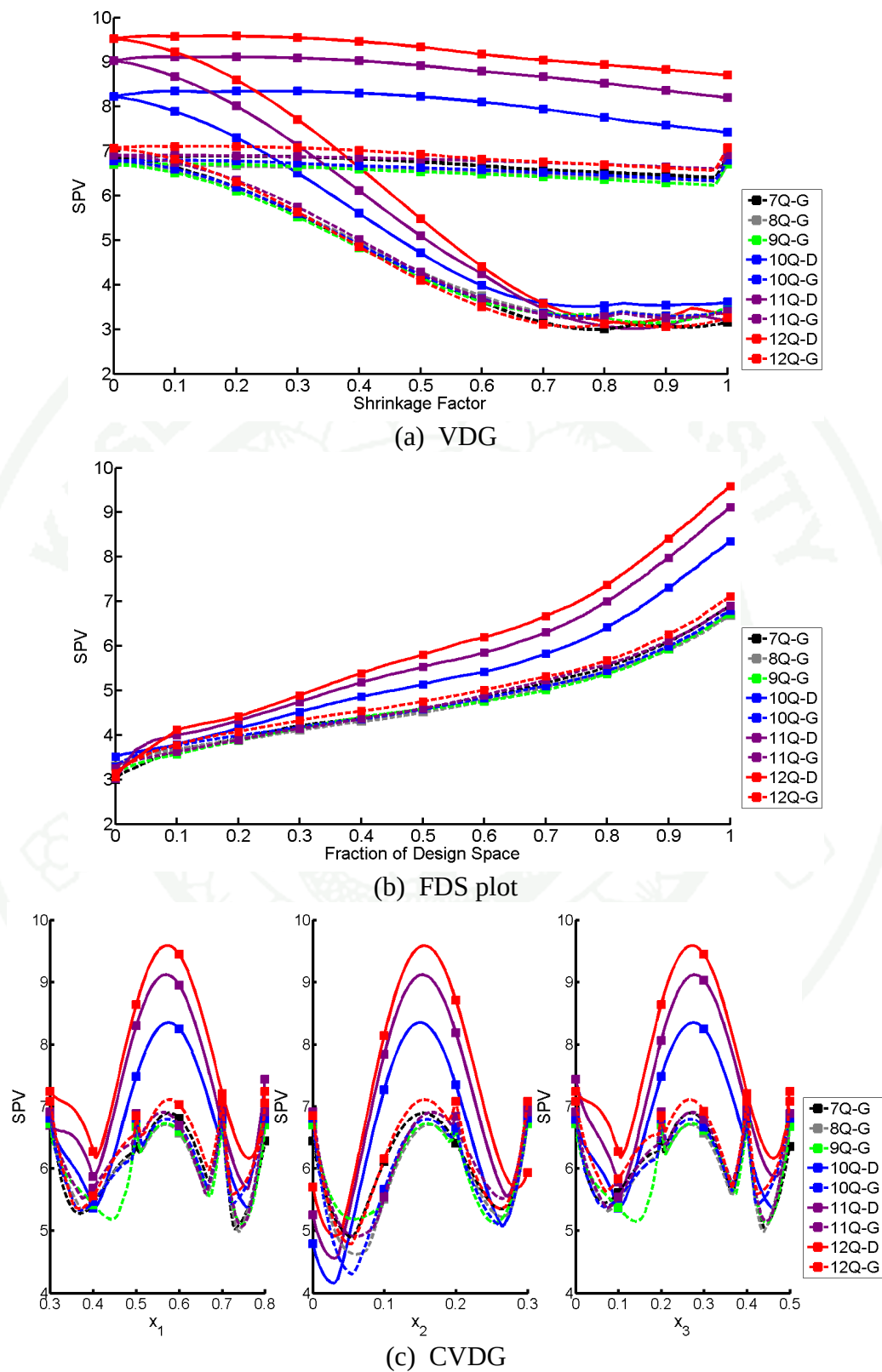


Figure 35 Graphical approaches for comparing 9 mixture designs for assuming the quadratic model for the poultry experiment.

In Table 19, $D_w - S$, $D_w - W$, $G_w - S$ and $G_w - W$ represent the weighted D -optimality criteria based on SH and WH and the weighted G -optimality criteria based on SH and WH, respectively. The weighted D -optimal exact designs under SH with $8 \leq n \leq 13$ points have high $D_w - S$ and $D_w - W$ values and quite low $G_w - S$ and $G_w - W$ values, while the weighted D -optimal exact designs under WH with $8 \leq n \leq 13$ points have high $D_w - S$ values and quite low $G_w - S$ and $G_w - W$ values. The weighted G -optimal exact designs under SH and WH with $8 \leq n \leq 13$ points, however, have high $D_w - W$ values as well as high $G_w - S$ and $G_w - W$ values.

The weighted G -optimal exact designs under SH with $n = 8, 10$ and 12 points are identical to the weighted G -optimal exact designs under WH or have relative efficiencies very close to 100%. Theoretically, the relative efficiencies should be 100%, but the GA terminated before finding the true weighted optimal exact designs under SH or WH. For $8 \leq n \leq 13$ points, the weighted D -optimal exact designs under SH and WH have D -efficiencies greater than 99%, while the weighted G -optimal exact designs under SH and WH have D - and G -efficiencies greater than 89% under SH and WH. As the number of design points increases, the objective function values of the weighted optimal exact designs increase accordingly for the weighted D -optimal exact designs based on SH and WH except when $n = 13$. As the number of design points increases, the objective function values of the weighted G -optimal exact designs based on SH and WH do not yield a significant advantage in SPV.

In Figure 36, the VDGs are plotted for the weighted D -optimal and weighted G -optimal exact designs assuming the special cubic model for the poultry experiment. The minimum and maximum of the SPV are plotted for shrinkage levels between 0 and 1. Figure 37 displays the FDS plot of weighted D -optimal and weighted G -optimal exact designs assuming the special cubic model for the poultry experiment. In the FDS plot, the fraction of the design space at or below any SPV value is shown. Figure 38 contains CVDGs of weighted D -optimal and weighted G -optimal exact designs for the special cubic model for the poultry experiment. The maximum of the SPV for allowable mixtures with $x_i = a$ where $L_i \leq a \leq U_i$ are shown. Table 20

presents the maximum SPV for the weighted D -optimal and weighted G -optimal exact designs assuming the special cubic model for the poultry experiment.

In Figure 36, the VDG lines are quite similar for all of the weighted G -optimal exact designs, while the others are also quite similar for the weighted D -optimal exact designs. From the VDG on shrunken boundaries, the SPV for the weighted D -optimal exact designs are greater than that of the weighted G -optimal exact designs at the perimeter of the region; however, at the design center, the SPV for the weighted D -optimal exact designs and weighted G -optimal exact designs are close to one another. The weighted G -optimal exact designs show an advantage with a lower maximum for shrinkage levels between 0 and 1.

In Figure 37, the FDS plot also provides useful information. We see that for almost 100% of the design space, the weighted G -optimal exact designs are superior to the weighted D -optimal exact designs. Like the quadratic model case, the weighted G -optimal exact designs begin to separate themselves from the weighted D -optimal exact designs once the fraction of the design space about 10%. The weighted D -optimal exact designs show a clear disadvantage throughout the design space, because for any chosen fraction of the design space, the corresponding SPV values are larger than those of the weighted G -optimal exact designs.

The SPV values for the worse case of the weighted D -optimal designs (the 13SC-W-D design) are less than 7 (the G -optimal bound) for approximately 50% of the design region, while for the best case of the weighted D -optimal exact designs (the 8SC-S-D design) the SPV values are less than 7 for approximately 80% of the design region. The SPV values for the worse case of the weighted G -optimal designs (the 8SC-W-G design) are less than 7 for approximately 80% of the design region, while for the best case of the weighted G -optimal exact designs (the 9SC-W-G design) the SPV values are less than 7 for approximately 98% of the design region. It is clear that the weighted G -optimal exact designs have much flatter and lower FDS curves throughout the design region, indicating more desirable SPV distribution.

Table 19 Performance comparison of objective function and relative efficiencies based on D - and G -criterion of optimal exact designs assuming the special cubic model for the poultry experiment.

n	Design	Objective function values				Relative efficiencies (%)			
		D_w -S	D_w -W	G_w -S	G_w -W	D_w^{eff} -S	D_w^{eff} -W	G_w^{eff} -S	G_w^{eff} -W
8	8SC-S-D	0.6035	0.5454	59.2414	58.3445	100	99.96	78.22	76.35
	8SC-W-D	0.6033	0.5456	57.9146	57.0102	99.97	100	76.47	74.60
	8SC-S-G	0.5415	0.4948	72.7775	72.0598	89.73	90.69	96.10	94.30
	8SC-W-G	0.5569	0.5080	75.7325	76.4169	92.28	93.11	100	100
9	9SC-S-D	0.6057	0.5482	53.2739	53.4946	100	99.96	62.39	64.08
	9SC-W-D	0.6055	0.5484	52.2245	52.4614	99.97	100	61.16	62.85
	9SC-S-G	0.5820	0.5299	85.3896	83.2501	96.09	96.63	100	99.73
	9SC-W-G	0.5847	0.5319	84.9635	83.4761	96.53	96.99	99.50	100
10	10SC-S-D	0.6143	0.5558	54.9698	55.3807	100	99.96	68.82	70.89
	10SC-W-D	0.6141	0.5560	54.1472	54.7503	99.97	100	67.79	70.09
	10SC-S-G	0.5770	0.5263	79.8722	78.1176	93.93	94.66	100	100
	10SC-W-G	0.5782	0.5272	79.6589	78.0611	94.12	94.82	99.73	99.93
11	11SC-S-D	0.6142	0.5560	51.4688	52.0112	100	99.78	65.76	66.73
	11SC-W-D	0.6139	0.5572	50.8426	52.2324	99.95	100	64.96	67.01
	11SC-S-G	0.5670	0.5178	78.2705	76.6860	92.32	92.93	100	98.39
	11SC-W-G	0.5543	0.5068	77.4339	77.9426	90.25	90.95	98.93	100
12	12SC-S-D	0.6176	0.5606	51.9885	52.3187	100	99.96	64.54	65.83
	12SC-W-D	0.6174	0.5608	51.3854	52.0796	99.97	100	63.79	65.53
	12SC-S-G	0.5524	0.5059	80.5527	79.4713	89.44	90.21	100	100
	12SC-W-G	0.5576	0.5099	80.2264	78.8811	90.28	90.92	99.59	99.26
13	13SC-S-D	0.6156	0.5576	49.6264	50.2336	100	99.95	62.36	64.08
	13SC-W-D	0.6154	0.5579	49.0031	50.1508	99.97	100	61.57	64.18
	13SC-S-G	0.5526	0.5034	79.5852	78.1394	89.77	90.23	100	99.68
	13SC-W-G	0.5489	0.5002	78.6395	78.3922	89.17	89.66	98.81	100

*Boldface indicates optimal exact value of D_w^{opt} and G_w^{opt} .

In Figure 38, the CVDG depicts the variability in the entire mixture design space. The weighted G -optimal exact designs perform well with respect to the weighted D -optimal designs. The maximum of SPV for the weighted D -optimal and weighted G -optimal exact designs occurs at mixture (x_1, x_2, x_3) given in the last column of Table 20. For the weighted D -optimal designs, the mixture (x_1, x_2, x_3) at which the maximum of SPV occurs is quite similar for each design. However, for the weighted G -optimal designs, the mixture (x_1, x_2, x_3) at which the maximum of SPV occurs is quite different for each design.

In Figures 36 through 38, the designs that are created based on SH have the same curve pattern seen in the VDG, FDS plot or CVDG as those plots for the designs that are created based on WH, while the pattern of each graphical approach for the weighted D -optimal exact designs differs from those of the weighted G -optimal exact designs. For D_w and G_w , the design points of the weighted optimal exact designs based on SH and WH are quite similar. Based on the maximum SPV, the weighted D -optimal exact design under SH and WH are also similar. Similarly, the weighted G -optimal exact design under SH and WH are comparable. For SH and WH, the weighted D -optimal exact design and weighted G -optimal exact designs are comparable at the design center for each design points; however, the weighted D -optimal exact designs are no longer competitive at the perimeter of the region for each design point. Based on the maximum SPV, the weighted D -optimal exact designs are not similar to the weighted G -optimal exact designs. In Table 20, the 8SC-S-D design is the best with smaller maximum SPVs for the weighted D -optimal exact designs, while the 9SC-S-G design is the best with smaller maximum SPV for the weighted G -optimal exact designs, whereas for the weighted optimal exact design the 9SC-S-G design is the best with smaller maximum SPV. Assuming the special cubic model, the additional design points do not yield a significant advantage in SPV which can be seen in Figures 36 to Figure 38.

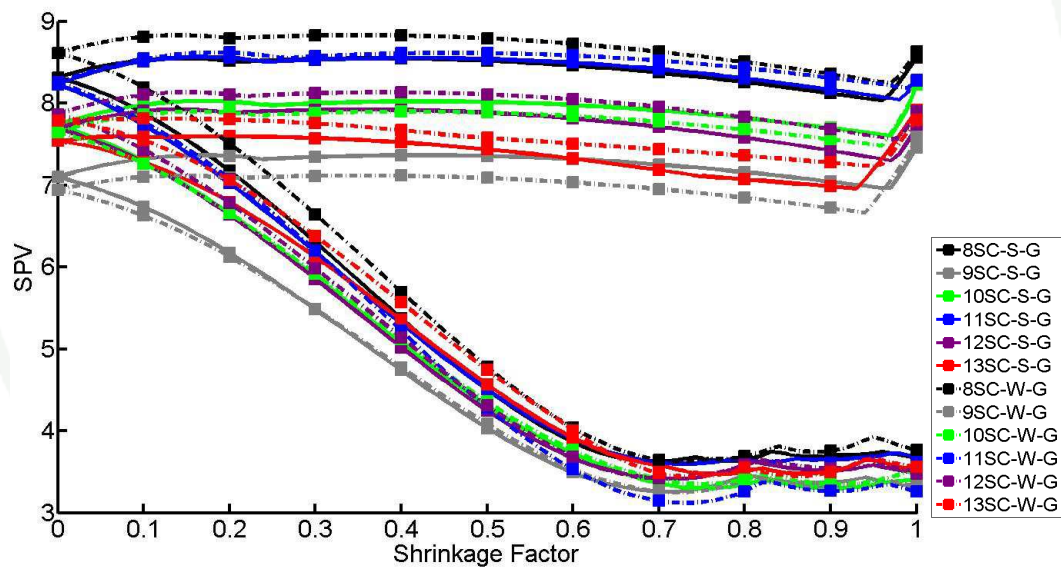
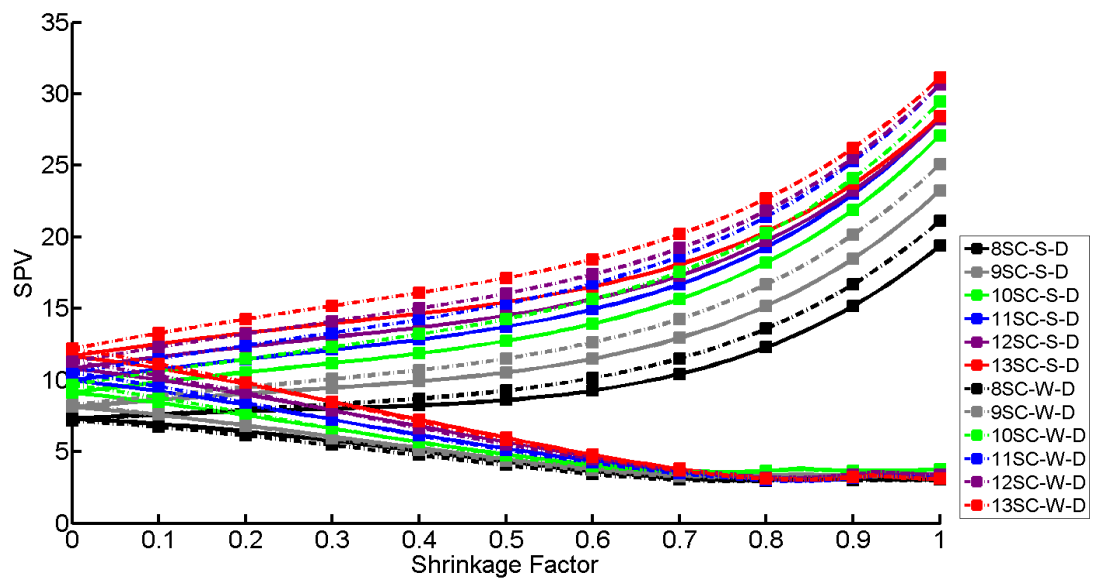


Figure 36 VDGs for the weighted optimal exact designs assuming the special cubic model for the poultry experiment.

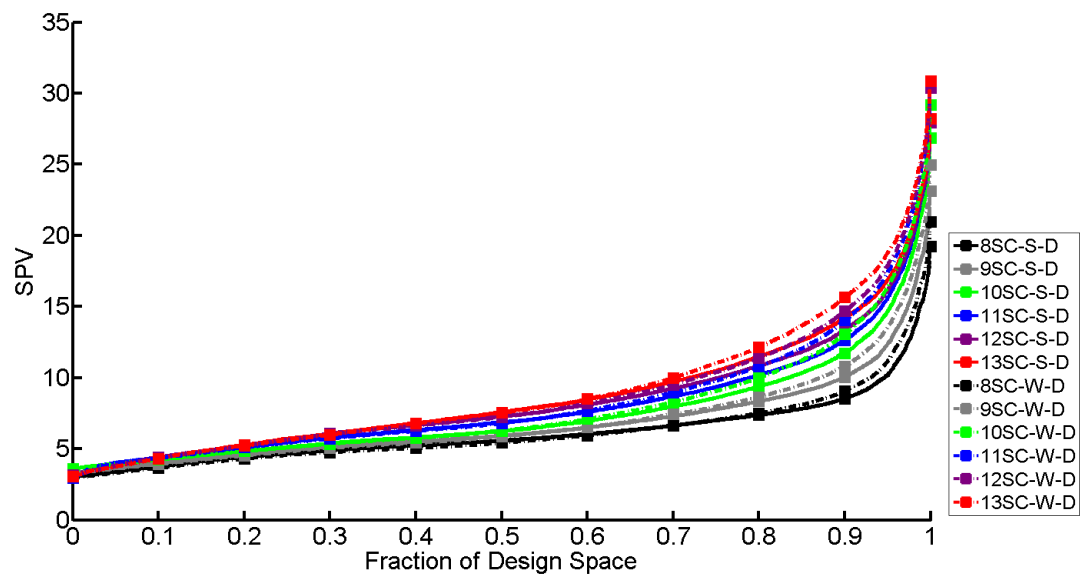
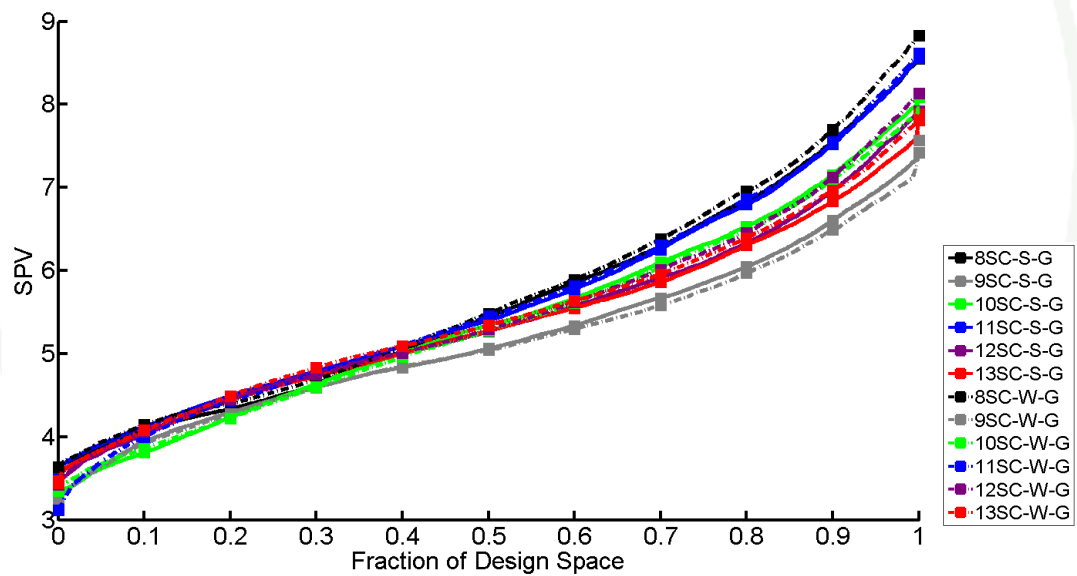
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 37 FDS plot for the weighted optimal exact design assuming the special cubic model for the poultry experiment.

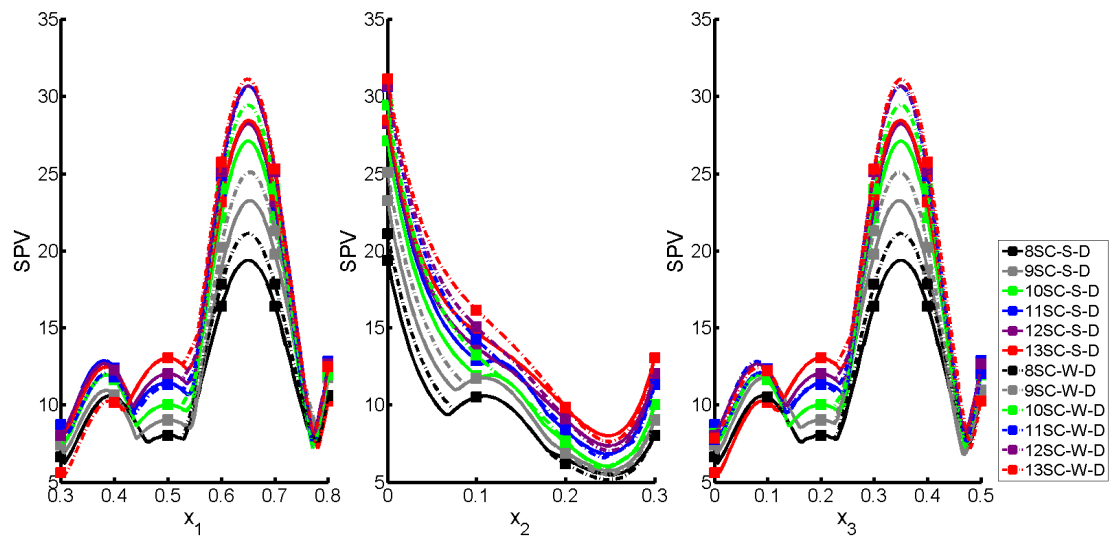
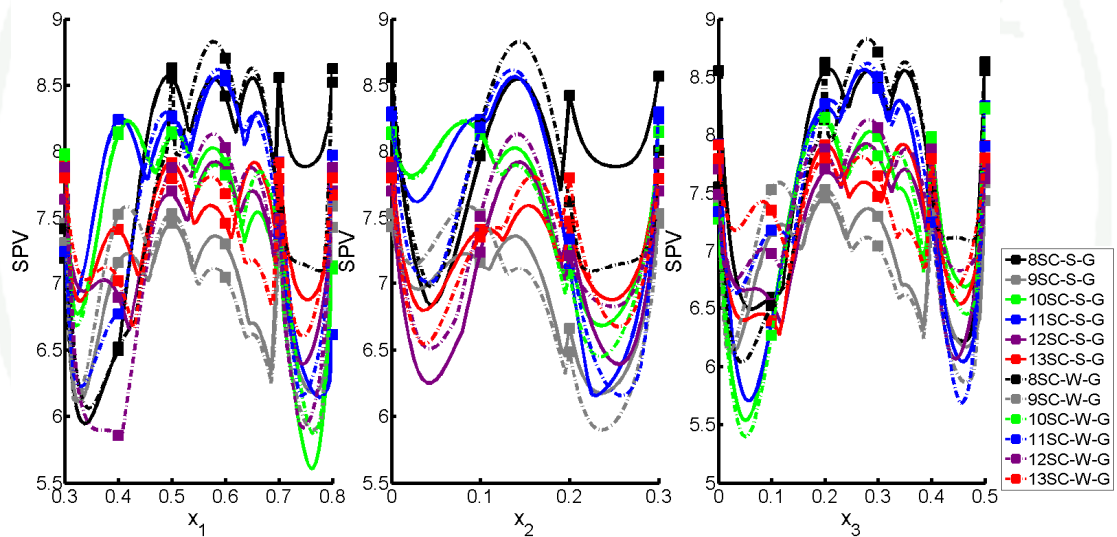
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 38 CVDGs for the weighted optimal exact design assuming the special cubic model for the poultry experiment.

Table 20 The maximum SPV for the poultry experiment assuming the special cubic model.

	Design	Max SPV	Max SPV occurs that (x_1, x_2, x_3)
The weighted <i>D</i> -optimal exact designs based on SH	8SC-S-D	19.22	(0.65, 0, 0.35)
	9SC-S-D	23.11	(0.655, 0, 0.345)
	10SC-S-D	26.84	(0.65, 0, 0.35)
	11SC-S-D	27.98	(0.65, 0, 0.35)
	12SC-S-D	27.96	(0.65, 0, 0.35)
	13SC-S-D	28.24	(0.65, 0, 0.35)
The weighted <i>D</i> -optimal exact designs based on WH	8SC-W-D	20.94	(0.65, 0, 0.35)
	9SC-W-D	24.94	(0.655, 0, 0.345)
	10SC-W-D	29.17	(0.65, 0, 0.35)
	11SC-W-D	30.39	(0.65, 0, 0.35)
	12SC-W-D	30.39	(0.65, 0, 0.35)
	13SC-W-D	30.85	(0.65, 0, 0.35)
The weighted <i>G</i> -optimal exact designs based on SH	8SC-S-G	8.55	(0.495, 0.3, 0.205)
	9SC-S-G	7.42	(0.5, 0.3, 0.2)
	10SC-S-G	8.09	(0.42, 0.08, 0.5)
	11SC-S-G	8.56	(0.585, 0.14, 0.275)
	12SC-S-G	7.92	(0.58, 0.145, 0.275)
	13SC-S-G	7.88	(0.655, 0, 0.345)
The weighted <i>G</i> -optimal exact designs based on WH	8SC-W-G	8.83	(0.575, 0.145, 0.28)
	9SC-W-G	7.56	(0.8, 0.085, 0.115)
	10SC-W-G	8.11	(0.415, 0.085, 0.5)
	11SC-W-G	8.62	(0.585, 0.135, 0.28)
	12SC-W-G	8.13	(0.58, 0.14, 0.28)
	13SC-W-G	7.81	(0.57, 0.16, 0.27)

For the special cubic model, we conclude that (1) the weighted G -optimal exact designs have better prediction properties than the weighted D -optimal exact designs throughout the design region, (2) the weighted G -optimal exact designs under SH and WH have similar profiles, whereas the weighted D -optimal exact designs under SH and WH have similar profiles as well, (3) the maximum SPV for the weighted D -optimal exact designs results in higher value than that of the weighted G -optimal exact designs in all cases, (4) the maximum SPV for the weighted D -optimal exact designs under SH and WH are quite similar, whereas the maximum SPV for the weighted G -optimal exact designs under SH and WH are also similar, and (5) as the design size increases, the weighted D -optimal designs have poorer prediction properties, whereas as the design size increases, the weighted G -optimal designs do not yield better prediction properties.

4. Examining model robustness for Case 1

Frequently, after the data are collected, the model may be subsequently changed because the experimenter finds that some effects may not be significant in the model and likely decide to choose a reduced model in the analysis phase. When the full model does not turn out to be the final model selected in the analysis phase, the prediction variance properties may be less desirable than for the initial design. The experimenter needs a tool to help him/her select the best design regardless of the final model selected. A serious problem occurs if the final model does not have sufficient complexity to adequately approximate the true underlying relationship which results in fitting an inappropriate model to our data. In this section, the FDS plots are used to study the robustness of a design to model change.

Suppose that **the quadratic model** corresponds to the most complex model that the experimenter might need to adequately model the data. For $q = 3$, there are 8 models nested within the full model. Table 21 gives a number of possible nested models for quadratic model which might be of interest when examining the mixture designs. In Figure 39, the corresponding FDS curves for the 7Q-D design shows that (1) the quadratic and linear model are enveloped around other models considered (2)

the plots for Model A to Model F are located between plots for quadratic and plots for the linear model and (3) any model that is nested within another model must have FDS curves that are at or below the curves for the larger model. The quadratic model FDS curve has a rather different slope than the remaining curves. Thus, addition of quadratic terms has a much larger affect on the stability of the SPV values. The last column of Table 21 shows the maximum SPV values for each model of the 7Q-D design.

We will look at a few common classes of models on the single FDS plot: only the quadratic model and the linear model are considered because these models give a manageable summary of the prediction performance of the design across a set of candidate models.

Table 21 Summary information for the possible reduced models assuming the quadratic model for the poultry experiment.

Type of model	Term in model	p	Max SPV
Quadratic	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3$	6	33.62
Model A	$x_1, x_2, x_3, x_1x_3, x_2x_3$	5	6.27
Model B	$x_1, x_2, x_3, x_1x_2, x_2x_3$	5	6.45
Model C	$x_1, x_2, x_3, x_1x_2, x_1x_3$	5	6.32
Model D	x_1, x_2, x_3, x_2x_3	4	6.23
Model E	x_1, x_2, x_3, x_1x_3	4	5.26
Model F	x_1, x_2, x_3, x_1x_2	4	6.29
Linear	x_1, x_2, x_3	3	3.81

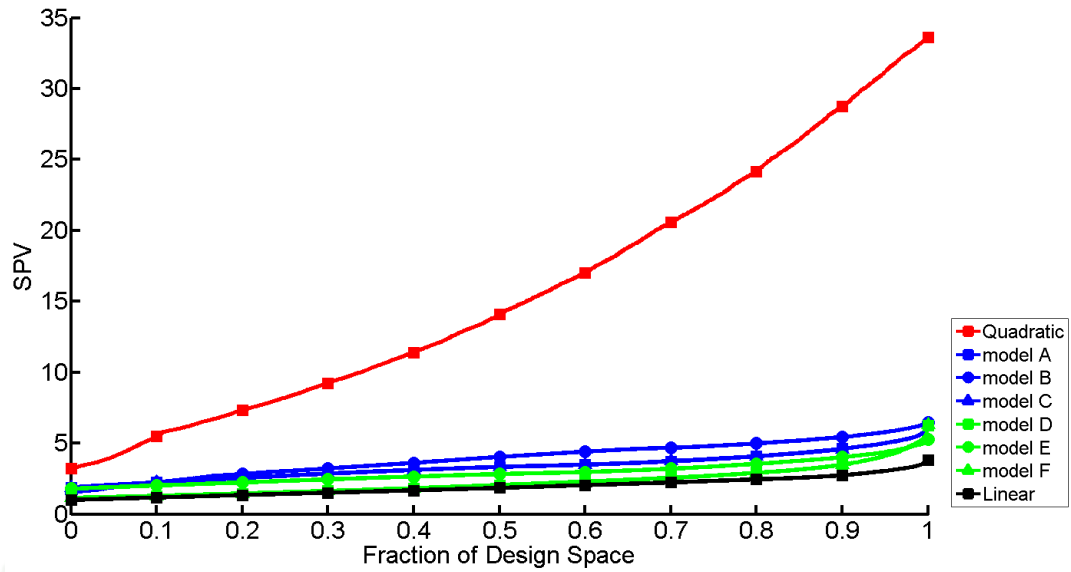


Figure 39 FDS plot for 7Q-D design for several models for the poultry experiment.

Figure 40 shows the comparison between the weighted D -optimal and weighted G -optimal exact designs for each design size. The comparison for all of the weighted D -optimal exact designs is shown in Figure 41 while Figure 42 displays the comparison for all of the weighted G -optimal exact designs. Table 22 contains the G -efficiency and the maximum SPV values for each design. In the previous section, the weighted G -optimal exact designs were shown to be superior to the weighted D -optimal exact designs and the 7Q-D, 8Q-D and 9Q-D designs were no longer competitive. That is, the VDG, FDS plot and CVDG curves for the quadratic model for the weighted G -optimal exact designs are lower than the corresponding curves for the weighted D -optimal exact designs for most of the design space.

As shown in Figure 40, for the linear model, the weighted D -optimal and weighted G -optimal exact designs are quite similar in performance for most of the design space. Only the maximum SPV values of the weighted G -optimal exact designs are larger than those for the weighted D -optimal exact designs for the linear model resulting in lower G -efficiencies except for $n = 7$ as shown in Table 22. For the quadratic model, the weighted G -optimal designs perform better than the weighted D -optimal designs for the entire design space because they maintain better stability

for large SPV values. As previously stated, the 7Q-D, 8Q-D and 9Q-D designs are no longer competitive for the quadratic model. The weighted *G*-optimal exact designs perform the best for the quadratic and linear models.

Figure 41 shows that 10Q-D, 11Q-D and 12Q-D designs seem to perform equally well and maintain better stability for large SPV values for the quadratic model and linear model. For the weighted *D*-optimal design, the 10Q-D design performs the best for the quadratic model and linear model because it has the best *G*-efficiencies for both model types. In Figure 42, all weighted *G*-optimal designs perform equally well and maintain better stability for large values of SPV for the quadratic model and linear model. For the weighted *G*-optimal design, the 8Q-G, 9Q-G and 10Q-G designs perform very well for the quadratic model and linear model because they have the best *G*-efficiencies for both model types.

Table 22 The maximum SPV values and approximate *G*-efficiencies for the weighted *D*-optimal and weighted *G*-optimal exact designs for two model types, assuming the quadratic model for the poultry experiment.

Design	Model type	G-eff	Max SPV	Design	Model type	G-eff	Max SPV
7Q-D	Quadratic	17.85%	33.61	7Q-G	Quadratic	87.08%	6.89
	Linear	78.74%	3.81		Linear	79.58%	3.77
8Q-D	Quadratic	15.63%	38.40	8Q-G	Quadratic	89.69%	6.69
	Linear	81.97%	3.66		Linear	78.53%	3.82
9Q-D	Quadratic	13.89%	43.19	9Q-G	Quadratic	89.42%	6.71
	Linear	85.23%	3.52		Linear	77.92%	3.85
10Q-D	Quadratic	71.86%	8.35	10Q-G	Quadratic	88.37%	6.79
	Linear	79.79%	3.76		Linear	79.58%	3.77
11Q-D	Quadratic	65.79%	9.12	11Q-G	Quadratic	86.83%	6.91
	Linear	77.72%	3.86		Linear	74.63%	4.02
12Q-D	Quadratic	63.03%	9.52	12Q-G	Quadratic	84.39%	7.11
	Linear	87.46%	3.43		Linear	78.33%	3.83

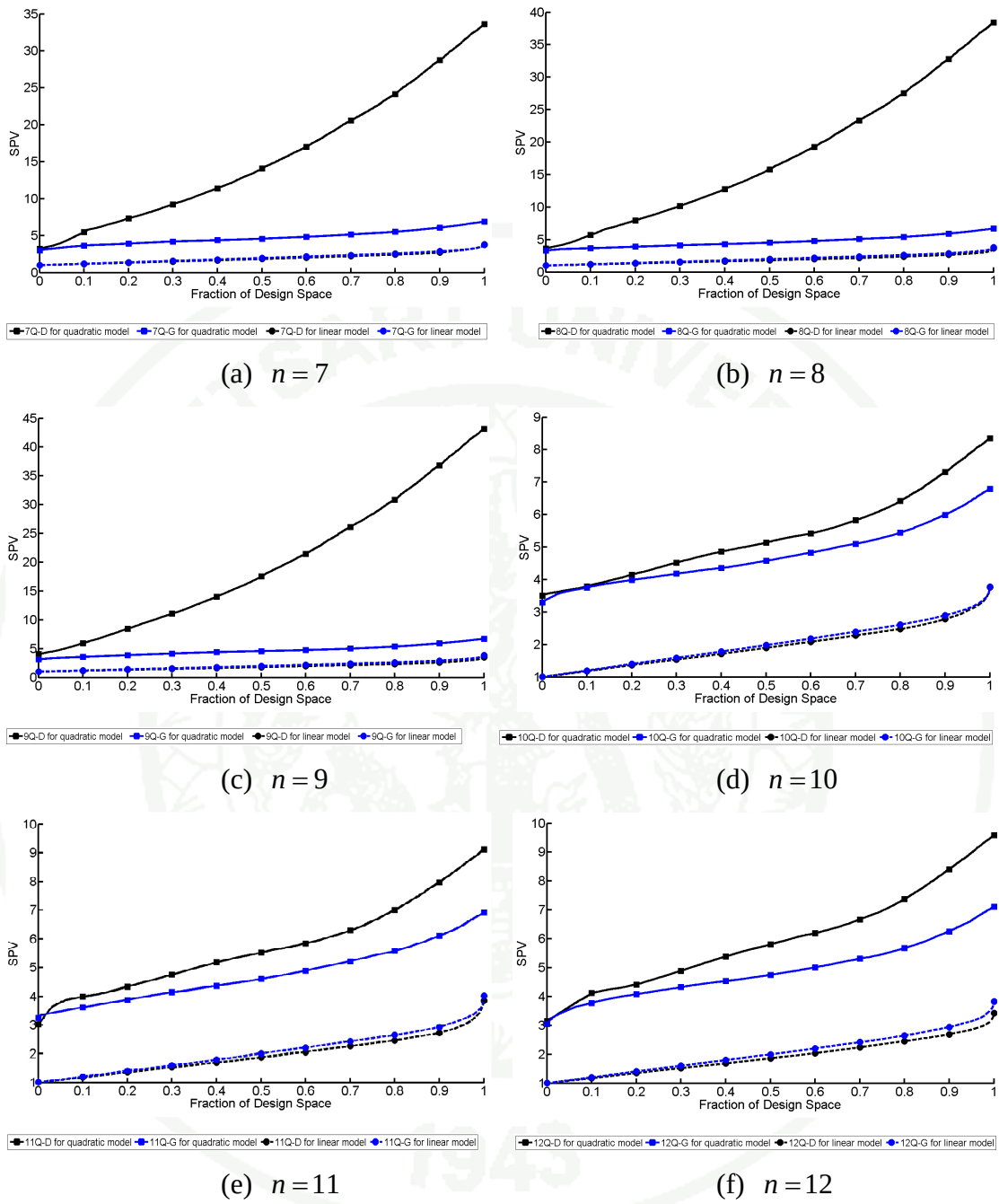


Figure 40 FDS plots for comparing the weighted D -optimal exact design and weighted G -optimal exact design for two types of models assuming the quadratic model for the poultry experiment.

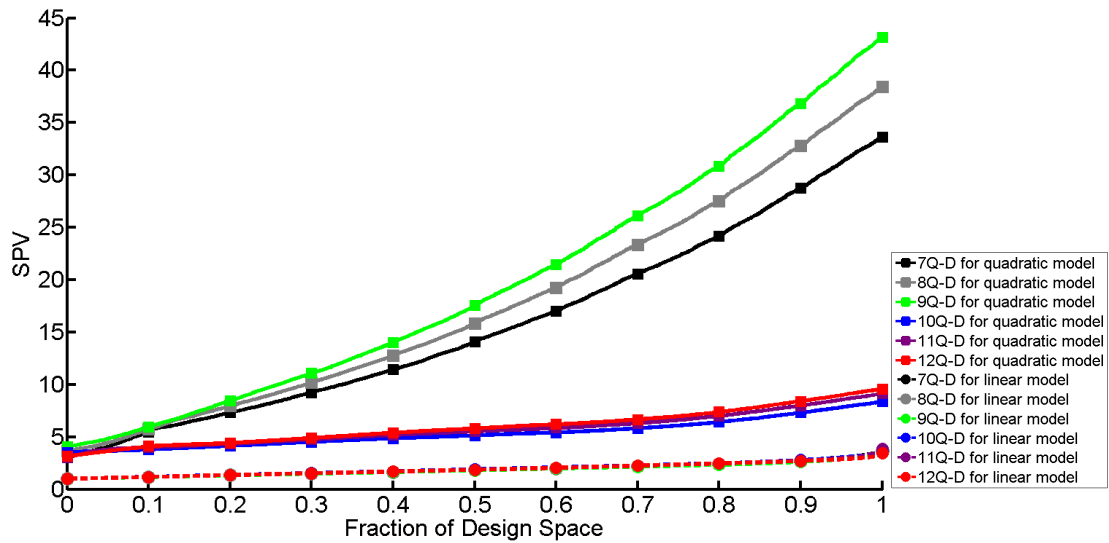


Figure 41 FDS plots for comparing the D -optimal exact designs for two types of models assuming the quadratic model for the poultry experiment.

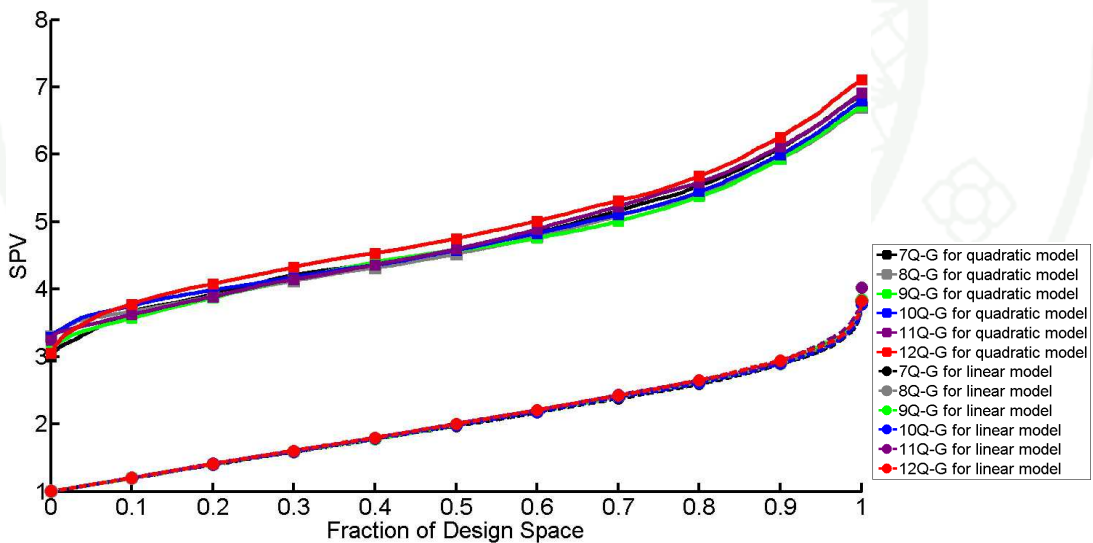


Figure 42 FDS plots for comparing the G -optimal exact designs for two types of models assuming the quadratic model for the poultry experiment.

For the majority of the design space, the weighted G -optimal designs and some of the weighted D -optimal designs, such as the 10Q-D, 11Q-D and 12Q-D designs, appear to have good robustness properties because they have much flatter and lower FDS curves for both model types, indicating more desirable SPV distributions. However, the weighted G -optimal designs are recommended for model robustness over the weighted D -optimal exact designs because (1) all of the curves associated with both models for the weighted G -optimal designs are closer together on the FDS plot than for the weighted D -optimal exact designs, and (2) the weighted G -optimal designs appear to outperform the weighted D -optimal exact designs.

Now suppose that **the special cubic model** corresponds to the most complex model that the experimenter might need to adequately model the data. For $q = 3$, there are 9 SH models and 15 WH models that are nested within the special cubic model. A number of possible nested models for the special cubic model under SH and WH, which might be of interest when examining the mixture designs, are given in Table 23. The corresponding FDS curves for the 8SC-S-D and 8SC-W-D designs are shown in Figures 43 and 44, respectively. The full model is the purple line and there are 7 parameters in the model, while there are 6 parameters in the model shown in red, 5 parameters in the model shown in blue, and 4 parameters in the model shown in green. The black line corresponds to the linear model which has an FDS curve that is at or below the green lines (linear models with one quadratic term), while the green lines are FDS curves that are at or below the blue lines (linear models with two quadratic terms), whereas the blue lines are FDS curves that are at or below the purple line for the special cubic model. We see that the special cubic model, the quadratic model and the linear model are enveloped around other models and the larger models have FDS curves that are at or on the top of the nested models for all fractions of the design space. The special cubic model FDS curve has a very different slope from the remaining curves. Thus, the addition of cubic terms have a much larger effect on the stability of the SPV values.

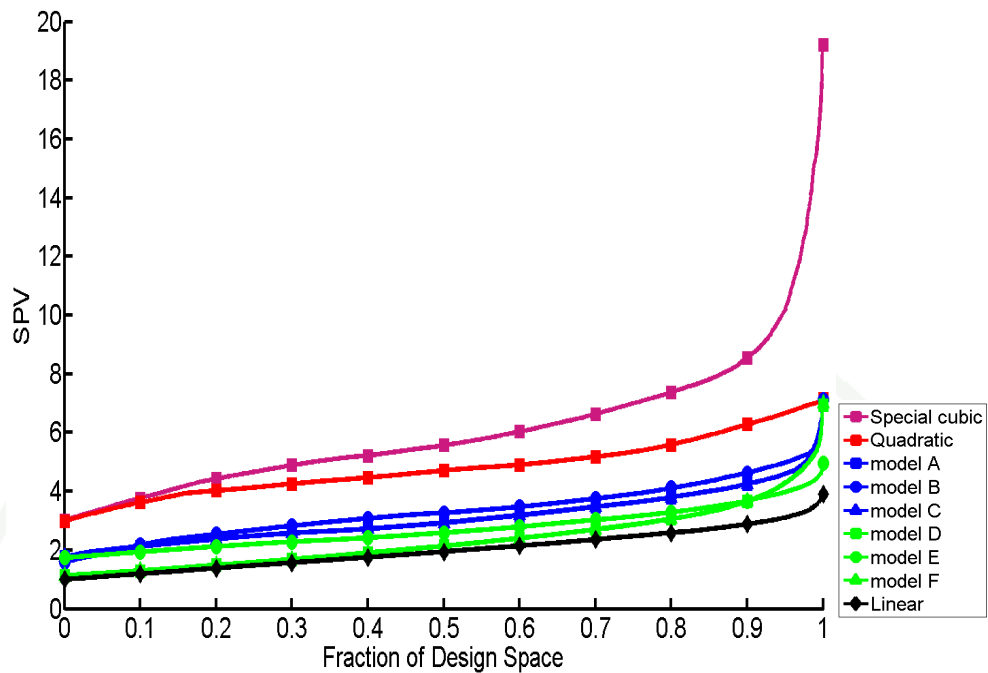


Figure 43 FDS plot for 8SC-S-D design for several models for the poultry experiment.

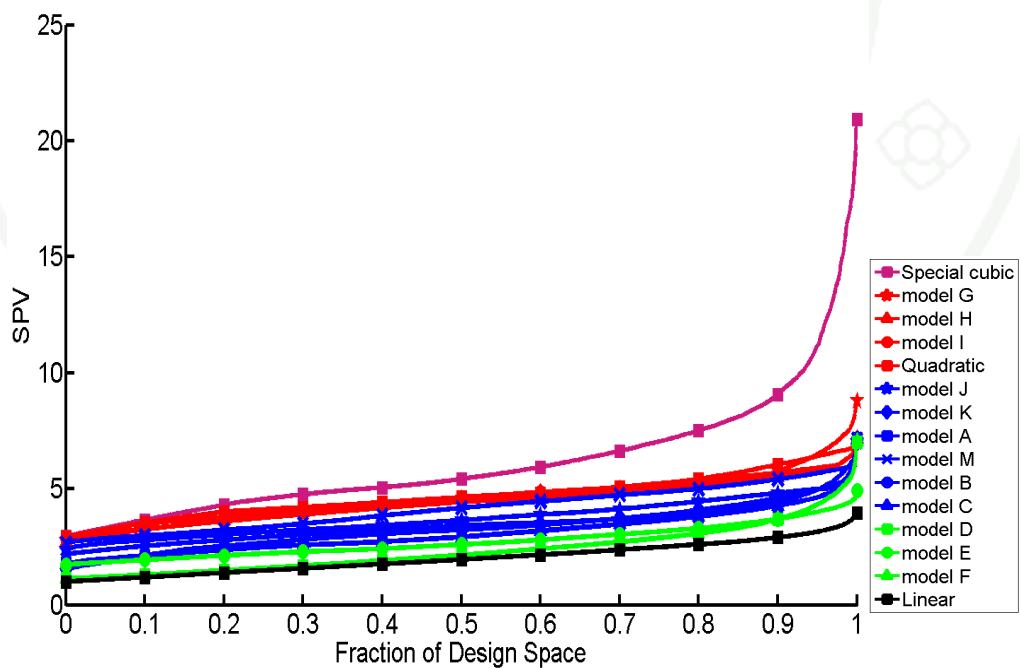


Figure 44 FDS plot for 8SC-W-D design for several models for the poultry experiment.

Table 23 Summary information for the possible SH and WH reduced models for assuming the special cubic model for the poultry experiment.

Heredity Type	Type of model	Term in model	p
SH	Special cubic	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2x_3$	7
	Quadratic	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3$	6
	Model A	$x_1, x_2, x_3, x_1x_3, x_2x_3$	5
	Model B	$x_1, x_2, x_3, x_1x_2, x_2x_3$	5
	Model C	$x_1, x_2, x_3, x_1x_2, x_1x_3$	5
	Model D	x_1, x_2, x_3, x_2x_3	4
	Model E	x_1, x_2, x_3, x_1x_3	4
	Model F	x_1, x_2, x_3, x_1x_2	4
	Linear	x_1, x_2, x_3	3
WH	Special cubic	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2x_3$	7
	Model G	$x_1, x_2, x_3, x_1x_3, x_2x_3, x_1x_2x_3$	6
	Model H	$x_1, x_2, x_3, x_1x_2, x_2x_3, x_1x_2x_3$	6
	Model I	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_1x_2x_3$	6
	Quadratic	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3$	6
	Model J	$x_1, x_2, x_3, x_2x_3, x_1x_2x_3$	5
	Model K	$x_1, x_2, x_3, x_1x_3, x_1x_2x_3$	5
	Model A	$x_1, x_2, x_3, x_1x_3, x_2x_3$	5
	Model M	$x_1, x_2, x_3, x_1x_2, x_1x_2x_3$	5
	Model B	$x_1, x_2, x_3, x_1x_2, x_2x_3$	5
	Model C	$x_1, x_2, x_3, x_1x_2, x_1x_3$	5
	Model D	x_1, x_2, x_3, x_2x_3	4
	Model E	x_1, x_2, x_3, x_1x_3	4
	Model F	x_1, x_2, x_3, x_1x_2	4
	Linear	x_1, x_2, x_3	3

We will now study several common classes of models on a single FDS plot: the special cubic model, the quadratic model and the linear model. Specifically, we are assuming that the experimenter would like to have a design that can fit each of these three models. Figure 45 shows the comparison of the weighted D -optimal exact design under SH, the weighted D -optimal exact design under WH, the weighted G -optimal exact design under SH, and the weighted G -optimal exact design under WH for the three model types. The comparison of the weighted D -optimal exact designs

under SH and WH are shown in Figure 41. Figure 42 displays the comparison of the weighted G -optimal exact designs under SH and WH. The G -efficiency and the maximum SPV values for each design are given in Table 24. In the previous section, we see that (1) the weighted G -optimal exact designs are superior to the weighted D -optimal exact designs (2) the weighted G -optimal exact designs under SH and WH are quite comparable (3) the weighted D -optimal exact designs under SH and WH are quite competitive.

As shown in Figure 45, for the linear model, the weighted D -optimal exact designs under SH, weighted D -optimal exact designs under WH, weighted G -optimal exact designs under SH and weighted G -optimal exact designs under WH are similar for the whole design space. For SH, only the maximum SPV of the weighted G -optimal exact designs are higher than that of the weighted D -optimal exact designs for the linear model resulting in lower G -efficiency except for $n = 9$ as shown in Table 24. For WH with $n = 10, 12$ and 13 points, the maximum SPV of the weighted G -optimal exact designs are higher than that of the weighted D -optimal exact designs for the linear model. Otherwise, the maximum SPV of the weighted G -optimal exact designs are lower than those for the weighted D -optimal exact designs for the linear model.

For the quadratic model, the weighted D -optimal exact designs under SH perform as well as the weighted D -optimal exact designs under WH, while the weighted G -optimal exact designs under SH are quite similar in performance to the weighted G -optimal exact designs under WH, whereas the weighted G -optimal exact designs perform better the weighted D -optimal exact designs for most of the design space except for $n = 8$ points. For SH and WH with quadratic model, only the maximum SPV of the weighted G -optimal exact designs are larger than that of the weighted D -optimal exact designs for the quadratic model for $n = 8$ points as shown in Table 24. However, when $n = 8$, the weighted D -optimal exact design performs as well as, if not slightly better than, the weighted G -optimal exact design.

For the special cubic model, the weighted D -optimal exact designs under SH compete well with the weighted D -optimal exact designs under WH for large values of SPV, while they are quite similar for small SPV values. While the weighted G -optimal exact designs under SH and WH are quite similar in performance for the majority of the design space. For SH and WH with special cubic model, it is quite clear from Figure 45 that the weighted G -optimal designs perform better than the weighted D -optimal designs for the entire design space because the stability is better maintained for large values of the SPV. As shown in Table 24, the maximum SPV of the weighted D -optimal exact designs are larger than those of the weighted G -optimal exact designs for SH and WH with the special cubic model. The maximum SPV of the weighted optimal exact designs under WH are larger than those for the weighted optimal exact designs under SH except in case of the 13SC-W-G design. For SH and WH, we note that (1) the weighted G -optimal exact designs for the special cubic model and the weighted D -optimal exact designs for the quadratic model are quite similar for $9 \leq n \leq 11$, and (2) the weighted G -optimal exact designs for the special cubic model perform better than the weighted D -optimal exact designs do for the quadratic model when $n = 12$ or 13 points.

Figure 46 shows that the 8SC-S-D design has lower and flatter FDS curves for all three model types, while the other designs are comparable. The 9SC-S-G and 9SC-W-G designs are quite similar and have lower and flatter FDS curves for all three model types, whereas the other designs are competitive as seen in Figure 47. In this case, the weighted G -optimal exact designs based on SH and WH appears to be more robust, because (1) all three lines for the special cubic model, quadratic model and linear model are quite similar, (2) they have much flatter and lower FDS curves for all the models considered, indicating more desirable SPV distribution and (3) they have a good G -efficiency for the special cubic and the nested model within the special cubic model. Although the weighted D -optimal designs based on SH and WH perform well for the quadratic model and linear model, their design performance depends on which final model is selected. In Figure 47, the SPV curves are quite similar for all three models. Therefore, the experimenter can choose the desired design points in the mixture experiments.

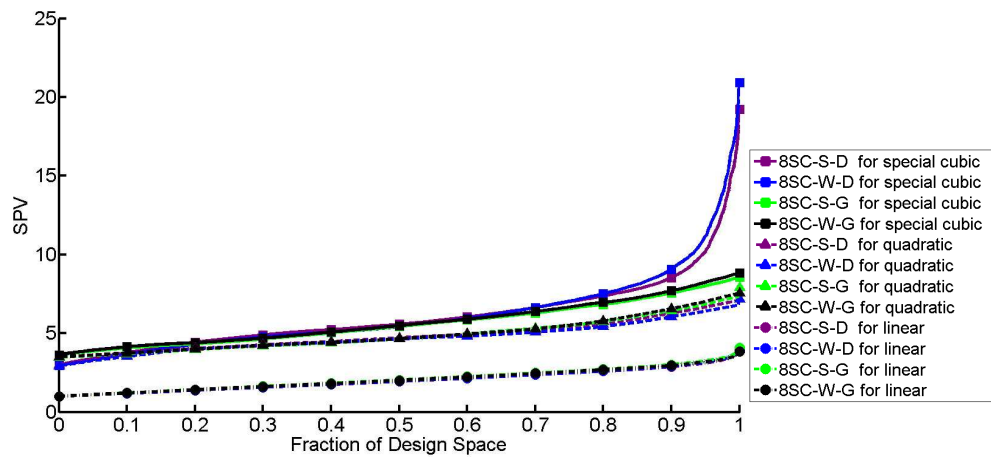
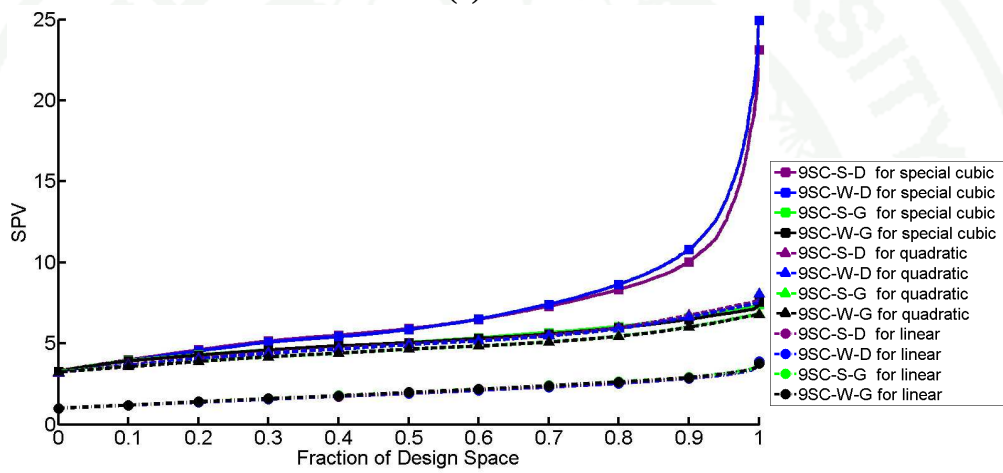
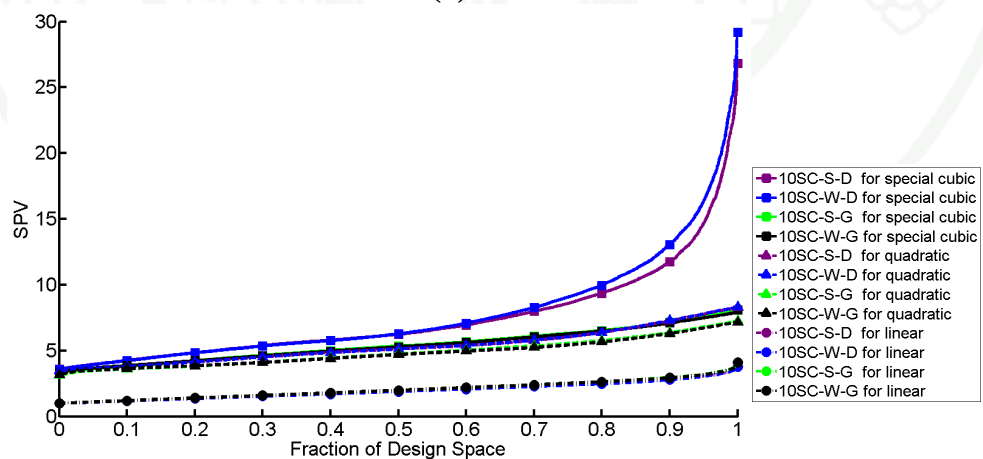
(a) $n = 8$ (b) $n = 9$ (c) $n = 10$

Figure 45 FDS Plot for comparing the weighted D - and G -optimal exact design for three types of models assuming the special cubic model for the poultry experiment.

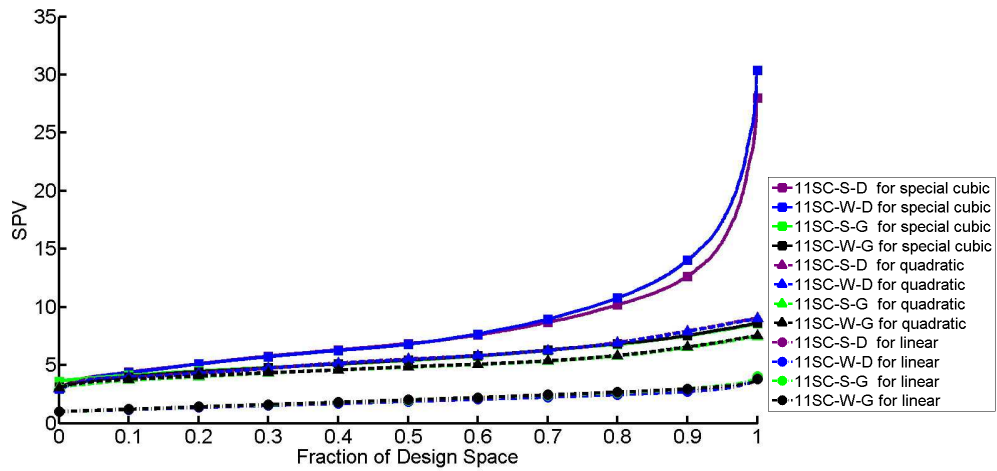
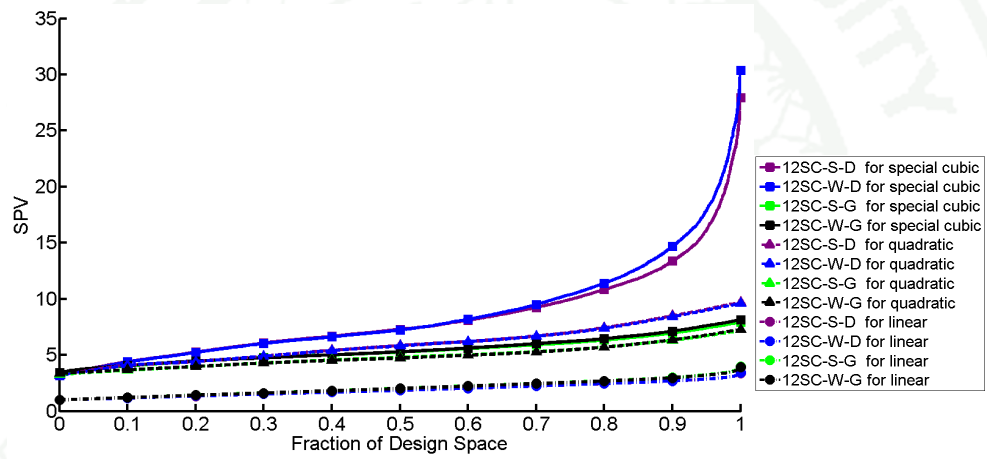
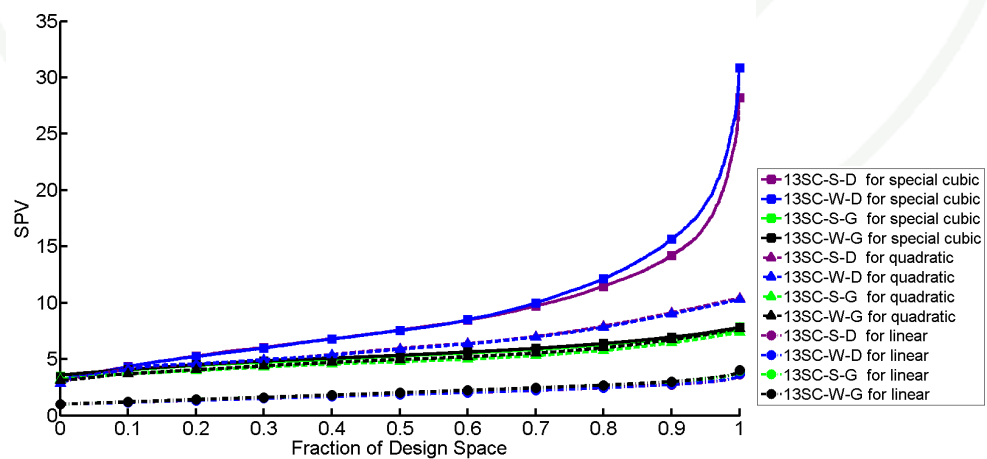
(d) $n = 11$ (e) $n = 12$ (f) $n = 13$

Figure 45 (Continued).

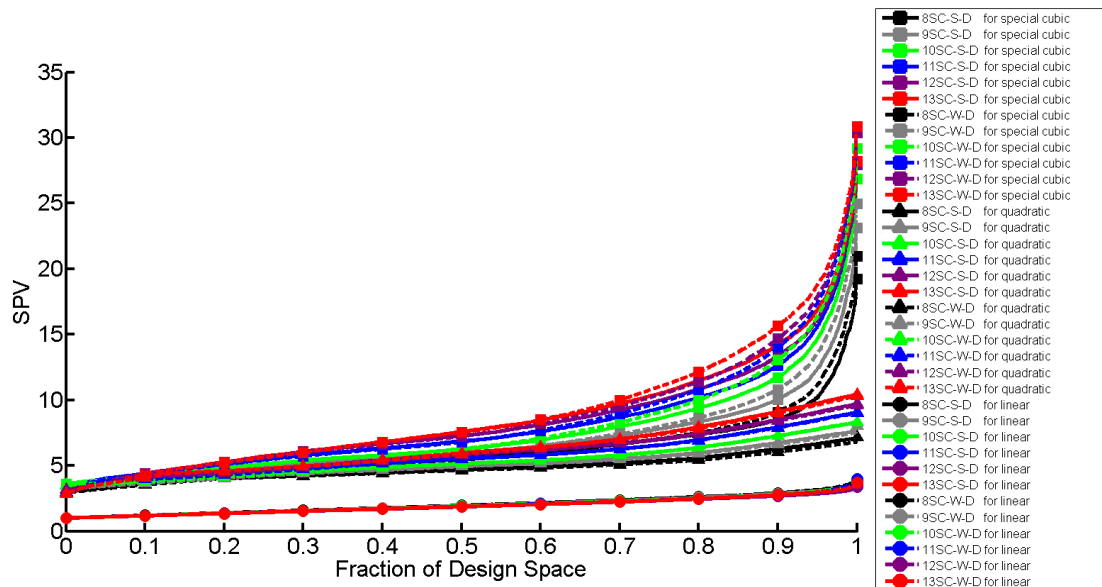


Figure 46 FDS Plot for comparing the D -optimal exact designs under SH and WH for three types of models assuming the special cubic model for the poultry experiment.

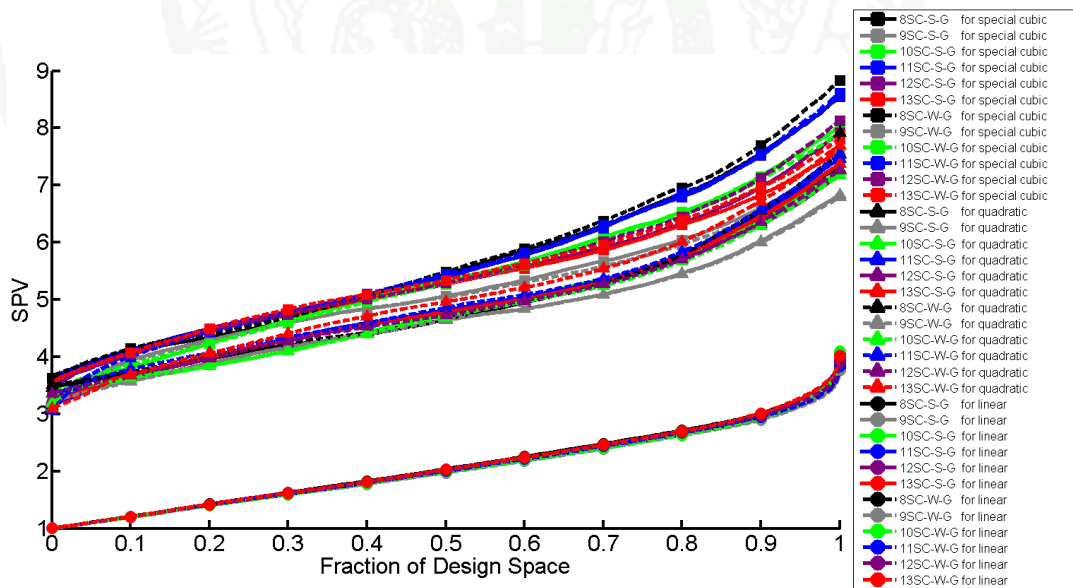


Figure 47 FDS Plot for comparing the G -optimal exact designs under SH and WH for three types of models assuming the special cubic model for the poultry experiment.

Table 24 The maximum SPV value and the approximate G -efficiencies for the weighted D -optimal and weighted G -optimal exact designs for three model types for the special cubic model for the poultry experiment.

Design	Model type	G-eff	Max SPV	Design	Model type	G-eff	Max SPV
8SC-S-D	SC	36.42%	19.22	8SC-S-G	SC	81.87%	8.55
	Q	83.80%	7.16		Q	75.76%	7.92
	L	76.73%	3.91		L	73.89%	4.06
9SC-S-D	SC	30.29%	23.11	9SC-S-G	SC	94.34%	7.42
	Q	74.63%	8.04		Q	87.85%	6.83
	L	78.13%	3.84		L	79.79%	3.76
10SC-S-D	SC	26.08%	26.84	10SC-S-G	SC	86.53%	8.09
	Q	72.38%	8.29		Q	82.76%	7.25
	L	79.16%	3.79		L	73.53%	4.08
11SC-S-D	SC	25.02%	27.98	11SC-S-G	SC	81.78%	8.56
	Q	66.23%	9.06		Q	80.43%	7.46
	L	75.95%	3.95		L	74.07%	4.05
12SC-S-D	SC	25.04%	27.96	12SC-S-G	SC	88.38%	7.92
	Q	61.98%	9.68		Q	82.53%	7.27
	L	88.50%	3.39		L	75.76%	3.96
13SC-S-D	SC	24.79%	28.24	13SC-S-G	SC	88.83%	7.88
	Q	58.59%	10.24		Q	81.41%	7.37
	L	82.42%	3.64		L	75.57%	3.97
8SC-W-D	SC	33.43%	20.94	8SC-W-G	SC	79.28%	8.83
	Q	83.68%	7.17		Q	79.47%	7.55
	L	75.38%	3.98		L	78.33%	3.83
9SC-W-D	SC	28.07%	24.94	9SC-W-G	SC	92.59%	7.56
	Q	74.53%	8.05		Q	88.37%	6.79
	L	77.32%	3.88		L	79.79%	3.76
10SC-W-D	SC	24.00%	29.17	10SC-W-G	SC	86.31%	8.11
	Q	72.20%	8.31		Q	83.68%	7.17
	L	79.79%	3.76		L	73.35%	4.09
11SC-W-D	SC	23.03%	30.39	11SC-W-G	SC	81.21%	8.62
	Q	66.59%	9.01		Q	79.58%	7.54
	L	75.57%	3.97		L	78.33%	3.83
12SC-W-D	SC	23.03%	30.39	12SC-W-G	SC	86.10%	8.13
	Q	62.63%	9.58		Q	82.53%	7.27
	L	87.72%	3.42		L	76.92%	3.90
13SC-W-D	SC	22.69%	30.85	13SC-W-G	SC	89.63%	7.81
	Q	58.37%	10.28		Q	78.02%	7.69
	L	81.52%	3.68		L	74.63%	4.02

Case 2: Single Component Constraints with Four Components

A four mixture component experiment was performed to study the amount of illumination produced by flares (McLean and Anderson 1966). The four SCCs are defined by the following constraints:

$$\begin{aligned} 0.4 &\leq x_1 \leq 0.6 \\ 0.1 &\leq x_2 \leq 0.47 \\ 0.1 &\leq x_3 \leq 0.47 \\ 0.03 &\leq x_4 \leq 0.08. \end{aligned} \quad (109)$$

where x_1 , x_2 , x_3 , and x_4 are, respectively, the mixture proportions of magnesium, sodium nitrate, strontium nitrate, and binder in a flare. The goal of the experiment is to determine the formulation of flare that yields maximum illumination level. The boundary formed by the SCCs has eight vertices, which are numbered 1 to 8 in Figure 48. The coordinates of these eight extreme vertices are listed in Table 25. The two full models under consideration are the Scheffé quadratic and special cubic mixture models. Respectively, these models are:

$$\begin{aligned} E(y) = & \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \\ & \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{14} x_1 x_4 + \beta_{23} x_2 x_3 + \beta_{24} x_2 x_4 + \beta_{34} x_3 x_4 \end{aligned}$$

and

$$\begin{aligned} E(y) = & \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \\ & \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{14} x_1 x_4 + \beta_{23} x_2 x_3 + \beta_{24} x_2 x_4 + \beta_{34} x_3 x_4 + \\ & \beta_{123} x_1 x_2 x_3 + \beta_{124} x_1 x_2 x_4 + \beta_{134} x_1 x_3 x_4 + \beta_{234} x_2 x_3 x_4. \end{aligned}$$

The models have ten and fourteen unknown parameters, respectively.

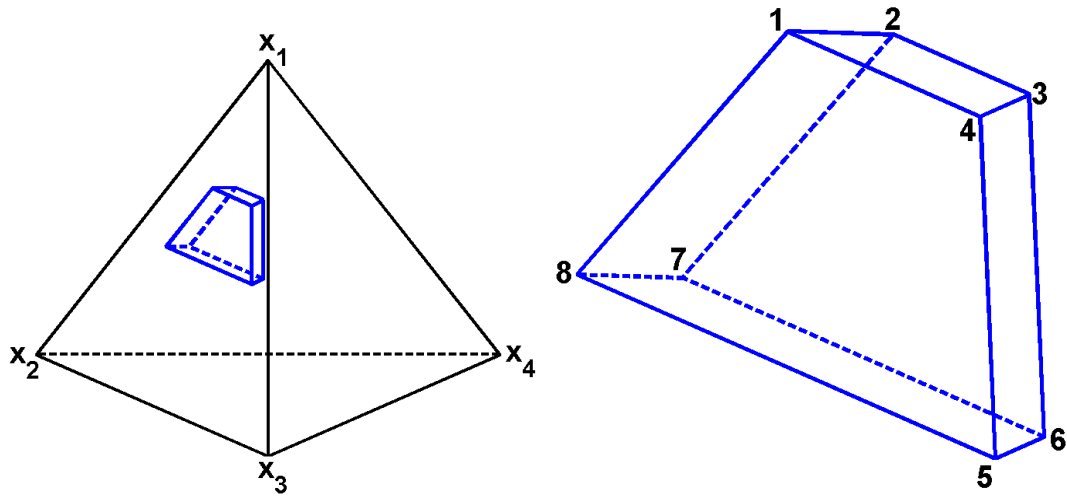


Figure 48 The four-component constrained region defined by the constraints $0.4 \leq x_1 \leq 0.6$, $0.1 \leq x_2 \leq 0.47$, $0.1 \leq x_3 \leq 0.47$, and $0.03 \leq x_4 \leq 0.08$.

Table 25 The coordinate points for the McLean and Anderson flare experiment.

Vertex	x_1	x_2	x_3	x_4
1	0.6000	0.2700	0.1000	0.0300
2	0.6000	0.2200	0.1000	0.0800
3	0.6000	0.1000	0.2200	0.0800
4	0.6000	0.1000	0.2700	0.0300
5	0.4000	0.1000	0.4700	0.0300
6	0.4000	0.1000	0.4200	0.0800
7	0.4000	0.4200	0.1000	0.0800
8	0.4000	0.4700	0.1000	0.0300

1. Appropriate genetic algorithm (GA) parameters for Case 2

In this section, the genetic algorithm parameters for Case 2 are considered. We would like to find appropriate values of α_i and σ to optimize the performance of the GA. We consider using 7,000 as the large number of iterations, $M = 7$ as the size of the population, and $n = 16$ runs as the number of design points. Mixture designs are then generated assuming a Scheffé quadratic model. However, when mixture designs

are generated assuming a Scheffé special cubic model, then $n = 20$ runs will be used for the number of design points considered under WH models.

The behaviors of D_w for the 8 sets of α_i and σ values when the model to be fitted is the **Scheffé quadratic model** are shown in Figure 49. Like Case 1, the results show that the best set of α_i and σ values is set 8, that is $0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.1$; $0.05 \leq \alpha_m \leq 0.2$; $0.1 \leq \sigma \leq 0.3$. This set produces the highest initial D_w values and after that the plot stabilizes and is superior to the plots for the other sets throughout the number of iterations. Subsequently, $M = 9$ with set 8 is used for examining the appropriate population size as well because increasing M reduces the chances of reporting a local optimum. In Figure 50, the result shows that $M = 7$ is appropriate based on the behavior of D_w because the initial improvement of D_w when $M = 7$ is superior to that of $M = 9$, and after that both have similar D_w values. As shown in Figure 50, there is no improvement for D_w after 5,000 iterations. On the other hand, the progression of G_w values with set 8 and $M = 7$ is shown in Figure 51. We see that the stability of G_w does not occur until the end of the large number of iterations.

When the model being fitted is the Scheffé quadratic model, we again choose $M = 7$ as the size of the population, use set 8 for the values of α_i and σ , 5,000 as the number of iterations when D_w is the objective function and 7,000 as the number of iterations when G_w is the objective function. Like Case 1, the values of α_i and σ are reset to smaller values after 250 iterations.

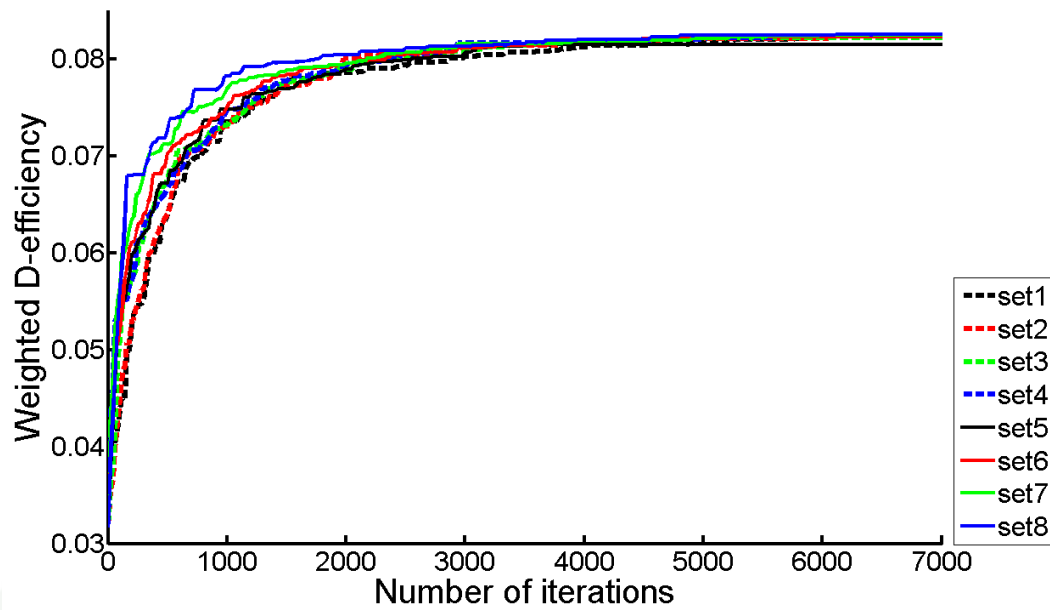


Figure 49 Progression of D_w values among 8 sets of α_i and σ values assuming the Scheffé quadratic model for Case 2.

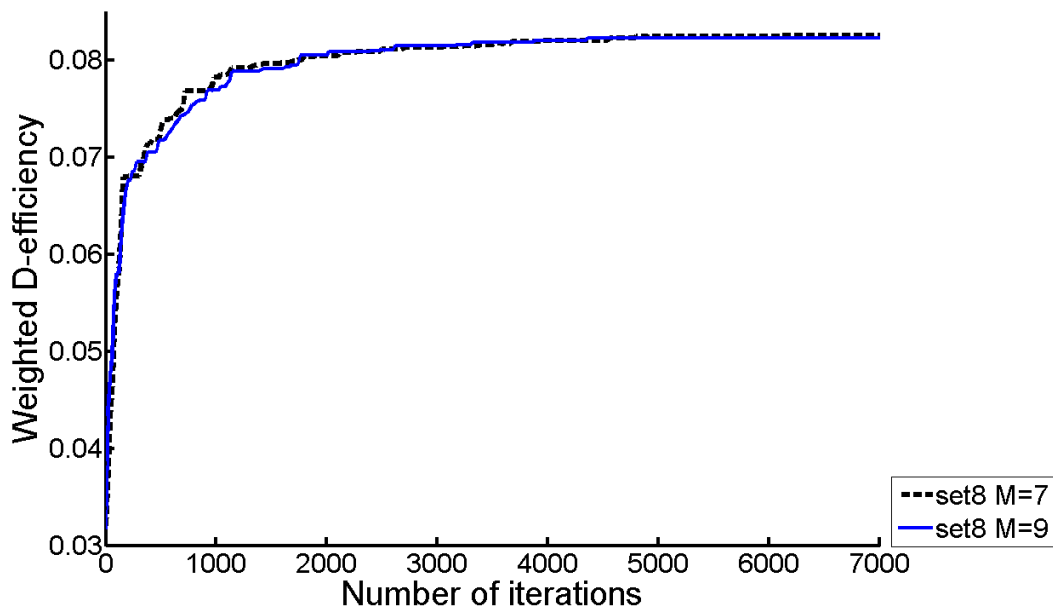


Figure 50 Behavior of D_w values of the best set of α_i and σ , with $M = 7$ and 9 assuming the Scheffé quadratic model for Case 2.

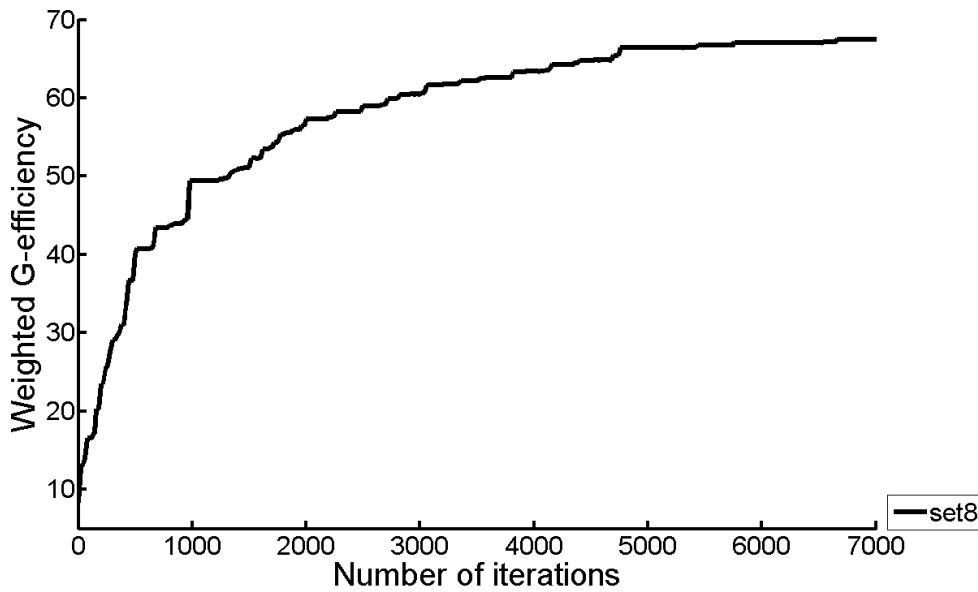


Figure 51 Progression for G_w values of the best set of α_i and σ , with $M = 7$, assuming the Scheffé quadratic model for Case 2.

Suppose that $M = 7$ is the population size and the α_i and σ values from set 8 are used to generate mixture designs assuming a **Scheffé special cubic model**. Figure 52 shows the behavior of D_w under these conditions. After 5,000 iterations, there is no improvement in D_w . On the other hand, Figure 53 displays the progression of G_w values for set 8 and $M = 7$ assuming the special cubic model. Like the quadratic model, the stability of G_w does not occur until the end of a large number of iterations.

Therefore, assuming the special cubic model, the decision was to use $M = 7$ as the size of the population, set 8 for the values of α_i and σ , 5,000 as the number of iterations when D_w is the objective function and 7,000 as the number of iterations when G_w is the objective function. Like Case 1, the values of α_i and σ are reset to smaller values after 250 iterations. Notice that the genetic algorithm parameters for the case of the special cubic model are identical to the case for the quadratic model.

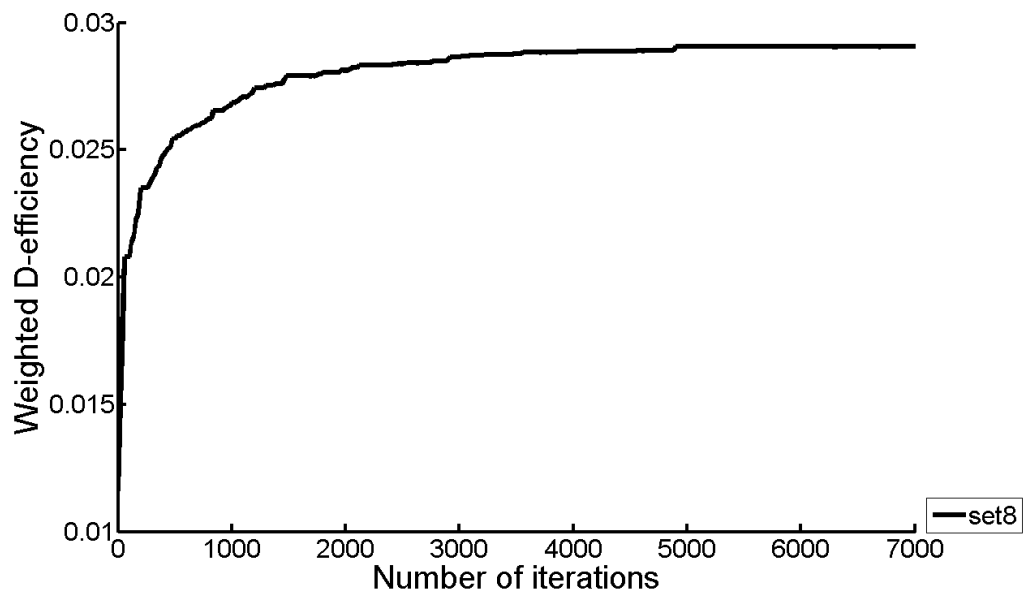


Figure 52 Behavior of D_w values with the best set of α_i and σ values and $M = 7$, assuming the full Scheffé special cubic model for Case 2.

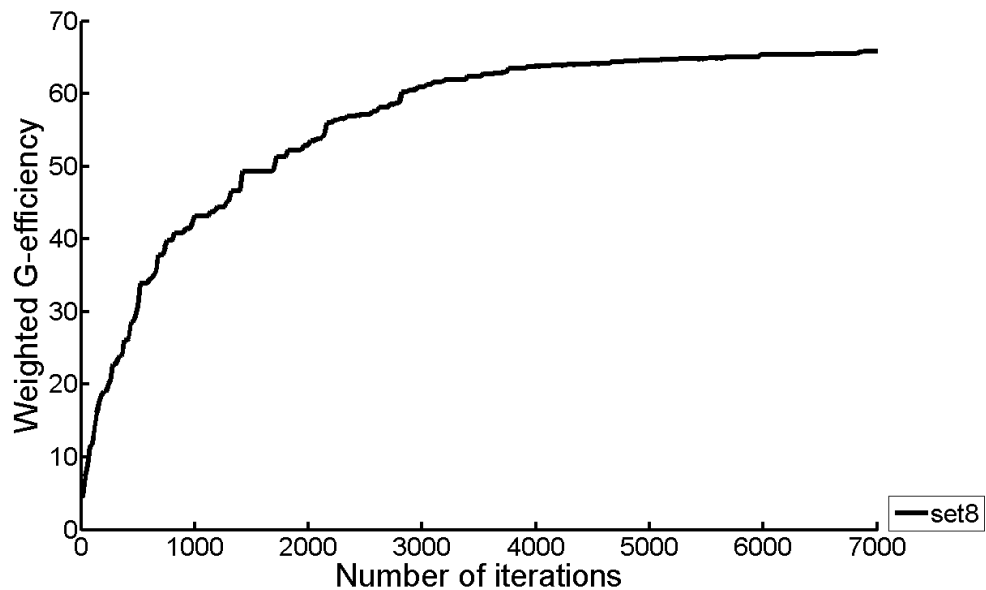


Figure 53 Progression of G_w values of the best set of α_i and σ , with $M = 7$, assuming the full Scheffé special cubic model for Case 2.

2. Generating optimal exact designs for Case 2

In this section, the most fit GA designs and the optimal exact designs are proposed for the four component flare experiment. The most fit GA design serves as the starting design for a local grid search to achieve the optimal exact design. Similar to Case 1, we want to find model-robust designs that are as efficient as possible over classes of reduced models. We first consider the mixture designs generated by the GA when the full model is **the Scheffé quadratic model**. There are 64 reduced models under SH and WH which are shown in Table 5. We focus on the following two cases that vary in terms of weighted design optimal criteria:

- For D_w , the GA generated designs and the optimal exact designs having 11 to 16 points for the quadratic model are shown in Appendix Tables B1 to B6.
- For G_w , the GA generated designs and the optimal exact designs having 11 to 16 points for the quadratic model are given in Appendix Tables B7 to B12.

The **Scheffé special cubic model** will also be considered as the full model. Tables 8 and 9, respectively, contain the 113 reduced SH models and 809 reduced WH models for the Scheffé special cubic model. The following four cases are examined that vary in the terms of weighted design optimal criteria and heredity concepts:

- For D_w with SH, the GA generated designs and the optimal exact designs having 15 to 20 points are given in Appendix Tables B13 to B18.
- For D_w with WH, the GA generated designs and the optimal exact designs having 15 to 20 points are given in Appendix Tables B19 to B24.
- For G_w with SH, the GA generated designs and the optimal exact designs having 15 to 20 points are shown in Appendix Tables B25 to B30.
- For G_w with WH, the GA generated designs and the optimal exact designs having 15 to 20 points are shown in Appendix Tables B31 to B36.

After the local grid search, most of D_w values under WH increase in the fifth decimal place. Thus, six decimal places is used to compare the percentage increase in D_w values. Otherwise, four decimal places is used. A local grid search led to increases in the objective D_w and G_w function values as shown at the bottoms of Appendix Tables B1 to B36. Tables 26 and 27 display the percentage increase in the objective function value when the full models are the quadratic and the special cubic models, respectively. The last column in Tables 26 and 27 represents the percentage change between the objective function of the best GA generated design and the optimal exact design for that model.

It is clear that the percentage changes in the D_w values are less than the percentage changes in the G_w values. As shown in Table 26, the largest percentage increases in D_w and G_w values occur for the 12-point design, while the smallest percentage increases in D_w and G_w values occur for the 16-point and 15-point designs, respectively. The D_w values of the optimal exact designs are very close, while the G_w values of the optimal exact designs are quite different.

Table 26 Percentage increase in objective function values assuming the quadratic model as the full model for the flare experiment.

Objective function	Run	Best GA generated design	Optimal exact design	Percentage increase (%)
D_w	11	0.080514	0.080757	0.3018
	12	0.080663	0.080990	0.4054
	13	0.080828	0.081060	0.2870
	14	0.081396	0.081560	0.2015
	15	0.081952	0.082119	0.2038
	16	0.082394	0.082530	0.1651
G_w	11	64.6127	71.7332	11.0203
	12	60.8486	73.2223	20.3352
	13	62.8829	68.7614	9.3483
	14	68.0784	71.5466	5.0944
	15	66.7775	68.9409	3.2397
	16	67.4434	73.5949	9.1210

As shown in Table 27, the smallest percentage increase in D_w occurs for the 20-point design, while the largest percentage increase under SH and WH occurs for the 19-point and 16-point designs, respectively. For G_w with SH, the smallest percentage increase occurs for the 16-point design, while the 15-point design has the largest percentage increase. For G_w with WH, the 16-point design has the largest percentage increase, while the smallest percentage increase occurs for the 17-point design. For SH and WH, the D_w values of the optimal exact designs are very close, while the G_w values of the optimal exact designs are quite different.

Table 27 Percentage increase in objective function values assuming the special cubic model as the full model for the flare experiment.

Objective function	Heredity	Run	Best GA generated design	Optimal exact design	Percentage increase (%)
D_w	SH	15	0.032547	0.032623	0.233508
		16	0.032880	0.032996	0.352798
		17	0.033104	0.033161	0.172185
		18	0.033177	0.033272	0.286343
		19	0.033265	0.033446	0.544115
		20	0.033385	0.033430	0.134791
	WH	15	0.028367	0.028429	0.218564
		16	0.028540	0.028672	0.462509
		17	0.028732	0.028741	0.031324
		18	0.028914	0.028974	0.207512
		19	0.029016	0.029124	0.372208
		20	0.029043	0.029087	0.1515
G_w	SH	15	60.1853	65.6713	9.115183
		16	63.9092	67.6680	5.881469
		17	64.5183	69.9795	8.464575
		18	66.4605	71.1533	7.061036
		19	66.1616	71.3235	7.801958
		20	65.3008	70.9548	8.658393
	WH	15	59.7899	63.3992	6.036638
		16	61.7374	67.1785	8.813296
		17	67.7739	70.5052	4.030017
		18	66.7748	71.4587	7.014473
		19	66.2622	71.6545	8.137822
		20	66.4675	71.2817	7.242938

Assuming the full model is the quadratic model, the following 12 optimal exact designs were generated: D_w -based designs 11Q-D, 12Q-D, 13Q-D, 14Q-D, 15Q-D, and 16Q-D for 11 to 16 points, respectively, and G_w -based designs 11Q-G, 12Q-G, 13Q-G, 14Q-G, 15Q-G, and 16Q-G for 11 to 16 points, respectively.

Assuming the full model is the special cubic model, the following 24 optimal exact designs were generated: D_w -based designs 15SC-S-D, 16SC-S-D, 17SC-S-D, 18SC-S-D, 19SC-S-D, 20SC-S-D for SH and 15 to 20 points, respectively; D_w -based designs 15SC-W-D, 16SC-W-D, 17SC-W-D, 18SC-W-D, 19SC-W-D, 20SC-W-D for WH and 15 to 20 points, respectively; G_w -based designs 15SC-S-G, 16SC-S-G, 17SC-S-G, 18SC-S-G, 19SC-S-G, 20SC-S-G for SH and 15 to 20 points, respectively; and G_w -based designs 15SC-W-G, 16SC-W-G, 17SC-W-G, 18SC-W-G, 19SC-W-G, 20SC-W-G for WH and 15 to 20 points, respectively.

For optimal exact designs, the set of points appearing in any one of these 36 designs is given in Table 28. Table 29 summarizes the sets of points in each of the 36 designs assuming a quadratic or a special cubic model. The boundary formed by the SCCs is indicated by the polyhedron inside the pyramid which has eight vertices, twelve edges and six faces is shown in Figure 48. The differences in the distributional patterns of points of the optimal exact designs for the quadratic model based on D_w and G_w are shown in Figure 54. For D_w and G_w , Figures 55 and 56, respectively, display the distributional patterns of the points in the optimal exact designs assuming the special cubic model.

Table 28 List of points appearing in any of the flare example designs.

Label	x_1	x_2	x_3	x_4	Label	x_1	x_2	x_3	x_4
Vertices					Other points				
V ₁	0.4000	0.4700	0.1000	0.0300	G ₁₃	0.5127	0.3573	0.1000	0.0300
V ₂	0.4000	0.1000	0.4700	0.0300	G ₁₄	0.4000	0.2867	0.2833	0.0300
V ₃	0.6000	0.1000	0.2700	0.0300	G ₁₅	0.5028	0.3172	0.1000	0.0800
V ₄	0.6000	0.2700	0.1000	0.0300	G ₁₆	0.5880	0.1000	0.2320	0.0800
V ₅	0.4000	0.4200	0.1000	0.0800	G ₁₇	0.6000	0.2345	0.1000	0.0655
V ₆	0.4000	0.1000	0.4200	0.0800	G ₁₈	0.4000	0.3883	0.1317	0.0800
V ₇	0.6000	0.1000	0.2200	0.0800	G ₁₉	0.5716	0.2984	0.1000	0.0300
V ₈	0.6000	0.2200	0.1000	0.0800	G ₂₀	0.4000	0.3887	0.1532	0.0581
Edge points					G ₂₁	0.4892	0.1190	0.3438	0.0480
E ₁	0.4000	0.1000	0.4450	0.0550	G ₂₂	0.5386	0.1000	0.3176	0.0438
E ₂	0.4000	0.4450	0.1000	0.0550	G ₂₃	0.4000	0.2834	0.2866	0.0300
E ₃	0.4000	0.2850	0.2850	0.0300	G ₂₄	0.5189	0.3511	0.1000	0.0300
E ₄	0.4000	0.2600	0.2600	0.0800	G ₂₅	0.4000	0.4500	0.1000	0.0500
E ₅	0.6000	0.1000	0.2450	0.0550	G ₂₆	0.4000	0.2884	0.2816	0.0300
E ₆	0.6000	0.2450	0.1000	0.0550	G ₂₇	0.6000	0.1000	0.2230	0.0770
E ₇	0.6000	0.1850	0.1850	0.0300	G ₂₈	0.4077	0.4123	0.1000	0.0800
E ₈	0.6000	0.1600	0.1600	0.0800	G ₂₉	0.4192	0.1000	0.4508	0.0300
E ₉	0.5000	0.1000	0.3700	0.0300	G ₃₀	0.4000	0.1000	0.4444	0.0556
E ₁₀	0.5000	0.1000	0.3200	0.0800	G ₃₁	0.5045	0.2289	0.2187	0.0479
E ₁₁	0.5000	0.3700	0.1000	0.0300	G ₃₂	0.4932	0.1000	0.3268	0.0800
E ₁₂	0.5000	0.3200	0.1000	0.0800	G ₃₃	0.4228	0.4472	0.1000	0.0300
Face points					G ₃₄	0.4000	0.1564	0.3636	0.0800
F ₁	0.4000	0.2725	0.2725	0.0550	G ₃₅	0.5838	0.2362	0.1000	0.0800
F ₂	0.6000	0.1725	0.1725	0.0550	G ₃₆	0.4000	0.2912	0.2788	0.0300
F ₃	0.5000	0.1000	0.3450	0.0550	G ₃₇	0.5871	0.1000	0.2700	0.0429
F ₄	0.5000	0.3450	0.1000	0.0550	G ₃₈	0.5120	0.3580	0.1000	0.0300
F ₅	0.5000	0.2350	0.2350	0.0300	G ₃₉	0.4000	0.2955	0.2745	0.0300
F ₆	0.5000	0.2100	0.2100	0.0800	G ₄₀	0.4025	0.4175	0.1000	0.0800
Overall centroid					G ₄₁	0.4000	0.1000	0.4610	0.0390
C	0.5000	0.2225	0.2225	0.0550	G ₄₂	0.4000	0.2779	0.2421	0.0800
Other Points					G ₄₃	0.5348	0.1000	0.2852	0.0800
G ₁	0.4000	0.1000	0.4307	0.0693	G ₄₄	0.4529	0.1000	0.4171	0.0300
G ₂	0.4000	0.2843	0.2857	0.0300	G ₄₅	0.5000	0.2371	0.2090	0.0539
G ₃	0.6000	0.1467	0.1733	0.0800	G ₄₆	0.6000	0.1000	0.2420	0.0580
G ₄	0.6000	0.1467	0.1733	0.0800	G ₄₇	0.5917	0.2783	0.1000	0.0300
G ₅	0.4374	0.3826	0.1000	0.0800	G ₄₈	0.4623	0.3895	0.1000	0.0482
G ₆	0.5452	0.3248	0.1000	0.0300	G ₄₉	0.6000	0.2563	0.1000	0.0437
G ₇	0.4000	0.2760	0.2940	0.0300	G ₅₀	0.5243	0.1000	0.3457	0.0300
G ₈	0.5067	0.1000	0.3291	0.0642	G ₅₁	0.4000	0.2859	0.2841	0.0300
G ₉	0.4000	0.4685	0.1000	0.0315	G ₅₂	0.4000	0.1453	0.3747	0.0800
G ₁₀	0.4000	0.3726	0.1584	0.0690	G ₅₃	0.4000	0.3205	0.2495	0.0300
G ₁₁	0.4000	0.2836	0.2864	0.0300	G ₅₄	0.4695	0.3505	0.1000	0.0800
G ₁₂	0.4000	0.1000	0.4312	0.0688	G ₅₅	0.5165	0.2535	0.2000	0.0300

Table 28 (Continued)

Label	x_1	x_2	x_3	x_4	Label	x_1	x_2	x_3	x_4
Other points					Other points				
G ₅₆	0.5925	0.1000	0.2775	0.0300	G ₁₀₀	0.4893	0.3200	0.1107	0.0800
G ₅₇	0.6000	0.1000	0.2326	0.0674	G ₁₀₁	0.6000	0.1370	0.2330	0.0300
G ₅₈	0.4000	0.3807	0.1393	0.0800	G ₁₀₂	0.5859	0.2817	0.1000	0.0324
G ₅₉	0.4230	0.4200	0.1000	0.0570	G ₁₀₃	0.5752	0.1000	0.2448	0.0800
G ₆₀	0.4607	0.2216	0.2700	0.0477	G ₁₀₄	0.5382	0.1473	0.2542	0.0603
G ₆₁	0.4915	0.1000	0.3285	0.0800	G ₁₀₅	0.5246	0.1000	0.3454	0.0300
G ₆₂	0.4000	0.1000	0.4415	0.0585	G ₁₀₆	0.4018	0.1000	0.4682	0.0300
G ₆₃	0.4000	0.2864	0.2836	0.0300	G ₁₀₇	0.6000	0.1222	0.2478	0.0300
G ₆₄	0.4000	0.2728	0.2721	0.0551	G ₁₀₈	0.4000	0.2857	0.2843	0.0300
G ₆₅	0.5232	0.1000	0.3468	0.0300	G ₁₀₉	0.4000	0.2385	0.2815	0.0800
G ₆₆	0.4652	0.4048	0.1000	0.0300	G ₁₁₀	0.4935	0.1000	0.3265	0.0800
G ₆₇	0.4515	0.1000	0.3685	0.0800	G ₁₁₁	0.6000	0.2577	0.1000	0.0423
G ₆₈	0.4000	0.1000	0.4510	0.0490	G ₁₁₂	0.4000	0.2455	0.2745	0.0800
G ₆₉	0.6000	0.2300	0.1000	0.0700	G ₁₁₃	0.4012	0.1000	0.4688	0.0300
G ₇₀	0.5015	0.3185	0.1000	0.0800	G ₁₁₄	0.6000	0.2648	0.1000	0.0352
G ₇₁	0.4479	0.2666	0.2470	0.0385	G ₁₁₅	0.4000	0.2852	0.2848	0.0300
G ₇₂	0.4000	0.3838	0.1583	0.0579	G ₁₁₆	0.6000	0.1152	0.2548	0.0300
G ₇₃	0.4000	0.2453	0.3247	0.0300	G ₁₁₇	0.4919	0.1869	0.2416	0.0796
G ₇₄	0.4000	0.1343	0.3857	0.0800	G ₁₁₈	0.6000	0.1061	0.2139	0.0800
G ₇₅	0.5293	0.1000	0.3260	0.0447	G ₁₁₉	0.5813	0.2887	0.1000	0.0300
G ₇₆	0.4000	0.4607	0.1000	0.0393	G ₁₂₀	0.6000	0.2200	0.1178	0.0622
G ₇₇	0.4827	0.3373	0.1000	0.0800	G ₁₂₁	0.5623	0.2577	0.1000	0.0800
G ₇₈	0.4000	0.2327	0.2873	0.0800	G ₁₂₂	0.4000	0.2500	0.2700	0.0800
G ₇₉	0.6000	0.1227	0.2473	0.0300	G ₁₂₃	0.4000	0.4264	0.1245	0.0491
G ₈₀	0.5521	0.3179	0.1000	0.0300	G ₁₂₄	0.5000	0.2611	0.2089	0.0300
G ₈₁	0.4000	0.2900	0.2800	0.0300	G ₁₂₅	0.4086	0.4614	0.1000	0.0300
G ₈₂	0.4000	0.1000	0.4677	0.0323	G ₁₂₆	0.6000	0.1159	0.2541	0.0300
G ₈₃	0.5819	0.1195	0.2686	0.0300	G ₁₂₇	0.4000	0.2641	0.3059	0.0300
G ₈₄	0.4000	0.2750	0.2450	0.0800	G ₁₂₈	0.4961	0.1000	0.3372	0.0667
G ₈₅	0.5022	0.3178	0.1000	0.0800	G ₁₂₉	0.5166	0.1000	0.3478	0.0356
G ₈₆	0.4000	0.2860	0.2840	0.0300	G ₁₃₀	0.4943	0.3257	0.1000	0.0800
G ₈₇	0.4000	0.2814	0.2817	0.0369	G ₁₃₁	0.4429	0.2752	0.2277	0.0542
G ₈₈	0.5905	0.2795	0.1000	0.0300	G ₁₃₂	0.5847	0.1000	0.2353	0.0800
G ₈₉	0.5856	0.2344	0.1000	0.0800	G ₁₃₃	0.5312	0.2511	0.1877	0.0300
G ₉₀	0.6000	0.1000	0.2270	0.0730	G ₁₃₄	0.4000	0.4200	0.1017	0.0783
G ₉₁	0.4567	0.2933	0.2200	0.0300	G ₁₃₅	0.6000	0.2493	0.1000	0.0507
G ₉₂	0.5442	0.1942	0.2076	0.0540	G ₁₃₆	0.5106	0.1629	0.2465	0.0800
G ₉₃	0.5425	0.1000	0.3275	0.0300	G ₁₃₇	0.4000	0.2912	0.2788	0.0300
G ₉₄	0.4000	0.1039	0.4200	0.0761	G ₁₃₈	0.4000	0.2682	0.2518	0.0800
G ₉₅	0.4122	0.2536	0.2542	0.0800	G ₁₃₉	0.5639	0.3061	0.1000	0.0300
G ₉₆	0.4937	0.3430	0.1000	0.0633	G ₁₄₀	0.6000	0.1221	0.2479	0.0300
G ₉₇	0.6000	0.1143	0.2427	0.0300	G ₁₄₁	0.6000	0.1893	0.1307	0.0800
G ₉₈	0.4000	0.2592	0.2608	0.0800	G ₁₄₂	0.5269	0.3431	0.1000	0.0300
G ₉₉	0.4986	0.2968	0.1746	0.0300	G ₁₄₃	0.4026	0.4174	0.1000	0.0800

Table 28 (Continued)

Label	x_1	x_2	x_3	x_4	Label	x_1	x_2	x_3	x_4
Other points					Other points				
G ₁₄₄	0.4000	0.2833	0.2867	0.0300	G ₁₈₈	0.4000	0.2959	0.2741	0.0300
G ₁₄₅	0.6000	0.1000	0.2604	0.0396	G ₁₈₉	0.4000	0.2745	0.2455	0.0800
G ₁₄₆	0.5411	0.2899	0.1390	0.0300	G ₁₉₀	0.6000	0.2332	0.1338	0.0330
G ₁₄₇	0.4000	0.2829	0.2871	0.0300	G ₁₉₁	0.4869	0.1000	0.3831	0.0300
G ₁₄₈	0.6000	0.2248	0.1000	0.0752	G ₁₉₂	0.4000	0.1628	0.3808	0.0564
G ₁₄₉	0.4000	0.2490	0.2710	0.0800	G ₁₉₃	0.4886	0.1444	0.2870	0.0800
G ₁₅₀	0.4810	0.1000	0.3390	0.0800	G ₁₉₄	0.5659	0.3041	0.1000	0.0300
G ₁₅₁	0.4923	0.2361	0.2416	0.0300	G ₁₉₅	0.6000	0.1319	0.2029	0.0652
G ₁₅₂	0.4155	0.1446	0.3874	0.0525	G ₁₉₆	0.4400	0.4106	0.1000	0.0494
G ₁₅₃	0.5650	0.1000	0.3050	0.0300	G ₁₉₇	0.4000	0.2618	0.2582	0.0800
G ₁₅₄	0.4000	0.2626	0.2574	0.0800	G ₁₉₈	0.4970	0.1000	0.3730	0.0300
G ₁₅₅	0.5010	0.2718	0.1472	0.0800	G ₁₉₉	0.4000	0.4460	0.1000	0.0540
G ₁₅₆	0.4985	0.3715	0.1000	0.0300	G ₂₀₀	0.4000	0.1428	0.4015	0.0557
G ₁₅₇	0.6000	0.2603	0.1097	0.0300	G ₂₀₁	0.6000	0.2350	0.1350	0.0300
G ₁₅₈	0.4970	0.1000	0.3230	0.0800	G ₂₀₂	0.4791	0.2254	0.2277	0.0678
G ₁₅₉	0.4000	0.2755	0.2945	0.0300	G ₂₀₃	0.6000	0.1000	0.2680	0.0320
G ₁₆₀	0.6000	0.1418	0.2200	0.0382	G ₂₀₄	0.4749	0.2251	0.2700	0.0300
G ₁₆₁	0.4508	0.3942	0.1000	0.0550	G ₂₀₅	0.5500	0.3200	0.1000	0.0300
G ₁₆₂	0.5970	0.1000	0.2230	0.0800	G ₂₀₆	0.5160	0.1000	0.3040	0.0800
G ₁₆₃	0.4967	0.1000	0.3733	0.0300	G ₂₀₇	0.4000	0.2876	0.2824	0.0300
G ₁₆₄	0.4517	0.1074	0.3814	0.0595	G ₂₀₈	0.6000	0.2250	0.1000	0.0750
G ₁₆₅	0.4921	0.3279	0.1000	0.0800	G ₂₀₉	0.5377	0.2823	0.1000	0.0800
G ₁₆₆	0.4000	0.2836	0.2864	0.0300	G ₂₁₀	0.6000	0.2183	0.1517	0.0300
G ₁₆₇	0.4000	0.2531	0.2669	0.0800	G ₂₁₁	0.6000	0.2327	0.1000	0.0673
G ₁₆₈	0.4000	0.3929	0.1538	0.0533	G ₂₁₂	0.5204	0.3496	0.1000	0.0300
G ₁₆₉	0.6000	0.2317	0.1297	0.0386	G ₂₁₃	0.5231	0.1000	0.2969	0.0800
G ₁₇₀	0.4996	0.2323	0.2381	0.0300	G ₂₁₄	0.4000	0.2828	0.2872	0.0300
G ₁₇₁	0.4975	0.1525	0.2700	0.0800	G ₂₁₅	0.4000	0.2642	0.2558	0.0800
G ₁₇₂	0.5600	0.3100	0.1000	0.0300	G ₂₁₆	0.4000	0.2847	0.2853	0.0300
G ₁₇₃	0.6000	0.1075	0.2625	0.0300	G ₂₁₇	0.4000	0.2627	0.2573	0.0800
G ₁₇₄	0.6000	0.1000	0.2571	0.0429	G ₂₁₈	0.6000	0.2250	0.1000	0.0750
G ₁₇₅	0.4000	0.2826	0.2874	0.0300	G ₂₁₉	0.4909	0.2412	0.2379	0.0300
G ₁₇₆	0.5119	0.3581	0.1000	0.0300	G ₂₂₀	0.5239	0.1000	0.2961	0.0800
G ₁₇₇	0.5962	0.2238	0.1000	0.0800	G ₂₂₁	0.5951	0.2749	0.1000	0.0300
G ₁₇₈	0.4000	0.2593	0.2607	0.0800	G ₂₂₂	0.4079	0.1000	0.4381	0.0540
G ₁₇₉	0.6000	0.2293	0.1407	0.0300	G ₂₂₃	0.4673	0.4027	0.1000	0.0300
G ₁₈₀	0.5975	0.1000	0.2725	0.0300	G ₂₂₄	0.4000	0.2565	0.2774	0.0661
G ₁₈₁	0.6000	0.2258	0.1000	0.0742	G ₂₂₅	0.6000	0.1744	0.1756	0.0500
G ₁₈₂	0.4000	0.2624	0.2576	0.0800	G ₂₂₆	0.4000	0.4236	0.1000	0.0764
G ₁₈₃	0.4000	0.2832	0.2868	0.0300	G ₂₂₇	0.6000	0.1049	0.2651	0.0300
G ₁₈₄	0.5221	0.1000	0.2979	0.0800	G ₂₂₈	0.4821	0.2457	0.2422	0.0300
G ₁₈₅	0.5365	0.2798	0.1537	0.0300	G ₂₂₉	0.4000	0.3642	0.1558	0.0800
G ₁₈₆	0.5826	0.1000	0.2374	0.0800	G ₂₃₀	0.4986	0.3293	0.1000	0.0721
G ₁₈₇	0.5000	0.2330	0.2370	0.0300	G ₂₃₁	0.5017	0.1000	0.3683	0.0300

Table 28 (Continued)

Label	x_1	x_2	x_3	x_4	Label	x_1	x_2	x_3	x_4
Other points					Other points				
G ₂₃₂	0.4000	0.2862	0.2838	0.0300	G ₂₅₇	0.6000	0.1000	0.2249	0.0751
G ₂₃₃	0.4477	0.2327	0.2396	0.0800	G ₂₅₈	0.4753	0.3947	0.1000	0.0300
G ₂₃₄	0.6000	0.1638	0.1822	0.0540	G ₂₅₉	0.6000	0.1000	0.2429	0.0571
G ₂₃₅	0.4116	0.1000	0.4337	0.0547	G ₂₆₀	0.6000	0.1131	0.2069	0.0800
G ₂₃₆	0.4659	0.2224	0.2317	0.0800	G ₂₆₁	0.4016	0.4425	0.1013	0.0546
G ₂₃₇	0.4613	0.3587	0.1000	0.0800	G ₂₆₂	0.4566	0.2434	0.2700	0.0300
G ₂₃₈	0.5987	0.2713	0.1000	0.0300	G ₂₆₃	0.4807	0.1000	0.3893	0.0300
G ₂₃₉	0.4000	0.4028	0.1573	0.0399	G ₂₆₄	0.6000	0.1915	0.1785	0.0300
G ₂₄₀	0.4000	0.2693	0.2507	0.0800	G ₂₆₅	0.4000	0.1000	0.4451	0.0549
G ₂₄₁	0.5150	0.2424	0.2126	0.0300	G ₂₆₆	0.5076	0.1000	0.3124	0.0800
G ₂₄₂	0.4000	0.2820	0.2880	0.0300	G ₂₆₇	0.4000	0.2855	0.2845	0.0300
G ₂₄₃	0.4930	0.1000	0.3270	0.0800	G ₂₆₈	0.4631	0.2377	0.2289	0.0703
G ₂₄₄	0.4953	0.1000	0.3747	0.0300	G ₂₆₉	0.4823	0.1000	0.3877	0.0300
G ₂₄₅	0.5088	0.3505	0.1000	0.0407	G ₂₇₀	0.4000	0.1000	0.4423	0.0577
G ₂₄₆	0.4000	0.2560	0.2640	0.0800	G ₂₇₁	0.4000	0.3659	0.1907	0.0434
G ₂₄₇	0.5190	0.1000	0.3510	0.0300	G ₂₇₂	0.5118	0.1489	0.2593	0.0800
G ₂₄₈	0.6000	0.2089	0.1611	0.0300	G ₂₇₃	0.4000	0.2247	0.2953	0.0800
G ₂₄₉	0.4000	0.2866	0.2834	0.0300	G ₂₇₄	0.4000	0.3570	0.1630	0.0800
G ₂₅₀	0.6000	0.1000	0.2510	0.0490	G ₂₇₅	0.4000	0.2729	0.2971	0.0300
G ₂₅₁	0.5154	0.3046	0.1000	0.0800	G ₂₇₆	0.4967	0.3233	0.1000	0.0800
G ₂₅₂	0.4941	0.2409	0.2350	0.0300	G ₂₇₇	0.5317	0.1000	0.3061	0.0622
G ₂₅₃	0.6000	0.2687	0.1013	0.0300	G ₂₇₈	0.6000	0.2040	0.1488	0.0472
G ₂₅₄	0.4000	0.2937	0.2763	0.0300	G ₂₇₉	0.5070	0.2286	0.2344	0.0300
G ₂₅₅	0.4000	0.2573	0.2627	0.0800	G ₂₈₀	0.4657	0.4043	0.1000	0.0300
G ₂₅₆	0.5242	0.2958	0.1000	0.0800					

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Table 29 Summary of the points appearing in each of the flare example designs.

Design	V ₁	V ₂	V ₃	V ₄	V ₅	V ₆	V ₇	V ₈	Edge	Other points
11Q-D	1	1	1	1	1	1	1	1	E ₆	G ₁ to G ₃
11Q-G		1	1			1				G ₄ to G ₁₀
12Q-D	1	1	1	1	2	1	1	1		G ₁₁ to G ₁₃
12Q-G	1	1	1			1				G ₁₄ to G ₂₁
13Q-D	1	1	1	1	2	2	1	1		G ₂₂ to G ₂₄
13Q-G			1	1						G ₂₅ to G ₃₅
14Q-D	1	2	1	1	2	2	1	1		G ₃₆ to G ₃₈
14Q-G	1		1			1		1		G ₃₉ to G ₄₈
15Q-D	2	2	1	1	2	2	1	1		G ₄₉ to G ₅₁
15Q-G	1	1		1				1		G ₅₂ to G ₆₂
16Q-D	2	2	1	2	2	2	1	1		G ₆₃ to G ₆₅
16Q-G	1	1	1	1	1		1			G ₆₆ to G ₇₅
15SC-S-D	1	2	1	1	1	1	1	1		G ₇₆ to G ₈₁
15SC-W-D	2	1	1	1	1	2	1	1		G ₈₂ to G ₈₆
15SC-S-G	1	1			1				E ₁₀	G ₈₇ to G ₉₇
15SC-W-G	1	1		1	1	1		1	E ₂	G ₉₈ to G ₁₀₅
16SC-S-D	2	1	1	1	2	1	1	1		G ₁₀₆ to G ₁₁₁
16SC-W-D	2	1	1	1	2	1	1	1	E ₁₀	G ₁₁₂ to G ₁₁₆
16SC-S-G		1			1	1			E ₉	G ₁₁₇ to G ₁₂₈
16SC-W-G	1	1				1		1		G ₁₂₉ to G ₁₄₀
17SC-S-D	2	2	1	1	1	2	1	1	E ₄	G ₁₄₁ to G ₁₄₅
17SC-W-D	2	2	2	1	2	1	1	1		G ₁₄₆ to G ₁₅₀
17SC-S-G	1	1			1	1	1	1		G ₁₅₁ to G ₁₆₁
17SC-W-G	1	1			1	1		1		G ₁₆₂ to G ₁₇₃
18SC-S-D	2	2	1	1	2	2	1	1		G ₁₇₄ to G ₁₇₉
18SC-W-D	2	2	1	1	2	2	1	1		G ₁₈₀ to G ₁₈₅
18SC-S-G	1	1	1		1	1		1	E ₁₂	G ₁₈₆ to G ₁₉₆
18SC-W-G	1	1			1	1	1			G ₁₉₇ to G ₂₀₉
19SC-S-D	2	2	2	1	2	2	1	1		G ₂₁₀ to G ₂₁₅
19SC-W-D	2	2	2	1	2	2	1	1		G ₂₁₆ to G ₂₂₁
19SC-S-G	1	1		1		1	1	1	E ₁₀	G ₂₂₂ to G ₂₃₃
19SC-W-G	1	1	1		1	1	1	1		G ₂₃₄ to G ₂₄₅
20SC-S-D	2	2	1	2	2	2	2	1		G ₂₄₆ to G ₂₅₁
20SC-W-D	2	3	2	1	2	2	1	1		G ₂₅₂ to G ₂₅₇
20SC-S-G	1	1	1	1	1	1		1	E ₄ ,E ₁₂	G ₂₅₈ to G ₂₆₈
20SC-W-G	1	1	1	1	1	1	1	1		G ₂₆₉ to G ₂₈₀

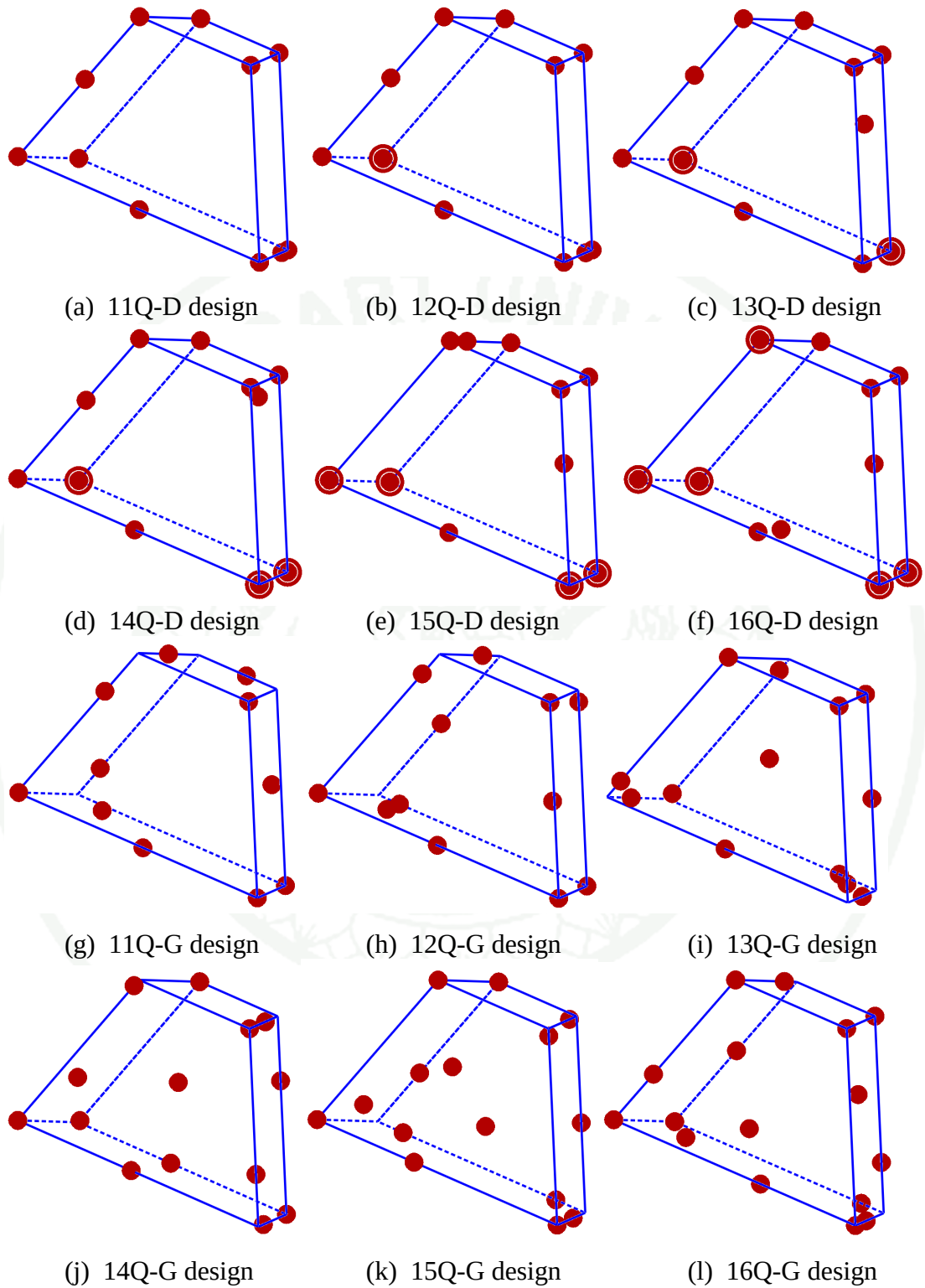


Figure 54 The optimal exact designs based on D_w and G_w assuming the Scheffé quadratic model for the flare experiment. $\bullet$ and $\odot$ represent 1 and 2 replicates of that design point, respectively.

For the quadratic model using D_w , there are obvious distributional patterns of the design points. The five designs (12Q-D, 13Q-D, 14Q-D, 15Q-D and 16Q-D) include all eight vertices. The remaining sets of design points each contain subsets of the vertices with varying levels of replication and additional points near vertices, near edge centroids and near face centroids. The 11Q-D design also includes the eight vertices, but it does not have replicated points. The 13Q-D design includes a face point. The 16Q-D design includes a near face centroid and has the most replicated points.

For the quadratic model using G_w , the six designs contain varying numbers of the eight vertices. The remaining points lie on near vertices, near edge centroids, on faces, and near the overall centroid. Only the 13Q-G and 14Q-G designs include a near overall centroid. The 11Q-G and 12Q-G designs include the same three vertices, the 13Q-G and 16Q-G designs have the same two vertices, the 14Q-G and 16Q-G designs include the same two vertices, and the 15Q-G and 16Q-G designs include the same two vertices as well. The third vertex $V_3 = (0.6, 0.1, 0.27, 0.03)$ occurs in all designs except for the 15Q-G design. However the 15Q-G design contains a point near V_3 . The 16Q-G design includes the most vertices, while the 13Q-G design includes the fewest vertices.

For the quadratic model, and like the poultry example, the geometries of the design based on D_w and G_w are very different. The patterns of points based on D_w are quite different as compared to those based on G_w in that they are all vertices with varying replication, near vertices, near edge centroids and near face centroids. Note that the designs based on D_w have no point near the overall centroid, while there are two G_w -based designs (13Q-G and 14Q-G), that do have a point near the overall centroid. Most of designs based on D_w have replicated points while all of designs based on G_w have no replicated points.

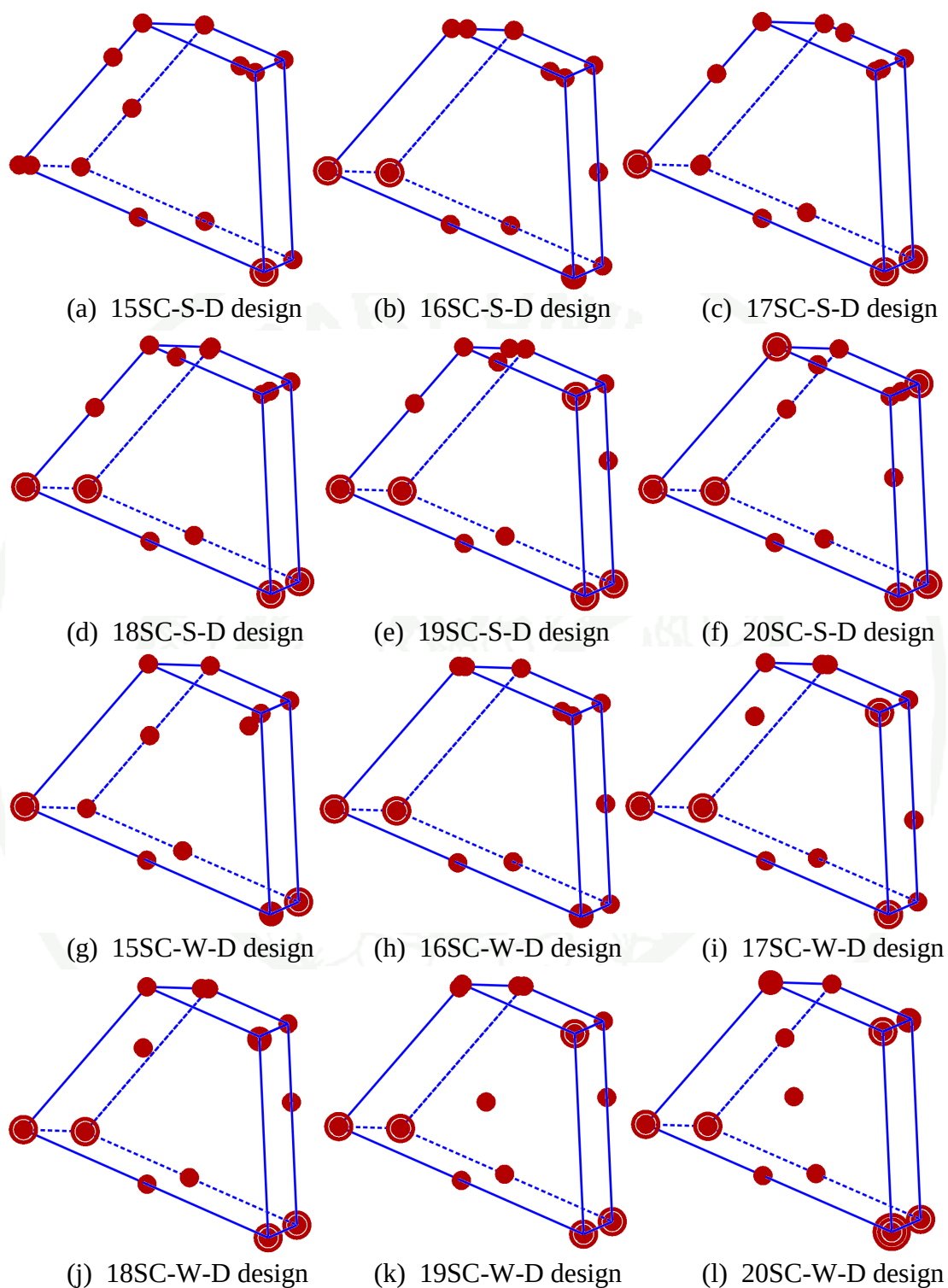


Figure 55 Optimal exact designs based on D_w assuming the Scheffé special cubic

model for the flare experiment. $\bullet$, $\odot$ and $\odot\odot$ represent 1, 2 and 3 replicates of that design point, respectively.

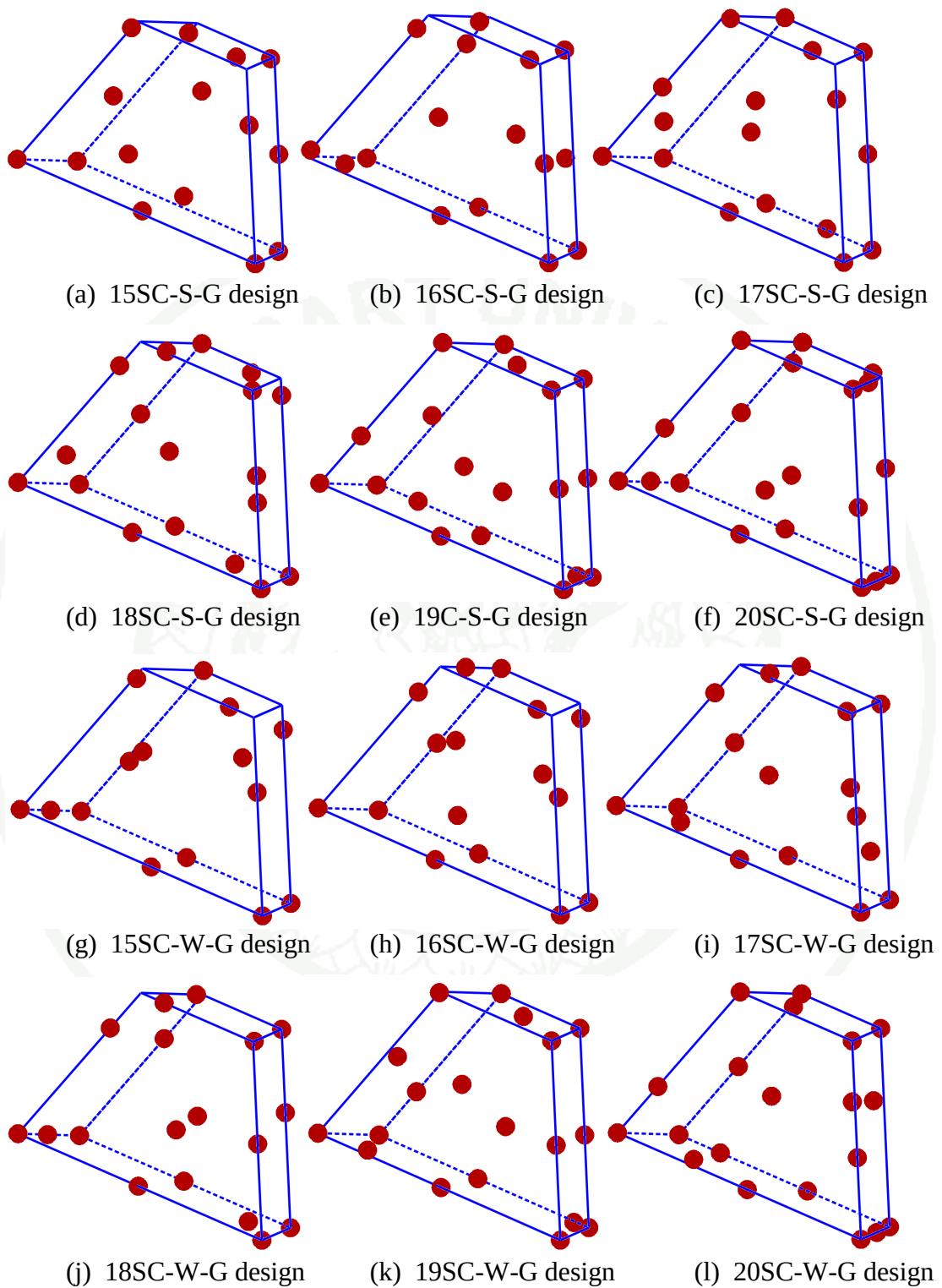


Figure 56 Optimal exact designs based on G_w assuming the Scheffé special cubic model for the flare experiment. ● represent 1 replicates of that design point.

For the special cubic model with D_w and under both SH and WH, there are similar distributional patterns of points. The twelve designs contain the eight vertices, and the remaining design points contain subsets of the vertices with varying levels of replication as well as additional points near vertices and near edge centroids. The 16SC-S-D, 17SC-S-D, 18SC-S-D, 15SC-W-D, 16SC-W-D, 18SC-W-D, and 20SC-W-D designs include replicated points at and very close to the vertices which is indicated by the larger size of these points in Figure 55. At least two replicated vertices are identical except for those of the 15SC-S-D design. The 15SC-S-D design includes only one replicated vertex, while the 20SC-S-D design has the most replicated vertices.

For the special cubic model with G_w and under both SH and WH, the twelve designs contain at least three unreplicated vertices plus various combinations of points near vertices, edge centroids, near edge centroids, near face centroids and on the faces. These designs do not include a near overall centroid. For $n = 15$, 15SC-S-G and 15SC-W-G do not include points lying on near face centroids of the two largest constraint planes. For $n = 17$ to 20, the 17SC-S-G, 17SC-W-G, 18SC-S-G, 18SC-W-G, 19SC-S-G, 19SC-W-G, 20SC-S-G and 20SC-W-G designs include points lying on near face centroids of the two largest constraint planes. The 20SC-W-G design includes all eight vertices, while the 20SC-S-G design includes seven vertices

For both SH and WH and the special cubic model as the full model, the distributions of points based on D_w is quite different than the distributions based on G_w . Specifically, designs based on D_w include all vertices with varying replication, and an edge or near edge centroid. As was the case for the quadratic model, the geometries of the points based on D_w and G_w are also different. For both D_w and G_w with the special cubic model, we see that the patterns of points under SH are quite similar to those under WH.

3. Evaluating designs for Case 2

When selecting a mixture design, there are many design criteria and characteristics that could be considered. Among the most important of the design criteria and characteristics is the stability of the prediction variance over the design region. When the experimenter is interested in the prediction variance throughout the design region, the design efficiency is not necessarily a good choice for comparing and evaluating designs. In this dissertation, we focus on D_w and G_w . The single number criteria, however, do not completely reflect a design's prediction variance properties throughout the entire experimental design region. Graphical techniques that are useful in evaluating experimental designs for any region of interest are the variance dispersion graph (VDG), the fraction of design space (FDS) plot, and the componentwise variance dispersion graph (CVDG).

When the experimenter would like to assess how good his/her n -point designs are relative to all possible n -point designs based for any optimality criterion, relative design efficiencies are considered. The optimal exact n -point designs have 100% relative efficiencies for their corresponding criterion. That is, over the set of all exact n -point designs, the weighted D -optimal design is 100% D -efficient for the weighted D criterion and the weighted G -optimal design is 100% G -efficient for the weighted G criterion. It is interesting to consider how both criteria affect the design. The summary of the objective function values and the relative design efficiencies for the flare experiment assuming the quadratic model and special cubic model are presented in Tables 30 and 32, respectively.

Table 30 Performance comparison of the objective function values and relative efficiencies of optimal exact designs assuming the quadratic model for the flare experiment.

Design points	Design	Objective function values		Relative efficiencies (%)	
		D_w	G_w	D_w^{eff}	G_w^{eff}
11	11Q-D	0.0808	35.1550	100	49.01
	11Q-G	0.0735	71.7333	90.97	100
12	12Q-D	0.0810	34.4341	100	47.03
	12Q-G	0.0733	73.2224	90.49	100
13	13Q-D	0.0811	38.4124	100	55.86
	13Q-G	0.0715	68.7614	88.16	100
14	14Q-D	0.0816	35.6939	100	49.89
	14Q-G	0.0724	71.5466	88.73	100
15	15Q-D	0.0821	33.0011	100	47.87
	15Q-G	0.0695	68.9410	84.65	100
16	16Q-D	0.0825	37.6864	100	51.21
	16Q-G	0.0719	73.5950	87.15	100

*Boldface indicates optimal exact value D_w^{opt} and G_w^{opt} .

In Table 30, assuming the quadratic model, the weighted D -optimal exact designs have low G_w values. However, the weighted G -optimal exact designs have high D_w values. As the number of design points increase, the D_w objective function values of the weighted exact optimal designs increase accordingly. The weighted G -optimal exact designs show otherwise. The weighted G -optimal exact designs have relative efficiencies greater than 84% for both criteria.

Figure 57 presents the VDG of the weighted D -optimal and weighted G -optimal exact designs assuming the quadratic model for the flare experiment. The minimum and maximum of the SPV for shrinkage levels between 0 and 1 are plotted. Figure 58 displays the FDS plot of the weighted D -optimal and weighted G -optimal exact designs, assuming the quadratic model for the flare experiment. The fraction of the design space at or below any SPV value is shown. Figure 59 shows the CVDG of the weighted D -optimal and weighted G -optimal exact designs, assuming the quadratic model for the flare experiment. The maximum of the SPV for allowable

mixtures with $x_i = a$ where $L_i \leq a \leq U_i$ are shown. The maximum SPV for the weighted D -optimal and weighted G -optimal exact designs for the flare experiment are displayed in Table 31.

Table 31 The maximum SPV for the flare experiment assuming the quadratic model.

Design	Design points	Max SPV	Max SPV occurs that (x_1, x_2, x_3)
11Q-D	11	60.23	(0.495, 0.22, 0.23, 0.055)
12Q-D	12	62.84	(0.5, 0.21, 0.235, 0.055)
13Q-D	13	78.02	(0.6, 0.245, 0.1, 0.055)
14Q-D	14	51.99	(0.4, 0.275, 0.27, 0.055)
15Q-D	15	59.75	(0.4, 0.275, 0.27, 0.055)
16Q-D	16	62.99	(0.505, 0.34, 0.1, 0.055)
11Q-G	11	12.69	(0.515, 0.1, 0.305, 0.08)
12Q-G	12	12.32	(0.48, 0.25, 0.24, 0.03)
13Q-G	13	13.12	(0.4, 0.47, 0.1, 0.03)
14Q-G	14	12.59	(0.515, 0.355, 0.1, 0.03)
15Q-G	15	12.75	(0.495, 0.1, 0.375, 0.03)
16Q-G	16	11.83	(0.6, 0.245, 0.1, 0.055)

As seen in Table 31, the 14Q-D design outperforms all of the weighted D -optimal designs with respect to the maximum SPV, while the 13Q-D design performs poorly with respect to the maximum SPV. The 16Q-G design outperforms all of the weighted G -optimal designs with respect to the maximum SPV, and all of the weighted G -optimal designs are quite comparable. The weighted D -optimal designs, however, are not comparable to the weighted G -optimal designs with respect to the maximum SPV in every situation considered.

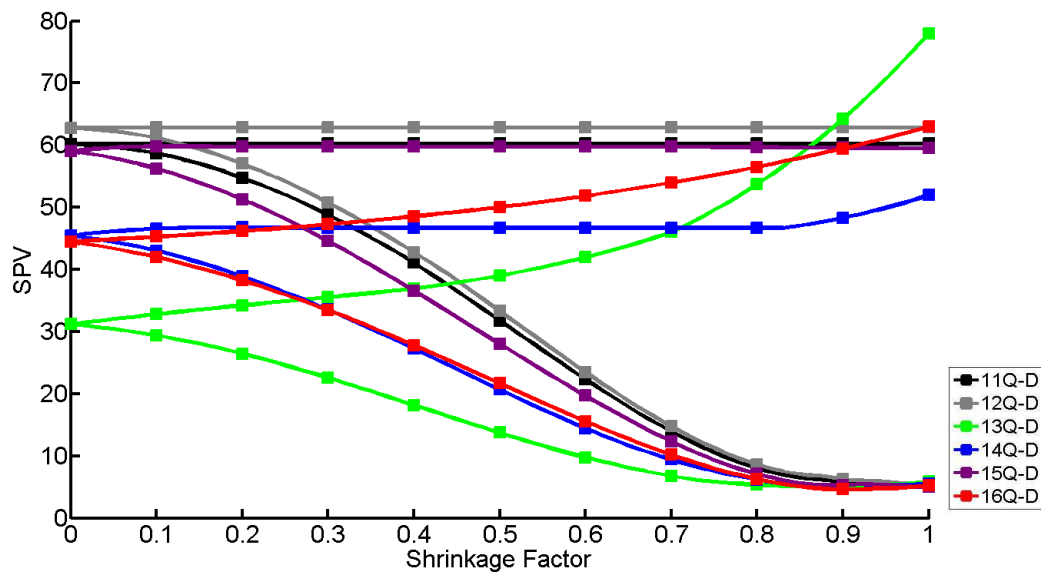
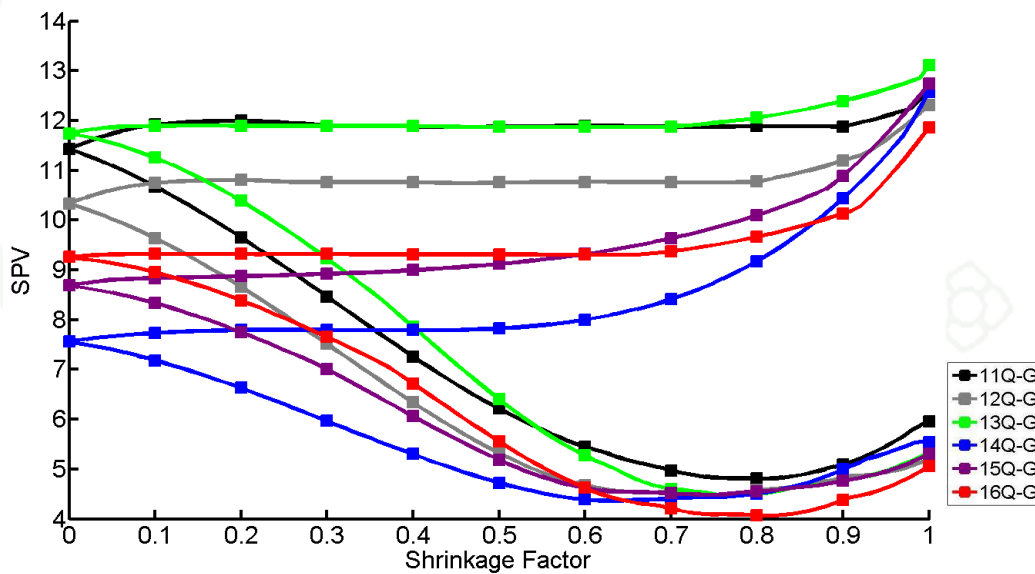
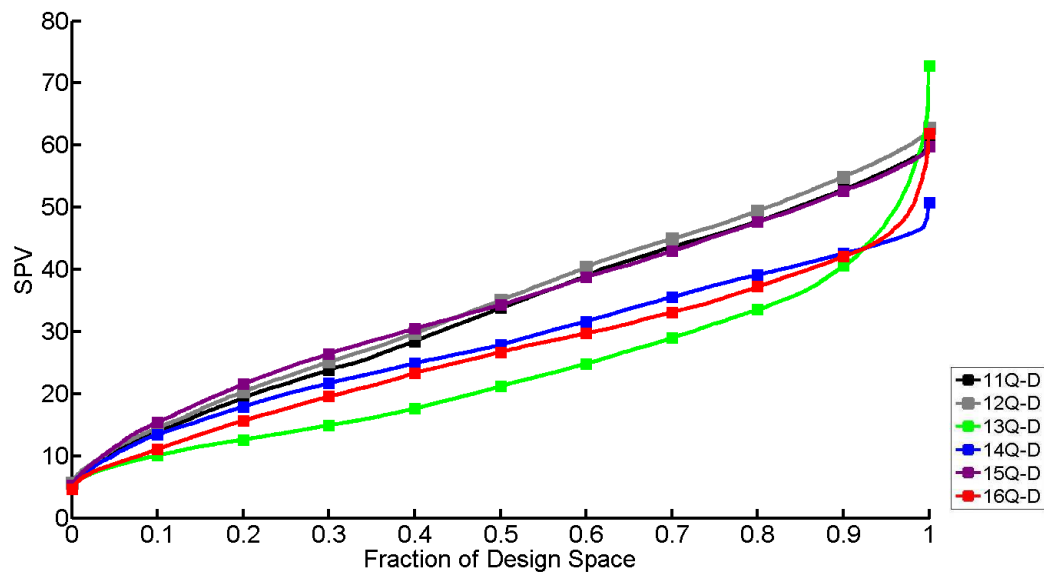
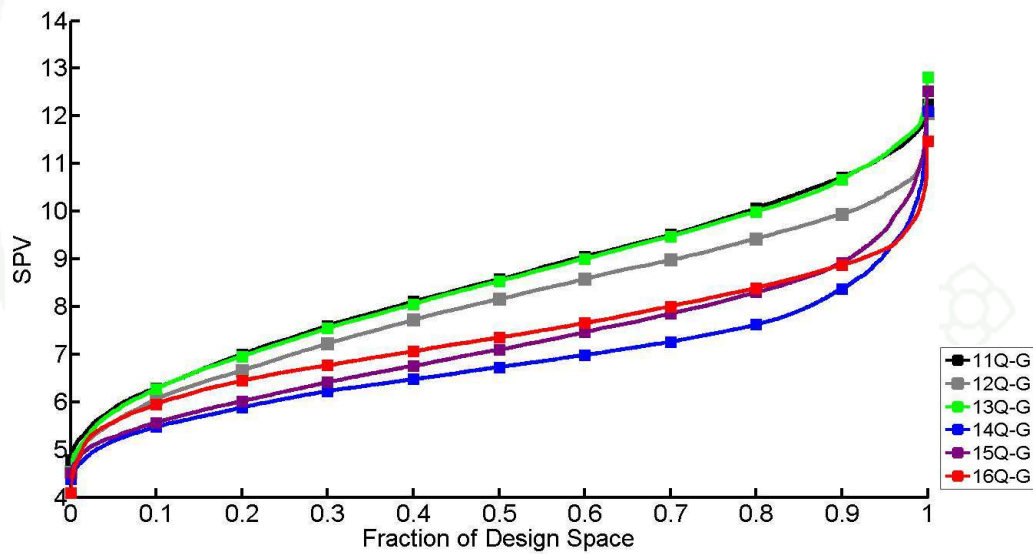
(a) VDGs of the weighted D -optimal exact designs(b) VDGs of the weighted G -optimal exact designs

Figure 57 VDGs for the weighted optimal exact designs assuming the quadratic model for the flare experiment.



(a) FDS plots of the weighted D -optimal exact designs



(b) FDS plots of the weighted G -optimal exact designs

Figure 58 FDS plot for the weighted optimal exact designs assuming the quadratic model for the flare experiment.

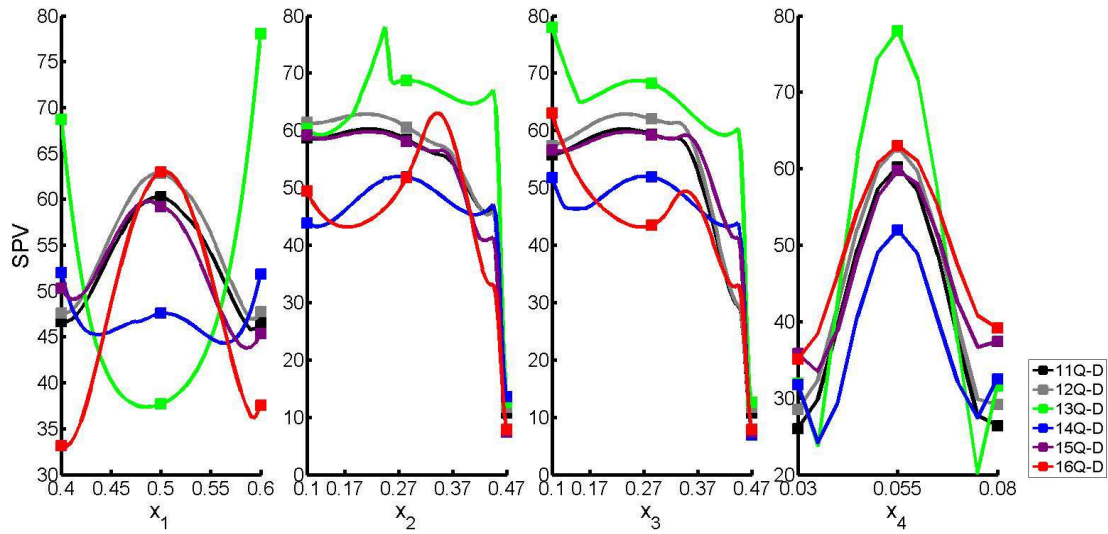
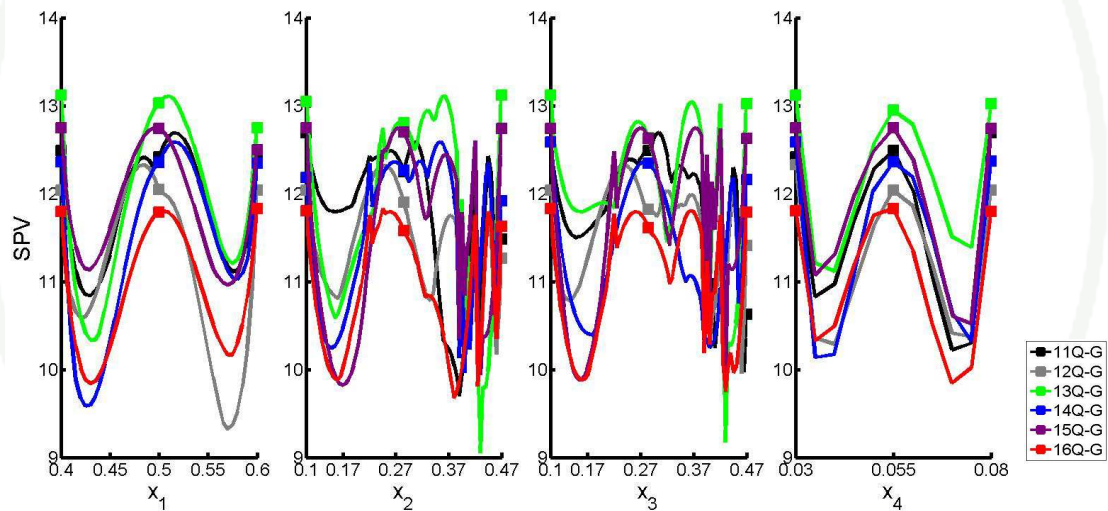
(a) CVDGs for the weighted D -optimal exact designs(b) CVDGs for the weighted G -optimal exact designs

Figure 59 CVDG for the weighted optimal exact designs assuming the quadratic model for the flare experiment.

As seen in Figure 57(a), the minimum SPV for the 13Q-D design is less than the minimum SPV for the other designs. However, at the outer regions, the maximum SPV for the 13Q-D design is noticeably larger while the maximum SPV for the 14Q-D design is clearly the smallest and is stable throughout the design region. In the FDS plots in Figure 58(a), the 13Q-D design performs better than the other designs over most of the design region but performs poorest for a small fraction of the design

space. The 14Q-D design is the most throughout the design space. In Figure 59(a), the CVDG profiles for x_1 for the 13Q-D and 14Q-D designs clearly differ from the other designs. For components x_2 and x_3 , the maximum SPV plots have similar patterns with a fairly stable, but poor, maximum SPV except when the component proportions are near 0.47. For component x_4 , the maximum SPV plots have similar patterns with the poorest performance when the component proportion is near its midlevel. The 14Q-D design performs as well as, if not better than, the 16Q-D design throughout the design region, as seen in Figures 57(a), 58(a) and 59(a). In Figures 57(b), 58(b) and 59(b), the weighted G -optimal designs have fairly similar profiles and outperformed all of the weighted D -optimal designs. The 14Q-G design performs well for the majority of the region but performs similarly to the other designs at the boundary of the design. The 14Q-G design has the larger fraction of the total design space at or below each SPV value considered. The weighted G -optimal designs have stable maximum SPV values for all components, as shown in Figure 59(b).

Figure 60 presents the VDG, FDS plot, and CVDG for the weighted D -optimal and weighted G -optimal exact designs for the flare experiment. Solid and dashed lines correspond to the weighted D -optimal and weighted G -optimal exact designs, respectively. In Figure 60(a), the VDG lines are similar for all of the weighted G -optimal exact designs, while those are quite different for the weighted D -optimal designs. The weighted G -optimal exact designs show an advantage with a lower maximum for shrinkage levels between 0 and 1. In Figure 60(b), the FDS plot shows additional evidence of the advantage of the G -optimal exact designs. Separation of FDS curves for the weighted G -optimal exact designs from the curves for the weighted D -optimal exact designs begins immediately at the design center. The weighted D -optimal exact designs show a clear disadvantage throughout the design space because for any chosen fraction of the design space, the corresponding SPV values are larger than those of the weighted G -optimal exact designs. The values of SPV for the weighted G -optimal designs are less than G -optimal bound of approximately 10 for approximately 80% of the design region for the 11Q-G and 13Q-G designs and more than 90% of the design region for the remaining designs. In Figure 60(c), the CVDG shows the variability over the entire mixture design space.

The weighted G -optimal exact designs outperformed all of the weighted D -optimal designs because they have the smallest SPV values and are competitive throughout the design space.

From the VDG on shrunken boundaries, the SPV for the weighted D -optimal exact designs is greater than that for the weighted G -optimal exact designs. From the FDS plot, the weighted G -optimal exact designs are superior to the weighted D -optimal exact designs throughout the design region. It is clear that the weighted G -optimal exact designs have much flatter and lower FDS curves, indicating a more desirable SPV distribution. In the CVDG, the maximum SPV occurs for the weighted D -optimal exact designs and weighted G -optimal exact design at (x_1, x_2, x_3, x_4) shown in the last column of Table 31. The SPV near $(x_1, x_2, x_3, x_4) = (0.6, 0.245, 0.1, 0.055)$, or E_6 , is inflated for the 13Q-D design. These designs can be improved by adding the mixture (x_1, x_2, x_3, x_4) at which the maxima SPV occurs.

Assuming the quadratic model, we conclude that (1) the weighted G -optimal exact designs have better prediction properties than the weighted D -optimal exact designs over nearly the entire design region, (2) the maximum SPVs for the weighted D -optimal exact designs are larger than the maximum SPVs of the weighted G -optimal exact designs for all cases, and (3) the additional design points do not provide significantly better SPV properties.

In Table 32, $D_w - S$, $D_w - W$, $G_w - S$ and $G_w - W$ represent the weighted D -optimality criteria based on SH and WH and the weighted G -optimality criteria based on SH and WH, respectively. The optimal exact design has 100% relative efficiencies for its corresponding criterion.

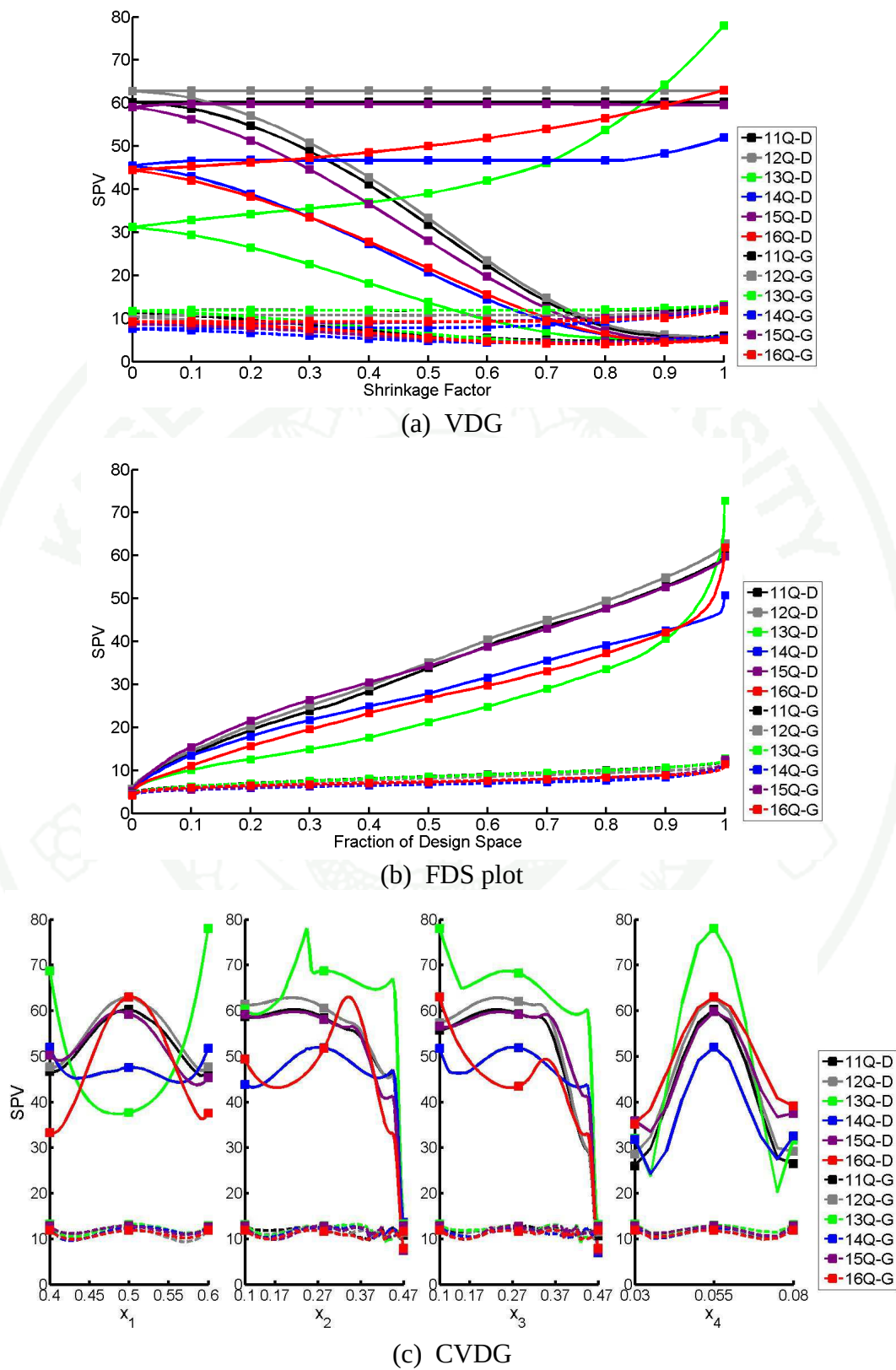


Figure 60 Graphical approaches for comparing the 12 mixture designs when assuming the quadratic model for the flare experiment.

Table 32 Performance comparison of objective function values and relative efficiencies based on D - and G -criterion of optimal exact designs assuming the special cubic model for the flare experiment.

n	Design	Objective function values				Relative efficiencies (%)			
		D_W -S	D_W -W	G_W -S	G_W -W	D_W^{eff} -S	D_W^{eff} -W	G_W^{eff} -S	G_W^{eff} -W
15	15SC-S-D	0.0326	0.0283	18.5928	20.5475	100	99.65	28.31	32.16
	15SC-W-D	0.0324	0.0284	13.2036	16.1591	99.39	100	20.10	25.29
	15SC-S-G	0.0289	0.0249	65.6713	63.9006	88.65	87.68	100	100
	15SC-W-G	0.0297	0.0256	63.1877	63.3993	91.10	90.14	96.21	99.22
16	16SC-S-D	0.0330	0.0286	17.0092	17.8516	100	99.65	25.13	26.50
	16SC-W-D	0.0321	0.0287	13.6663	15.6125	97.27	100	20.19	23.18
	16SC-S-G	0.0289	0.0249	67.6681	67.3593	87.58	86.76	100	100
	16SC-W-G	0.0288	0.0249	65.8326	67.1785	87.27	86.76	97.28	99.73
17	17SC-S-D	0.0332	0.0286	15.1121	15.3407	100	99.65	21.54	21.76
	17SC-W-D	0.0329	0.0287	16.5244	21.1941	99.10	100	23.55	30.06
	17SC-S-G	0.0291	0.0251	69.9795	69.4846	87.65	87.46	99.75	98.55
	17SC-W-G	0.0292	0.0252	70.1498	70.5053	87.95	87.80	100	100
18	18SC-S-D	0.0333	0.0287	17.4347	17.0881	100	98.97	24.42	23.91
	18SC-W-D	0.0332	0.0290	17.5003	22.3327	99.70	100	24.51	31.25
	18SC-S-G	0.0290	0.0250	71.1533	69.9943	87.09	86.21	99.68	97.95
	18SC-W-G	0.0294	0.0254	71.3808	71.4588	88.29	87.59	100	100
19	19SC-S-D	0.0334	0.0289	23.1649	24.8328	100	99.31	32.15	34.66
	19SC-W-D	0.0333	0.0291	18.5794	23.8477	99.70	100	25.79	33.28
	19SC-S-G	0.0291	0.0251	71.3235	70.4230	87.13	86.25	99.01	98.28
	19SC-W-G	0.0292	0.0252	72.0365	71.6545	87.43	86.60	100	100
20	20SC-S-D	0.0334	0.0288	26.0292	27.1442	100	98.97	36.68	38.08
	20SC-W-D	0.0333	0.0291	17.4019	22.5824	99.70	100	24.52	31.68
	20SC-S-G	0.0298	0.0257	70.9549	69.4018	89.22	88.32	99.99	97.36
	20SC-W-G	0.0293	0.0252	70.9596	71.2818	87.72	86.60	100	100

*Boldface indicates optimal exact value D_W^{opt} and G_W^{opt} .

Relative to the other designs, the weighted D -optimal exact designs under SH have high $D_w - W$ values as well as quite low $G_w - S$ and $G_w - W$ values. The weighted D -optimal exact designs under WH have relatively large $D_w - S$ values as well as quite small $G_w - S$ and $G_w - W$ values. The weighted G -optimal exact designs under SH have relatively high $D_w - S$, $D_w - W$, and $G_w - W$ values. The weighted G -optimal exact designs under SH have relatively high $D_w - S$, $D_w - W$, and $G_w - S$ values. The weighted G -optimal exact designs under SH are identical to the weighted G -optimal exact designs under WH or have relative efficiencies very close to 100%. Theoretically, the relative efficiencies should be 100%, but the GA terminated before finding the true weighted optimal exact designs under SH or WH. The weighted D -optimal exact designs under SH and WH have relative efficiencies greater than 97% for the D -criterion, while the weighted G -optimal exact designs under SH and WH have relative efficiencies greater than 86% and 96% for the D - and the G -criterion, respectively. As the number of design points increases, the objective function values of the weighted optimal exact designs increase slightly for the weighted D -optimal exact designs based on SH and WH. As the number of design points increases, the objective function values of the weighted optimal exact designs increase slightly for the weighted G -optimal exact designs based on SH and WH except when $n = 20$.

Figure 61 presents the VDGs of the weighted D -optimal and weighted G -optimal exact designs assuming the special cubic model for the flare experiment. The minimum and maximum of the SPV for shrinkage levels between 0 and 1 are shown. Figure 62 displays the FDS plot of weighted D -optimal and weighted G -optimal exact designs assuming the special cubic model for the poultry experiment. The fraction of the design space at or below any SPV value is shown in this figure. Figure 63 represents the CVDG of weighted D -optimal and weighted G -optimal exact designs for the special cubic model for the poultry experiment. The maximum of the SPV for allowable mixtures with $x_i = a$ where $L_i \leq a \leq U_i$ are shown in this figure. Table 33

presents the maximum SPV values for the weighted *D*-optimal and weighted *G*-optimal exact designs assuming the special cubic model for the flare experiment.

In Figures 61 through 66, the weighted *G*-optimal exact designs under SH have a similar pattern for each graphical approach as the designs under WH, while the pattern for each graphical approach for the weighted *D*-optimal exact designs differs from those of the weighted *G*-optimal exact designs. When examining the designs, we see that the SPV values for 16SC-S-D, 17SC-S-D, 18SC-S-D, 16SC-W-D, 18SC-W-D and 20SC-W-D designs are larger than the SPV values for the other designs throughout the design space. That is, these designs have inferior prediction properties compared to the other designs. These designs in Figures 64 to 66 are not further examined. As shown in Table 33, the maximum SPV for 16SC-S-D, 17SC-S-D, 18SC-S-D, 16SC-W-D, 18SC-W-D and 20SC-W-D design are significantly higher than the SPV of the other designs. The weighted *G*-optimal exact designs outperform all of the weighted *D*-optimal exact designs with respect to the maximum SPV. Based on the maximum SPV, the weighted *G*-optimal exact designs under SH and WH are quite comparable, while the weighted *D*-optimal exact designs under SH outperform the weighted *D*-optimal exact designs under WH. The weighted *D*-optimal exact designs are incomparable with the weighted *G*-optimal exact designs based on the maximum SPV. In Table 33, the 20SC-S-D design is the best with smaller maximum SPVs for all of the weighted *D*-optimal exact designs, while the 19SC-W-G design is the best with smaller maximum SPVs for all of the weighted *G*-optimal exact designs. Based on the graphical approaches, the weighted *G*-optimal exact designs under SH and WH are quite comparable, while the weighted *D*-optimal exact designs under SH outperform the weighted *D*-optimal exact designs under WH.

From the VDGs, the weighted *G*-optimal exact designs show an advantage with a lower maximum SPV for shrinkage levels between 0 and 1. The 20SC-S-D design is superior to the other designs based on the *D*-criterion, while the 17SC-W-D design is superior to the other designs based on the *D*-criterion under WH. The 19SC-W-D design does better at the center where shrinkage levels are small, while the 15SC-W-D design performs well at the larger shrinkage levels nearer the boundary of

the design space. Based on the G -criterion, at the design center, the SPV for the 15SC-S-G design has smaller SPV values than for the other designs, while the SPV for the 17SC-W-G design has larger SPV values than for the other designs. At the boundary of the design region, the 15SC-S-G design performs quite poorly, while the 17SC-W-G design performs well.

From the FDS plot, for almost 100% of the design space, the weighted G -optimal exact designs are superior to the weighted D -optimal exact designs. The weighted G -optimal exact designs begin to show separation from the weighted D -optimal exact designs at the design center. The weighted D -optimal exact designs show a clear disadvantage throughout the design space, because for any chosen fraction of the design space, the corresponding SPV values are larger than those of the weighted G -optimal exact designs. Like VDG, the 20SC-S-D design is superior to other designs based on the D -criterion, while the 17SC-W-D design is superior to other designs based on the D -criterion under WH. Based on the G -criterion, the 15SC-S-G design has the best prediction for small SPV values and is competitive throughout the design space, while the 19SC-W-G design performs well at the boundary of the design space, whereas the 15SC-W-G design is the worst case. The weighted G -optimal exact designs have similar SPV distributions. It is clear that the weighted G -optimal exact designs have much flatter and lower FDS curves throughout the design region, indicating a more desirable SPV distribution.

From the CVDGs, the maximum SPV for the weighted D -optimal and weighted G -optimal exact design occurs at (x_1, x_2, x_3, x_4) shown in the last column of Table 33. The mixture where maximum SPV occurs is quite different across designs for the weighted D - and G -optimal designs. Like the VDGs and FDS plots, the 20SC-S-D design is the superior design based on the D -criterion for all components, while the 17SC-W-D design is superior to the other designs based on the D -criterion under WH for all components. The 19SC-W-D is unstable for all components.

Table 33 Maximum SPV values for the poultry experiment assuming the special cubic model for the flare experiment.

	Design	Max SPV	Max SPV occurs that (x_1, x_2, x_3, x_4)
The weighted <i>D</i> -optimal exact designs based on SH	15SC-S-D	228.37	(0.51, 0.23, 0.23, 0.03)
	16SC-S-D	24,999.45	(0.5, 0.26, 0.21, 0.03)
	17SC-S-D	12,760.53	(0.5, 0.185, 0.235, 0.08)
	18SC-S-D	6,571.34	(0.5, 0.1, 0.32, 0.08)
	19SC-S-D	137.49	(0.5, 0.215, 0.235, 0.05)
	20SC-S-D	107.04	(0.5, 0.235, 0.215, 0.05)
The weighted <i>D</i> -optimal exact designs based on WH	15SC-W-D	1,730.57	(0.6, 0.175, 0.17, 0.055)
	16SC-W-D	56,123.18	(0.5, 0.255, 0.215, 0.03)
	17SC-W-D	559.79	(0.6, 0.17, 0.18, 0.05)
	18SC-W-D	14,809.42	(0.5, 0.37, 0.1, 0.03)
	19SC-W-D	4,180.39	(0.5, 0.1, 0.37, 0.03)
	20SC-W-D	67,248.05	(0.5, 0.37, 0.1, 0.03)
The weighted <i>G</i> -optimal exact designs based on SH	15SC-S-G	19.85	(0.515, 0.235, 0.22, 0.03)
	16SC-S-G	18.80	(0.51, 0.36, 0.1, 0.03)
	17SC-S-G	18.14	(0.515, 0.1, 0.355, 0.03)
	18SC-S-G	17.14	(0.51, 0.1, 0.33, 0.06)
	19SC-S-G	17.29	(0.515, 0.23, 0.225, 0.03)
	20SC-S-G	17.94	(0.515, 0.225, 0.23, 0.03)
The weighted <i>G</i> -optimal exact designs based on WH	15SC-W-G	20.19	(0.51, 0.36, 0.1, 0.03)
	16SC-W-G	18.52	(0.505, 0.1, 0.335, 0.06)
	17SC-W-G	17.63	(0.51, 0.1, 0.31, 0.08)
	18SC-W-G	17.00	(0.51, 0.36, 0.1, 0.03)
	19SC-W-G	16.91	(0.4, 0.27, 0.27, 0.06)
	20SC-W-G	17.16	(0.525, 0.345, 0.1, 0.03)

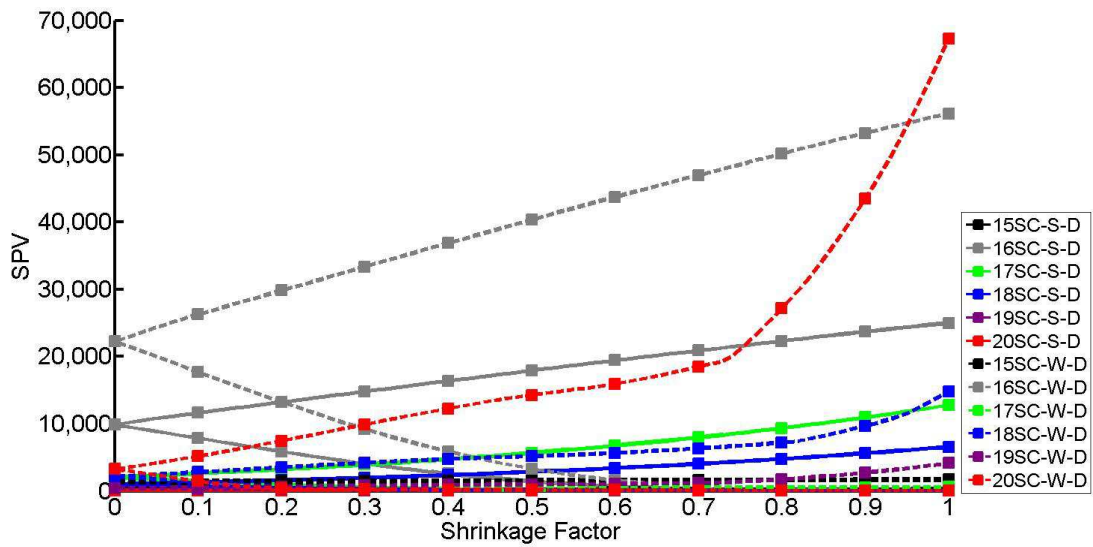
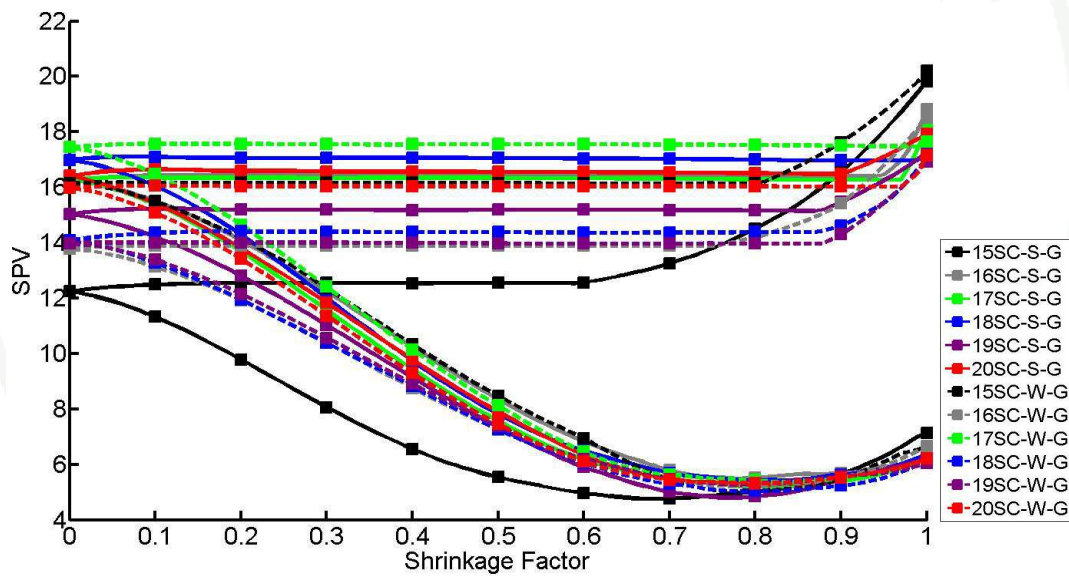
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 61 VDGs for the weighted optimal exact designs assuming the special cubic model for the flare experiment.

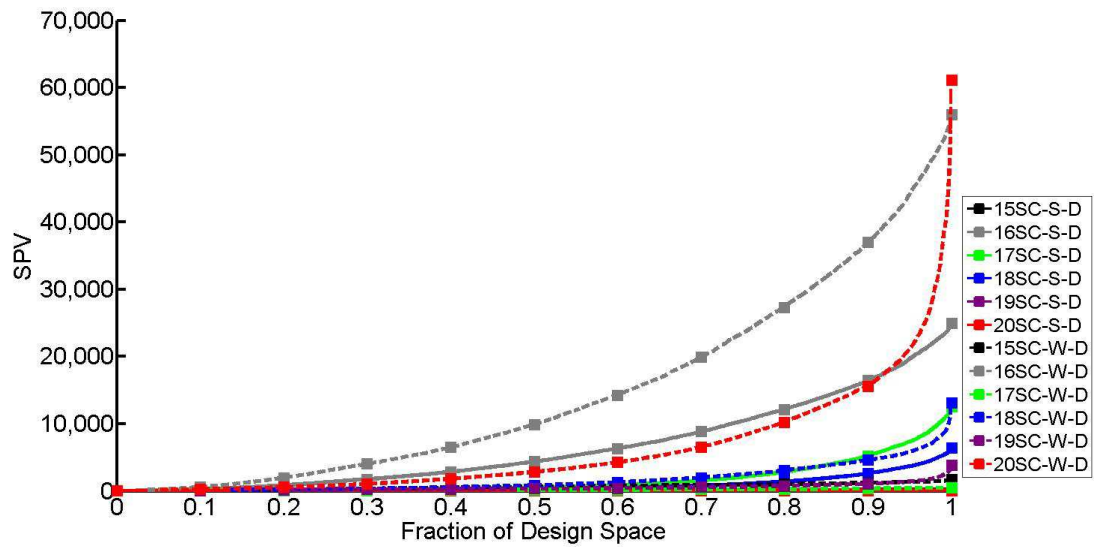
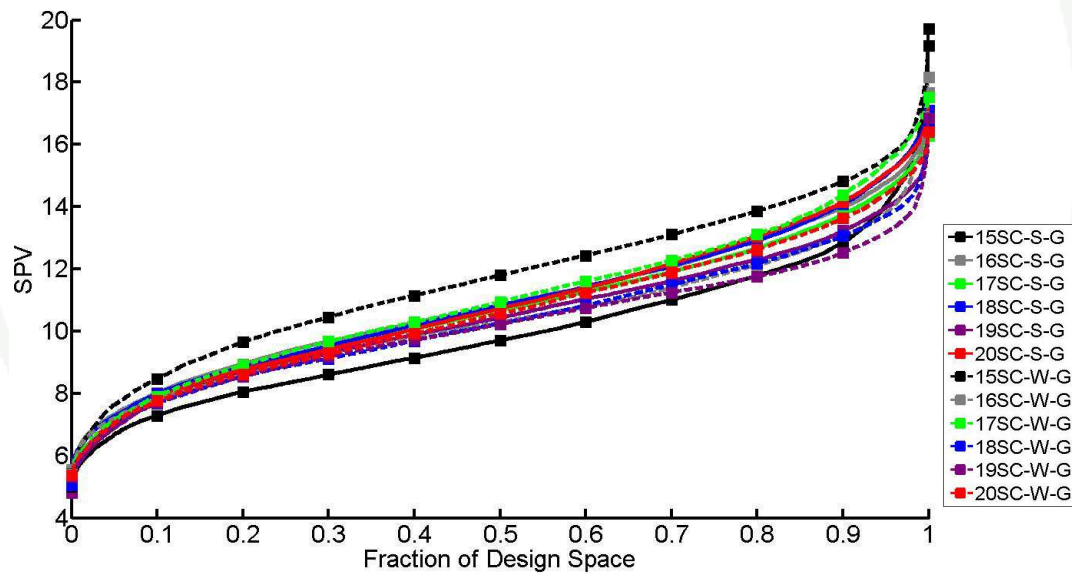
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 62 FDS plots for the weighted optimal exact design assuming the special cubic model for the flare experiment.

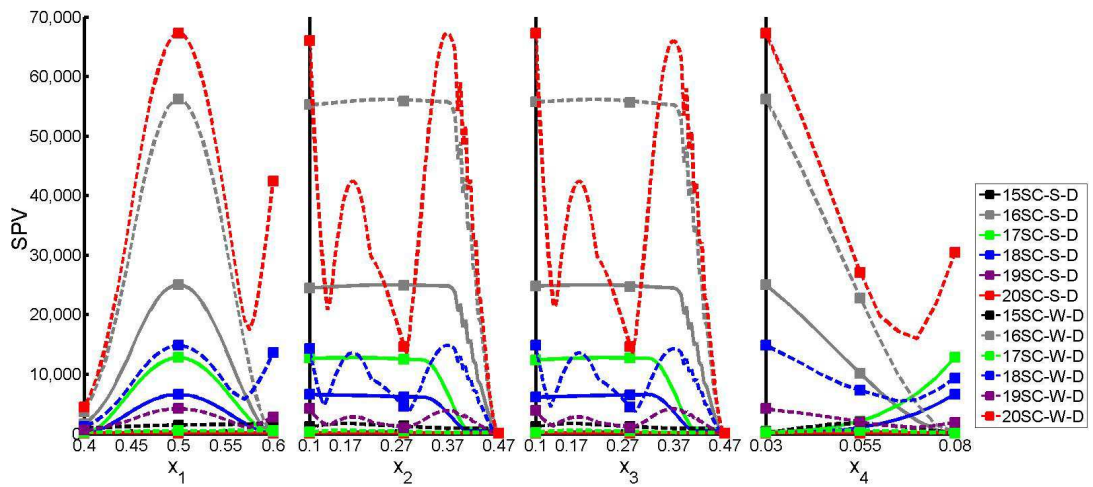
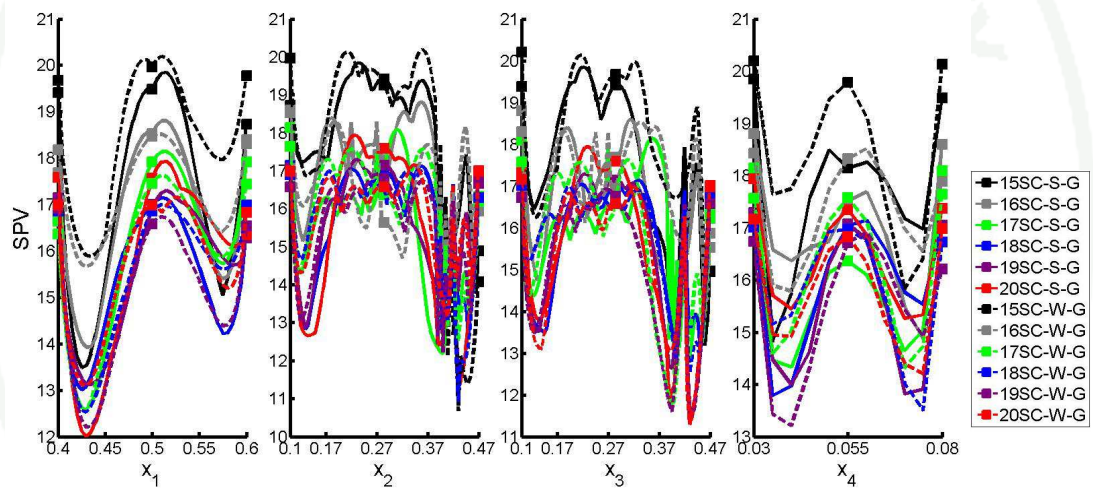
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 63 CVDGs for the weighted optimal exact design assuming the special cubic model for the flare experiment.

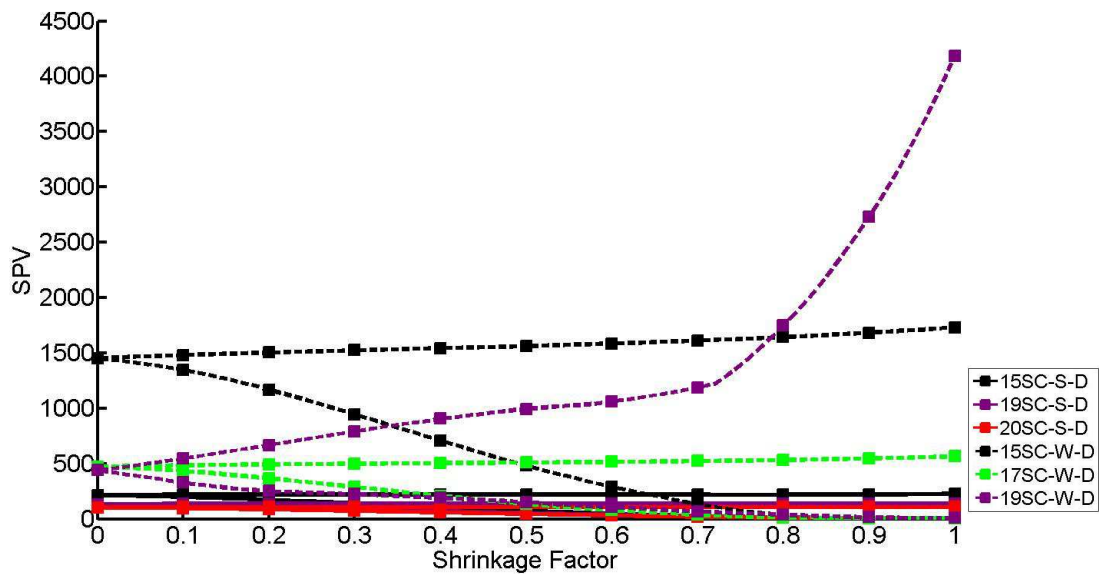


Figure 64 VDGs for some weighted D -optimal exact designs assuming the special cubic model for the flare experiment.

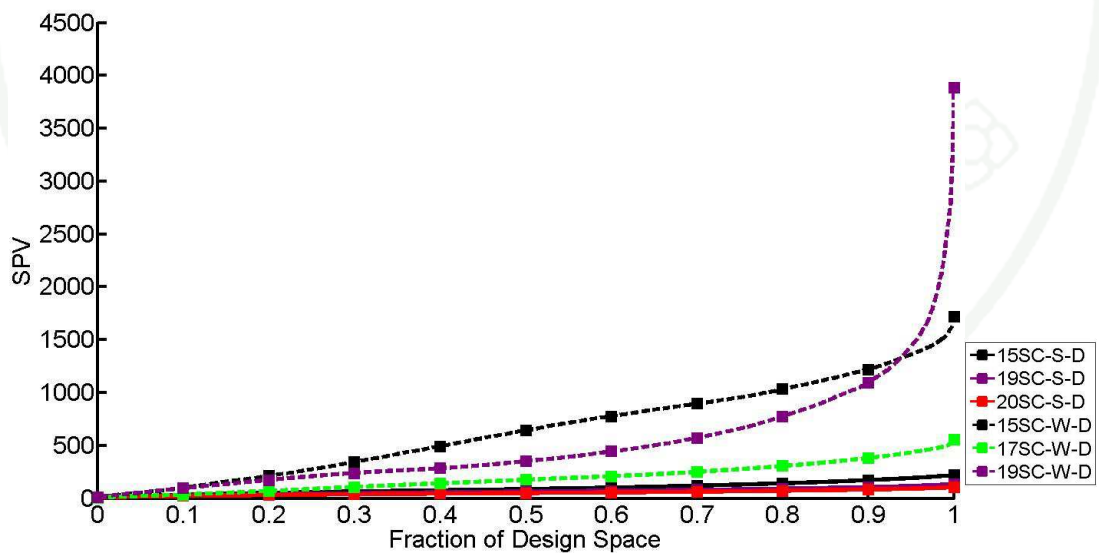


Figure 65 FDS plots for some weighted D -optimal exact designs assuming the special cubic model for the flare experiment.

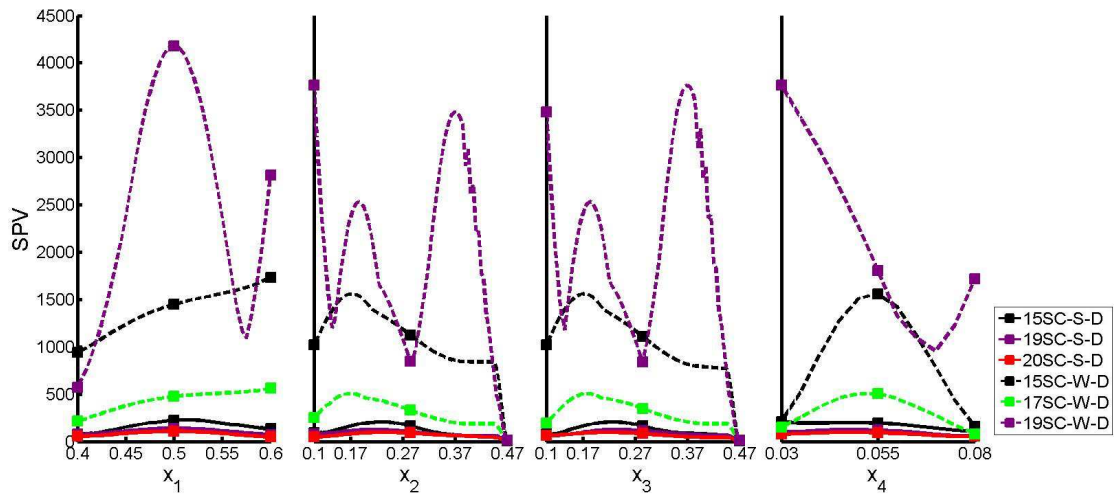


Figure 66 CVDGs for some weighted D -optimal exact designs assuming the special cubic model for the flare experiment.

For the special cubic model, we conclude that (1) the weighted G -optimal exact designs have better prediction variance properties than the weighted D -optimal exact designs throughout the design region, (2) the weighted G -optimal exact designs under SH and WH have similar profiles, whereas the weighted D -optimal exact designs under SH and WH have different profiles, (3) the maximum SPV values for the weighted D -optimal exact designs are larger than those for the weighted G -optimal exact designs in all cases, (4) the maximum SPV values for the weighted D -optimal exact designs under SH are smaller than those under WH, whereas the maximum SPV values for the weighted G -optimal exact designs under SH and WH are quite similar, and (5) as the design size increases, there is very little change in the prediction variance properties of the weighted D - and G -optimal designs.

4. Examining model robustness for Case 2

Frequently, after the data are collected and analyzed, the experimenter finds that some terms may not be significant in the model. As a result, the initial design may no longer have desirable prediction variance properties. The model robustness properties of a design should be a very important consideration when the final model

differs from the initial model. FDS plots can help the experimenter in choosing a design that performs well for a broad range of possible models within a specific model prior to data collection.

Now suppose that **the quadratic model** corresponds to the most complex model that the experimenter might need to adequately model the data. For $q = 4$, there are 64 models nested within the full model, which are shown in Table 5. Table 34 contains some nested models for the quadratic model which might be of interest when examining the 11Q-D design. The corresponding FDS curves for 7 models are shown in Figure 67. By observing Figure 67, we note that (1) the quadratic and linear model are enveloped around other models considered (2) the plots for Model A to Model E are located between the plots for the quadratic and linear models, and (3) any model that is nested within another model must have its FDS curve that is at or below the larger model. We consider the quadratic model and the linear model on the single FDS plot because these models give a manageable summary of the prediction performance of the design across a set of candidate models. The quadratic model FDS curves show rather different slopes than the remaining curves. The maximum SPV values for the larger model are higher than the nested models. Thus, the addition of many quadratic terms has a much larger effect on the stability of the SPV values and can only increase its SPV value. In Table 34 shows the maximum SPV values and G -efficiencies for each model of the 11Q-D design. The G -efficiencies between the linear and quadratic model are different because of the number of associated parameters in the model.

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Table 34 Summary information for the possible reduced models when assuming the quadratic model for the flare experiment.

Type of model	Term in model	Max SPV	G-eff (%)
Quadratic	$x_1, x_2, x_3, x_4, x_{12}, x_{13}, x_{14}, x_{23}, x_{24}, x_{34}$	60.23	16.60
Model A	$x_1, x_2, x_3, x_4, x_{13}, x_{14}, x_{23}, x_{24}, x_{34}$	46.43	19.38
Model B	$x_1, x_2, x_3, x_4, x_{14}, x_{23}, x_{24}, x_{34}$	45.61	17.54
Model C	$x_1, x_2, x_3, x_4, x_{23}, x_{24}, x_{34}$	13.56	51.62
Model D	$x_1, x_2, x_3, x_4, x_{24}, x_{34}$	9.31	64.45
Model E	$x_1, x_2, x_3, x_4, x_{34}$	6.67	74.96
Linear	x_1, x_2, x_3, x_4	5.38	74.35

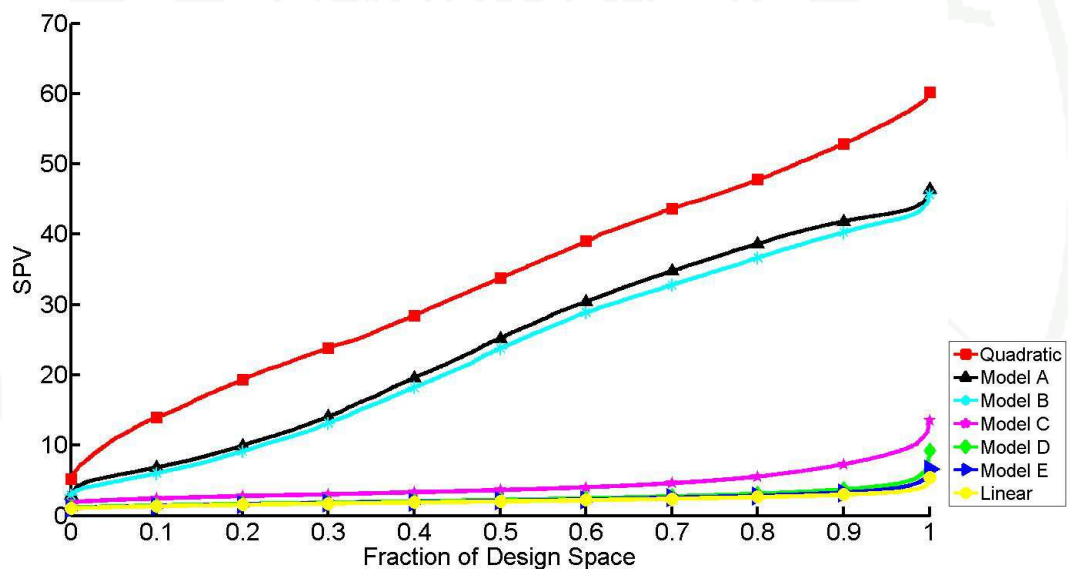


Figure 67 FDS plot for 11Q-D design for several models for the flare experiment.

In Figure 68, the weighted D -optimal and weighted G -optimal exact designs are compared for each design size. The comparison for all of the weighted D -optimal exact designs is shown in Figure 69. Figure 70 displays the comparison for all of the weighted G -optimal exact designs. Table 35 gives the G -efficiency for each design. In the previous section, the weighted G -optimal exact designs were seen to be superior to the weighted D -optimal exact designs. That is, the VDG, FDS and CVDG curves for

the quadratic model for the weighted G -optimal exact designs are lower than those of the weighted D -optimal exact designs for most of the design space.

As shown in Figure 68 and Table 35, for the linear model, the weighted D -optimal exact designs and weighted G -optimal exact designs are quite similar in performance for the most of the design space. For the linear model, the most of the G -efficiencies for the weighted D -optimal exact designs are higher than those of the weighted G -optimal exact designs except when $n=11$. However, for the quadratic model, all of the G -efficiencies for the weighted G -optimal exact designs are larger than those of the weighted D -optimal exact designs. For the linear and quadratic model, the weighted G -optimal designs perform better than the weighted D -optimal designs for the entire design space because they maintain better stability for large values of the SPV. The weighted G -optimal exact designs appear to be more robust than the weighted D -optimal exact designs because the two lines for the quadratic and linear models for each design maintain their stability throughout the design space. If the final model turns out to be the quadratic model, then the weighted G -optimal exact designs would have been the best choice.

In Figure 69, for the majority of the design space, all designs appear to have good robustness properties, while the 14Q-D design appears to be the more robust design because the two lines for the quadratic and linear models are more stable for large values of the SPV, while 13Q-D design appears to be the less robust design because the two lines for the quadratic and linear models do not maintain their stability throughout the design space. In this case, the 14Q-D design has the best performance based on the G -criterion and outperformed all of the weighted D -optimal exact designs with respect to the maximum SPV, while the 13Q-D design performs poorly with respect to the maximum SPV.

In Figure 70, all weighted G -optimal designs perform equally well and maintain better stability for large values of SPV for the quadratic model and linear model. That is, all of the weighted G -optimal designs appear to have good robustness properties. The 16Q-G design appears to be the more robust design and has the best

performance based on the maximum SPV. The 11Q-G and 13Q-G design are quite similar in the performance for the majority of the design space.

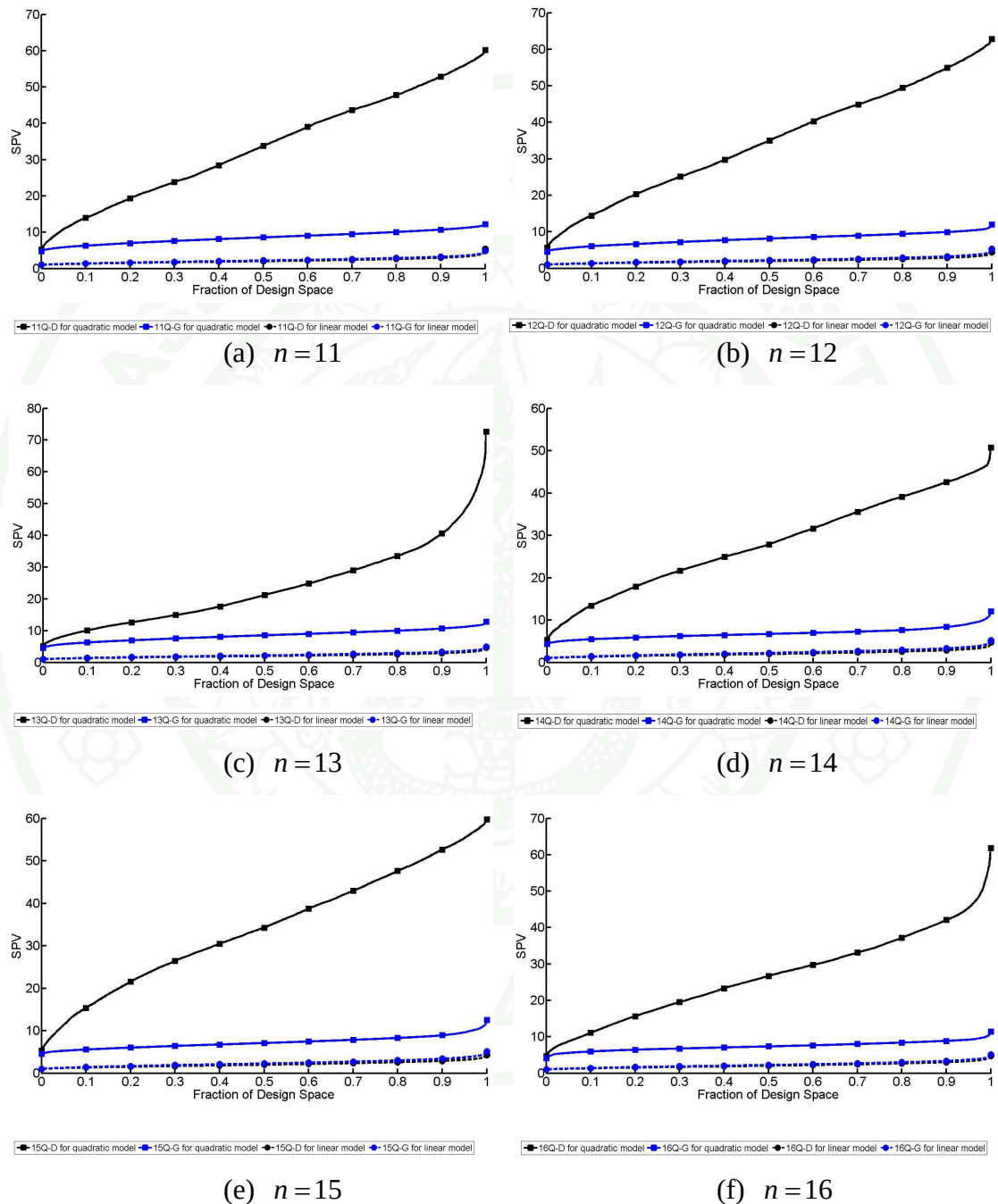


Figure 68 FDS plots for comparing the weighted D -optimal exact design and weighted G -optimal exact design for two types of models assuming the quadratic model ($q = 4$) for the flare experiment.

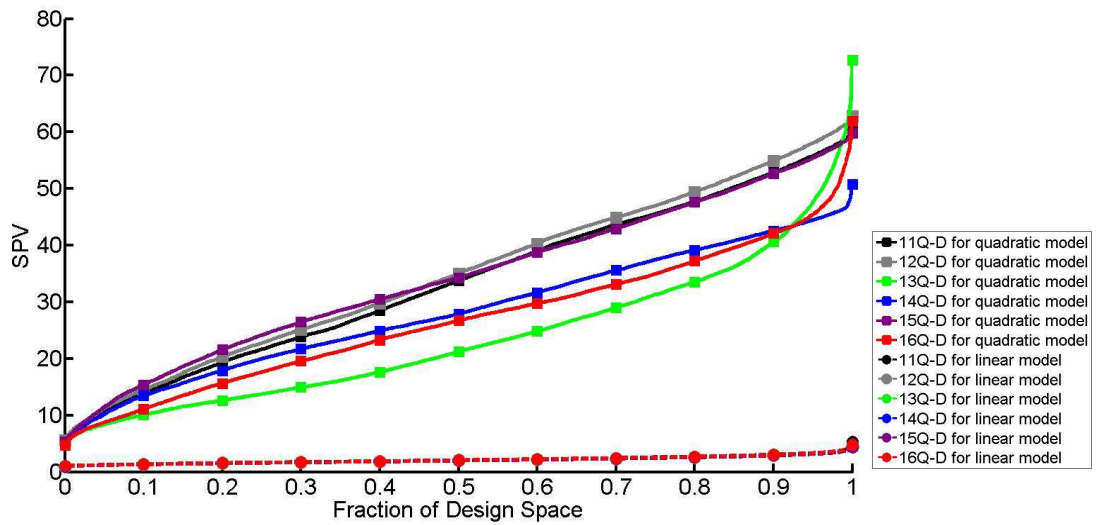


Figure 69 FDS plots for comparing the D -optimal exact designs for two types of models assuming the quadratic model ($q = 4$) for the flare experiment.

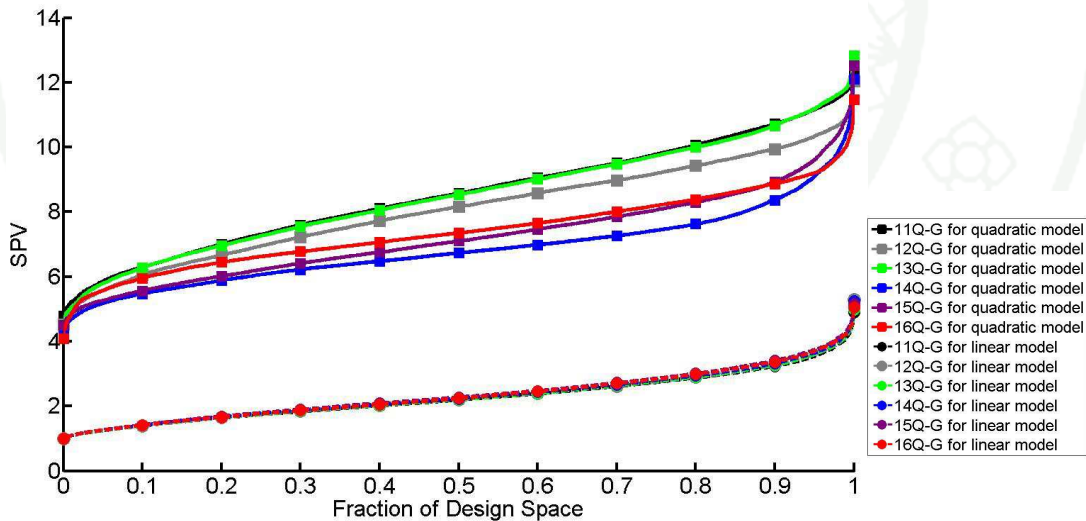


Figure 70 FDS plots for comparing the G -optimal exact designs for two types of models, assuming the quadratic model ($q = 4$) for the flare experiment.

Table 35 The maximum SPV values and approximate G -efficiencies for the weighted D -optimal and weighted G -optimal exact designs for two model types, assuming the quadratic model for the flare experiment.

Design	Model type	G-efficiency (%)	Design	Model type	G-efficiency (%)
11Q-D	Quadratic	16.61	11Q-G	Quadratic	81.70
	Linear	74.35		Linear	81.80
12Q-D	Quadratic	15.93	12Q-G	Quadratic	82.99
	Linear	90.50		Linear	75.61
13Q-D	Quadratic	13.75	13Q-G	Quadratic	78.06
	Linear	85.11		Linear	80.16
14Q-D	Quadratic	19.69	14Q-G	Quadratic	82.58
	Linear	84.39		Linear	76.19
15Q-D	Quadratic	16.73	15Q-G	Quadratic	79.87
	Linear	93.24		Linear	77.67
16Q-D	Quadratic	16.16	16Q-G	Quadratic	87.11
	Linear	83.16		Linear	79.21

For the majority of the design space, all of the weighted D - and G - optimal designs appear to have good robustness properties because they have much flatter and lower FDS curves for the two model types, indicating a more desirable SPV distribution. However, the weighted G -optimal designs are recommended for model robustness over the weighted D -optimal exact designs because (1) all of the curves associated with two models for the weighted G -optimal designs are closer together on FDS plot than the weighted D -optimal exact designs, and (2) the weighted G -optimal designs appear to outperform the weighted D -optimal exact designs.

Now suppose that **the special cubic model** corresponds to the most complex model that the experimenter might need to adequately model the data. For $q = 4$, there are 113 SH models and 809 WH models that are nested within the special cubic model. A number of possible nested models for the special cubic model, which might be of interest when examining the mixture designs are given in Table 36. The corresponding FDS curves for 15SC-S-D design are shown in Figure 71.

Table 36 Summary information for the possible reduced models assuming the special cubic model for the flare experiment.

Type of model	Term in model	p
Special cubic	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4, x_2x_3, x_2x_4, x_3x_4, x_1x_2x_3, x_1x_2x_4, x_1x_3x_4, x_2x_3x_4$	14
Model A	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4, x_2x_3, x_2x_4, x_3x_4, x_1x_2x_3, x_1x_2x_4, x_1x_3x_4$	13
Model B	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4, x_2x_3, x_2x_4, x_3x_4, x_1x_2x_3, x_1x_2x_4$	12
Model C	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4, x_2x_3, x_2x_4, x_3x_4, x_1x_2x_3$	11
Quadratic	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4, x_2x_3, x_2x_4, x_3x_4$	10
Model D	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4, x_2x_3, x_2x_4$	9
Model E	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4, x_2x_3$	8
Model F	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3, x_1x_4$	7
Model G	$x_1, x_2, x_3, x_4, x_1x_2, x_1x_3$	6
Model H	$x_1, x_2, x_3, x_4, x_1x_2$	5
Linear	x_1, x_2, x_3, x_4	4

There are 14 parameters in the special cubic model represented by the red line, while there are 10 parameters in the quadratic model represented in green, whereas there are 4 parameters in the linear model represented in yellow. The FDS plots of models A and B are quite similar to those for the special cubic model, while the FDS plot of model H is quite similar to the linear model. The yellow line (linear model) has a FDS curve that is below the green line (quadratic model), while the green line has a FDS curve that is underneath the red line (special cubic model). Models A, B and C, which have 13, 12 and 11 parameters in the model, respectively, have FDS curves that are at or below the special cubic model curve, which has 14 model parameters. Models D to H, which have 9 to 5 parameters in the model, respectively, have FDS curves that are below the quadratic model, which has 10 model parameters.

We see that the plots for the special cubic model, the quadratic model, and the linear model wrap around the plots for the other models, and the larger models have

FDS curves that are at or above curves for the nested models for all fractions of the design space. Models that have cubic terms have different slopes than the remaining curves. Thus, the addition of cubic terms provides a much larger effect on the stability of SPV values.

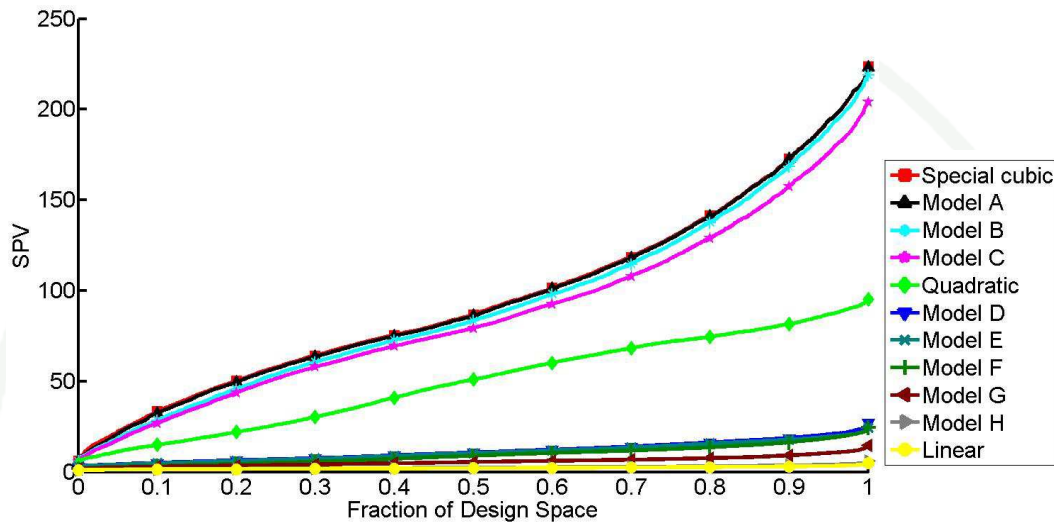


Figure 71 FDS plot for 15SC-S-D design for several models for the flare experiment.

When examining model robustness, if the experimenter has no prior information about which reduced models should be considered, we suggest looking at a few common classes of models on a single FDS plot. These classes include the special cubic model, the quadratic model and the linear model for the special cubic model. Figure 72 shows the comparison between the weighted D -optimal exact design under SH and WH for each design. The comparison between the weighted G -optimal exact design under SH and WH is shown in Figure 73. The comparison of the weighted D -optimal exact designs under SH and WH is shown in Figure 74. Figure 75 displays the comparison of the weighted G -optimal exact designs under SH and WH. Table 37 gives the G -efficiency for each design.

In the previous section, we see that (1) the weighted G -optimal exact designs are superior to the weighted D -optimal exact designs, (2) the weighted G -optimal exact designs under SH and WH have similar profiles and are quite comparable, (3) the weighted D -optimal exact designs under SH and WH have different profiles. However, most of the weighted D -optimal exact designs under SH perform better than those of under WH, and (4) as the design size increases, there is little change in the prediction variance properties for the weighted D - and G -optimal designs.

As shown in Table 37, for only the linear model, the G -efficiencies of the weighted D -optimal exact designs are higher than those of the weighted G -optimal designs, however, they are quite competitive. For the special cubic and quadratic model, the G -efficiencies of the weighted D -optimal exact designs are smaller than those of the weighted G -optimal designs. The G -efficiencies of the weighted D -optimal exact designs under SH and WH are quite comparable for the linear model, however, for the special cubic and quadratic models, the G -efficiencies of the weighted D -optimal exact designs under SH are higher than those under WH. The G -efficiencies of the weighted G -optimal exact designs under SH and WH are quite comparable for nested models within the special cubic model.

In Figures 72 and 74, the FDS curves for the special cubic for the weighted D -optimal exact designs under SH are significantly lower than those for the weighted D -optimal exact designs under WH for most of the design space except when $n=17$. However, the FDS curves for the quadratic model for the weighted D -optimal exact designs under SH are significantly lower than those for the weighted D -optimal exact designs under WH for most of the design space, while the FDS curves for the linear model for the weighted D -optimal exact designs under SH and WH are quite similar. The 16SC-S-D, 17SC-S-D, 18SC-S-D, 16SC-W-D, 18SC-W-D, 19SC-W-D and 20SC-W-D designs are not model robust because they have the worst FDS curves for the special cubic model and do not maintain stability for the three models. The remaining designs based on SH (15SC-S-D, 19SC-S-D, 20SC-S-D) appear to have better robustness properties than the remaining designs based on WH (15SC-W-D, 17SC-W-D). In these cases, the 20SC-S-D design appears to be a clear winner as the

most robust design because the FDS curves for the special cubic, quadratic and linear models of this design are closer than other designs.

In Figure 73 and 75, the FDS curves for the special cubic, quadratic, and linear models for the weighted G -optimal exact designs under SH and WH perform similarly. The weighted G -optimal designs under SH appears to be the slightly more robust designs than those under WH except when $n = 16$. The weighted G -optimal designs with $n \geq 17$ appear to be slightly more robust designs than the weighted G -optimal designs with $n \leq 16$. However, all twelve weighted G -optimal exact designs appear to be robust designs because they have the best G -efficiencies and lower and flatter FDS curves for the nested models within the special cubic model for the majority of the design space.

In this case, the weighted G -optimal exact designs based on SH and WH appears to be the more robust designs because (1) all three lines for the special cubic model, quadratic model and linear model are quite similar, (2) they have much flatter and lower FDS curves for all the models considered, indicating more desirable SPV distribution and (3) they have good G -efficiencies for the special cubic and the nested model within the special cubic model. Although the weighted D -optimal designs based on SH and WH perform well for the linear model, they perform poorly for the quadratic and special cubic models. Some weighted D -optimal designs (15SC-S-D, 19SC-S-D, 20SC-S-D, 15SC-W-D, 17SC-W-D) are mildly robust, however, they are no longer competitive in comparison to the weighted G -optimal designs with respect to their robustness properties. If the final model turns out to be either the special cubic or quadratic model, then the weighted G -optimal exact designs would have been the best choice.

Table 37 Maximum SPV values and approximate G -efficiencies for the weighted D - and G -optimal exact designs for three model types for the special cubic model for the flare experiment.

Design	Model type	G-efficiency (%)	Design	Model type	G-efficiency (%)
15SC-S-D	SC	6.26	15SC-S-G	SC	73.03
	Q	10.50		Q	59.99
	L	82.47		L	69.08
16SC-S-D	SC	0.06	16SC-S-G	SC	79.28
	Q	15.70		Q	68.17
	L	91.12		L	72.46
17SC-S-D	SC	0.11	17SC-S-G	SC	85.94
	Q	10.21		Q	71.28
	L	93.46		L	73.94
18SC-S-D	SC	0.22	18SC-S-G	SC	81.92
	Q	14.77		Q	73.05
	L	89.09		L	69.08
19SC-S-D	SC	10.20	19SC-S-G	SC	83.04
	Q	14.28		Q	71.79
	L	85.29		L	71.68
20SC-S-D	SC	13.09	20SC-S-G	SC	79.95
	Q	19.94		Q	67.11
	L	79.84		L	75.90
15SC-W-D	SC	0.81	15SC-W-G	SC	70.99
	Q	1.08		Q	61.69
	L	88.69		L	71.94
16SC-W-D	SC	0.03	16SC-W-G	SC	77.13
	Q	4.74		Q	62.62
	L	90.70		L	65.25
17SC-W-D	SC	2.52	17SC-W-G	SC	79.95
	Q	4.06		Q	72.15
	L	86.77		L	69.93
18SC-W-D	SC	0.11	18SC-W-G	SC	84.39
	Q	5.16		Q	69.16
	L	86.39		L	72.73
19SC-W-D	SC	0.36	19SC-W-G	SC	83.09
	Q	4.05		Q	73.69
	L	84.21		L	72.99
20SC-W-D	SC	0.02	20SC-W-G	SC	85.42
	Q	3.73		Q	70.72
	L	81.30		L	72.99

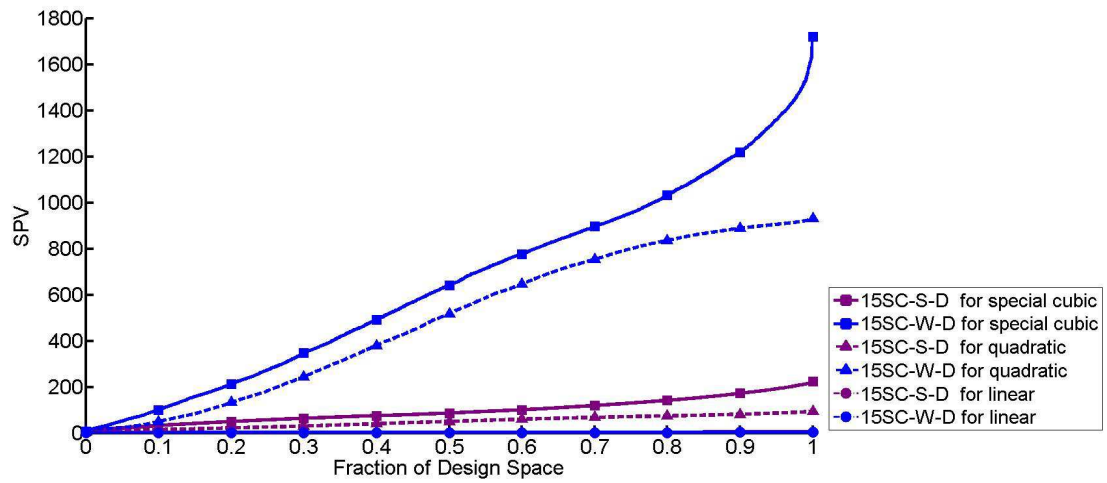
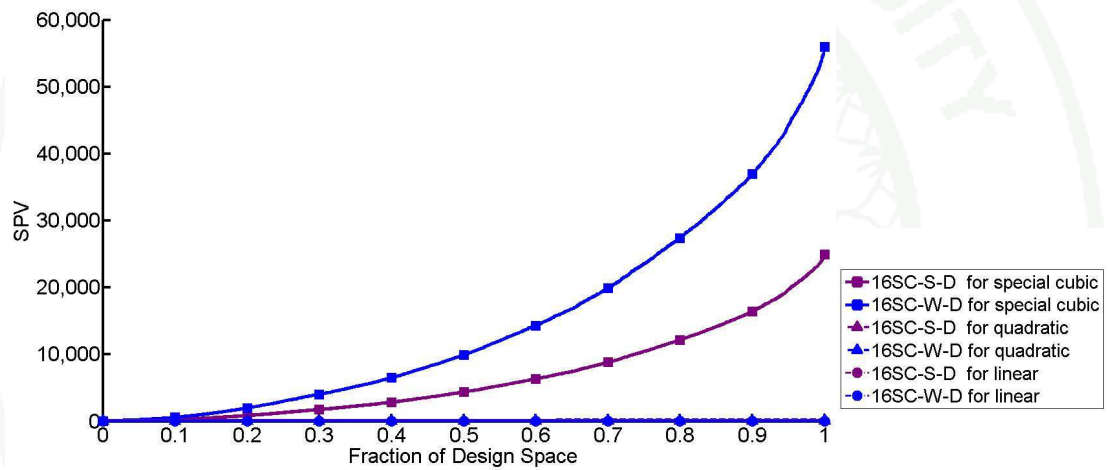
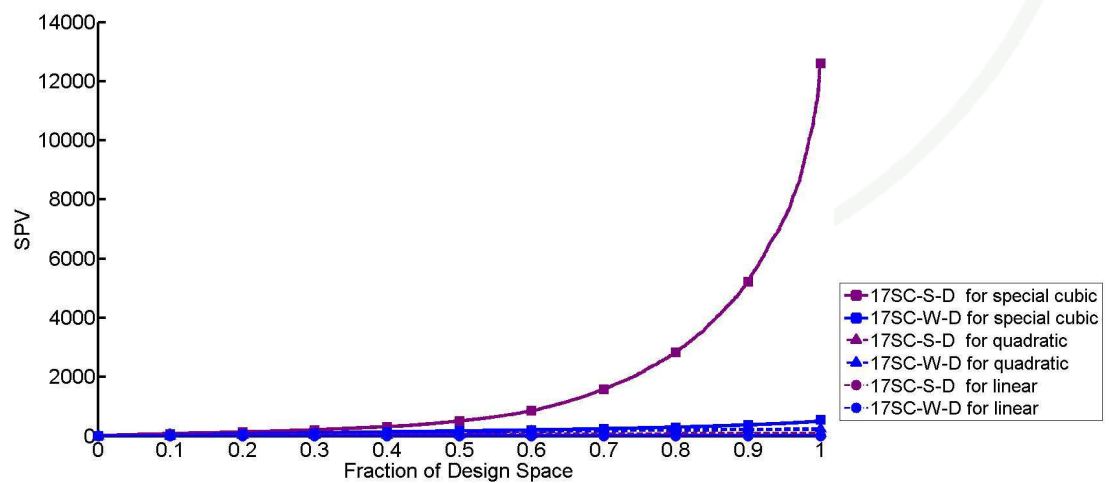
(a) $n = 15$ (b) $n = 16$ (c) $n = 17$

Figure 72 FDS plots for comparing the weighted D -optimal exact designs for three model types assuming the special cubic model for the flare experiment.

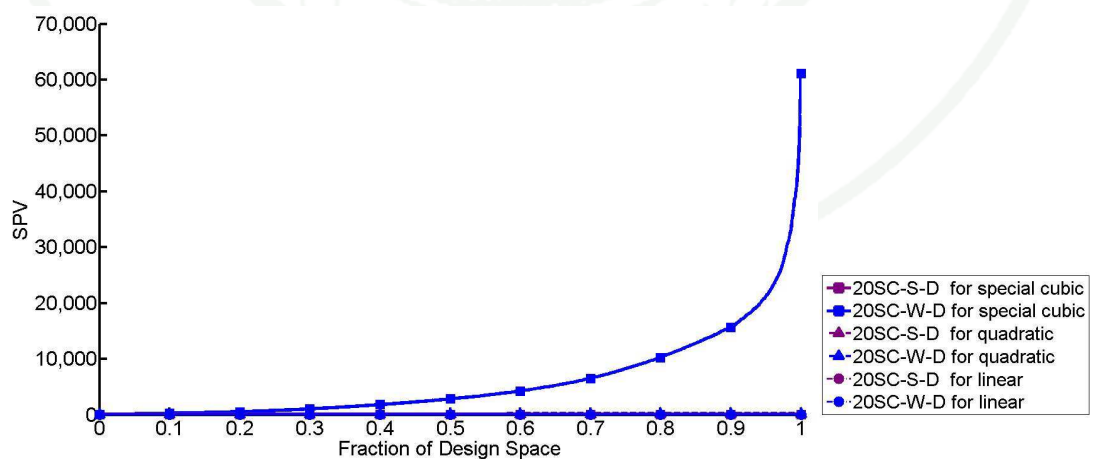
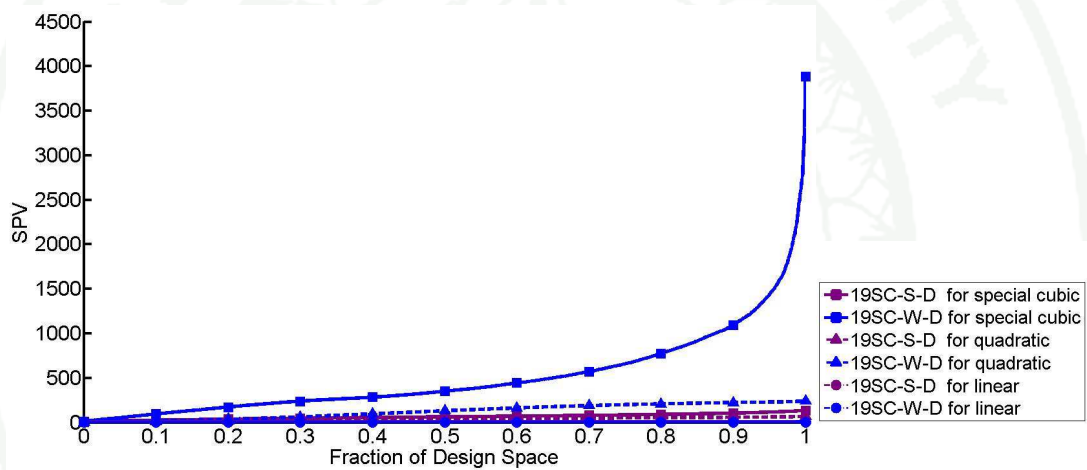
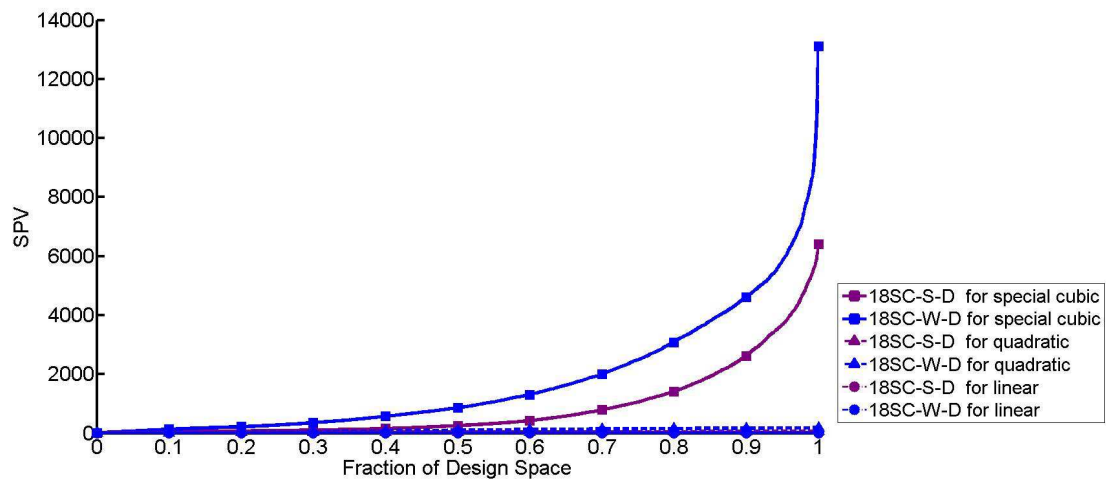


Figure 72 (Continued).

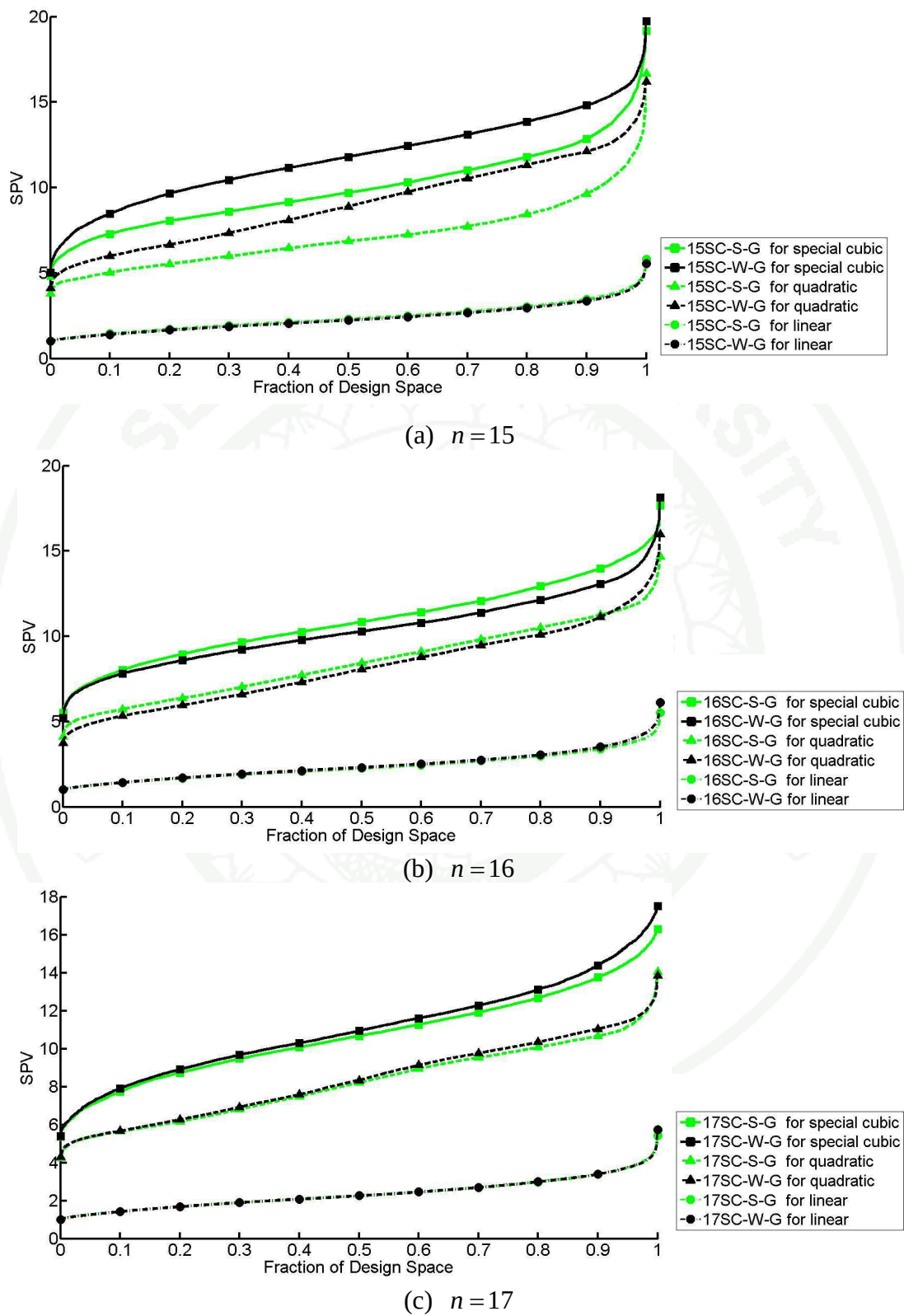
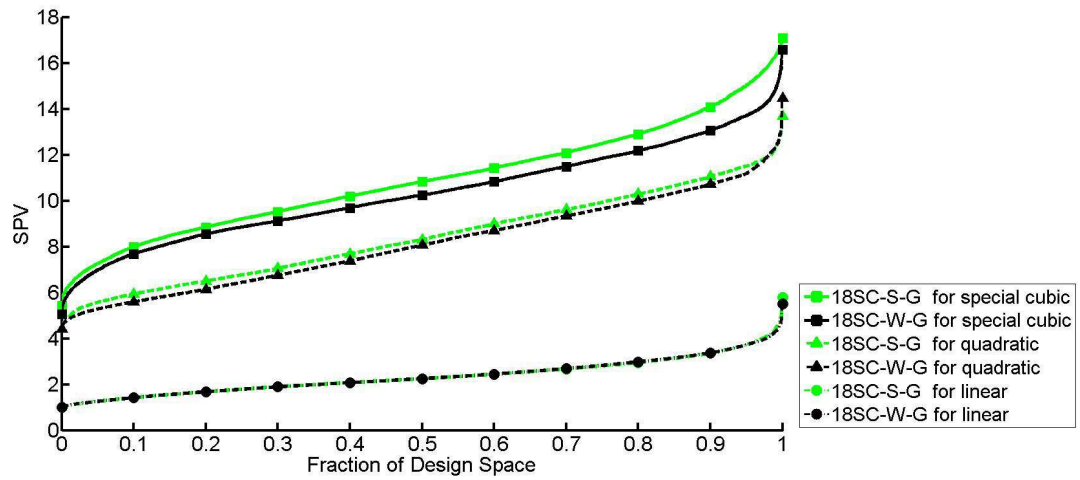
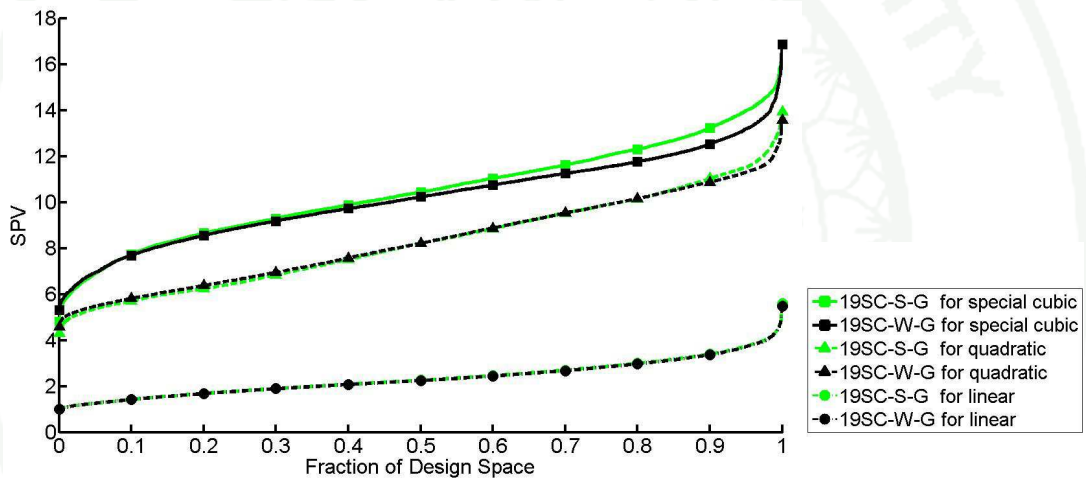
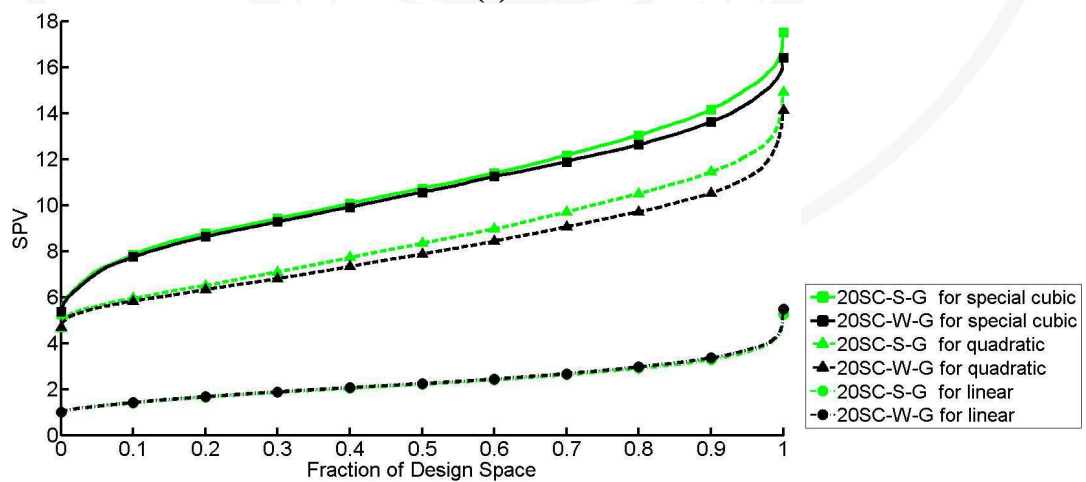


Figure 73 FDS plots for comparing the weighted G-optimal exact design for three model types assuming the special cubic model for the flare experiment.

(d) $n = 18$ (e) $n = 19$ (f) $n = 20$ **Figure 73** (Continued).

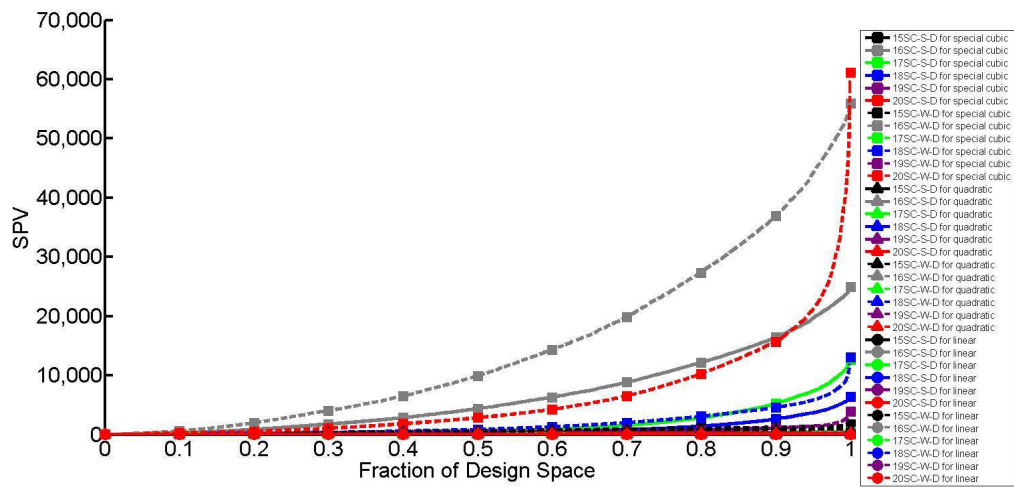
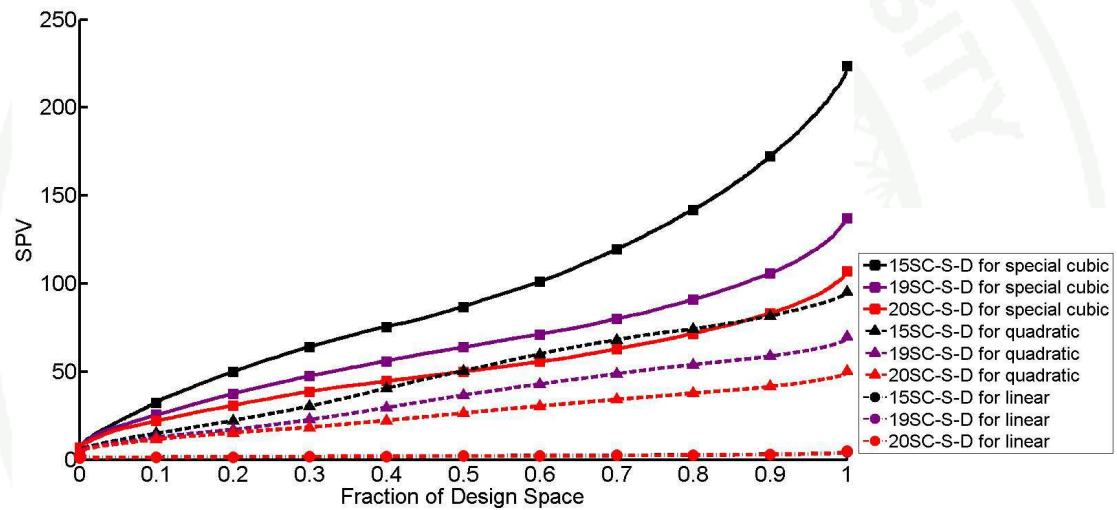
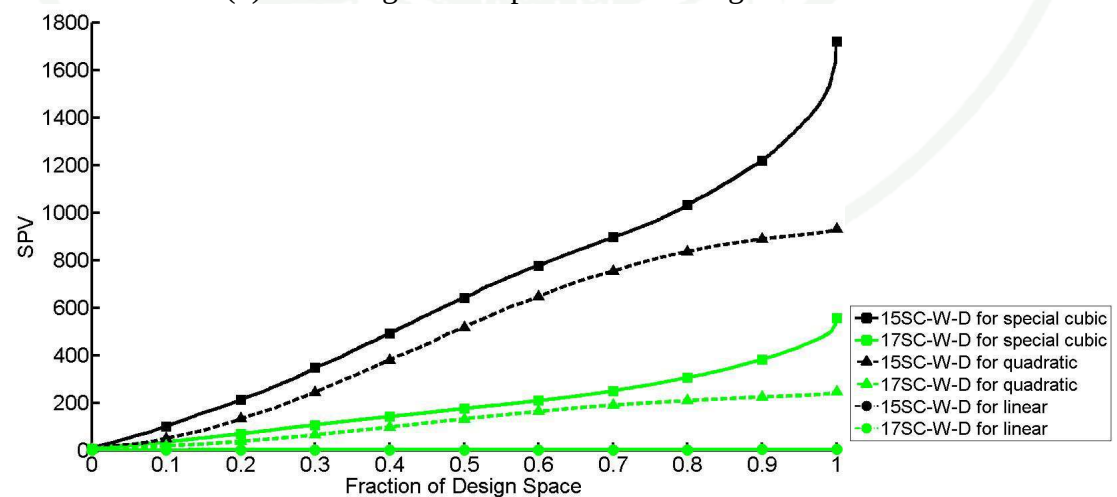
(a) The weighted D -optimal exact designs(b) The weighted D -optimal exact designs under SH(c) The weighted D -optimal exact designs under WH

Figure 74 FDS plots for comparing the D -optimal exact designs for three types of models assuming the special cubic model for the flare experiment.

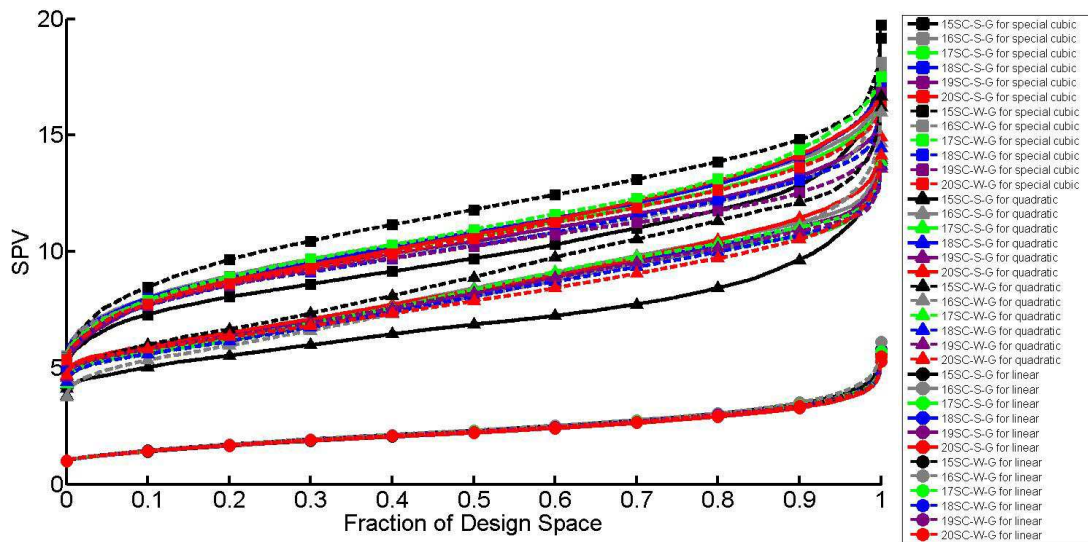
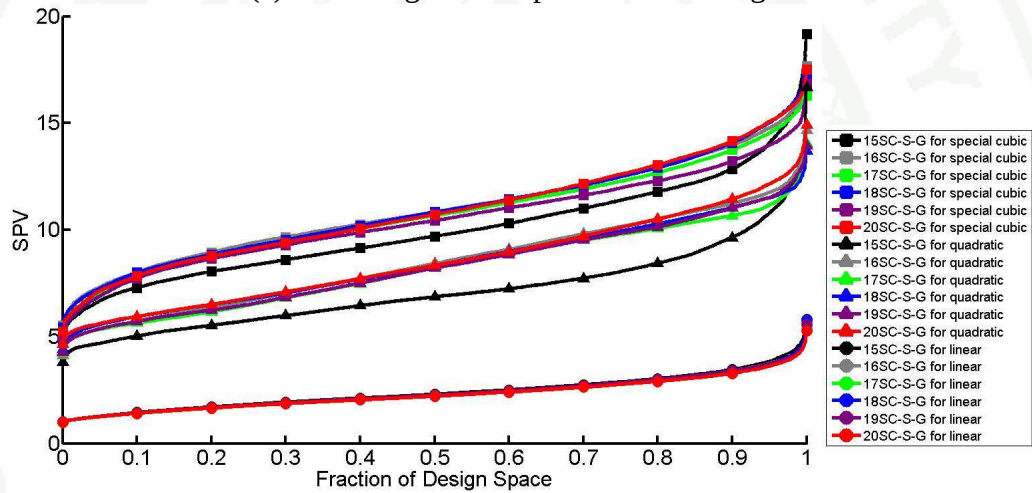
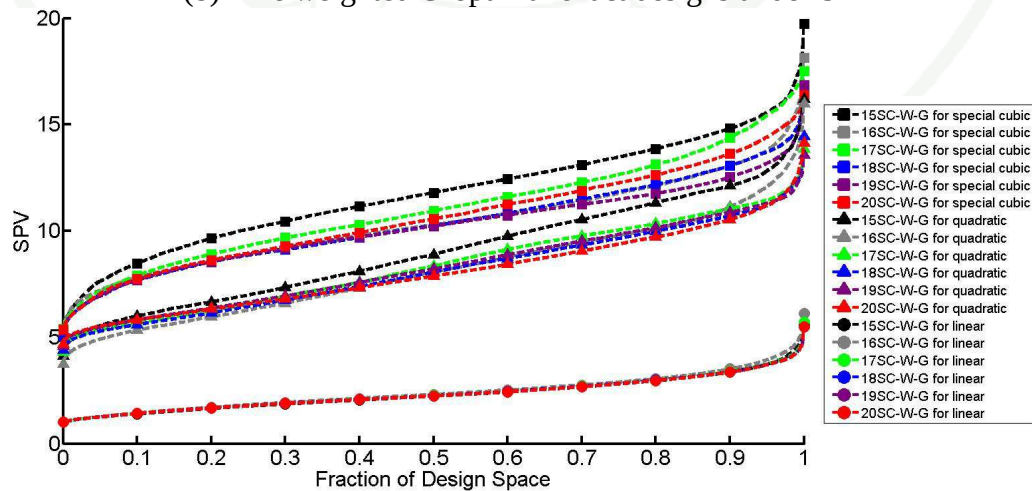
(a) The weighted G -optimal exact designs(b) The weighted G -optimal exact designs under SH(c) The weighted G -optimal exact designs under WH

Figure 75 FDS plots for comparing the G -optimal exact designs for three types of models assuming the special cubic model for the flare experiment.

Case 3: Single and Linear Multi Component Constraints with Three Components

The final case study is a three-component mixture experiment with both SCCs and MCCs (Snee, 1979) and is defined by the following constraints:

$$\begin{aligned}
 0.1 &\leq x_1 \leq 0.5 \\
 0.1 &\leq x_2 \leq 0.7 \\
 0.0 &\leq x_3 \leq 0.7 \\
 0.9 &\leq 0.85x_1 + 0.9x_2 + x_3 \leq 0.95 \\
 0.4 &\leq 0.7x_1 + x_3.
 \end{aligned} \tag{110}$$

The boundary defined by only the SCCs is indicated by the dashed line inside the simplex that has six vertices denoted alphabetically as A to F in Figure 76. After the two linear MCCs are imposed, the boundary of the experimental region is indicated by the dashed line which has six vertices denoted 1 to 6 in Figure 76. The six extreme vertices of the resulting region are listed in Table 38.

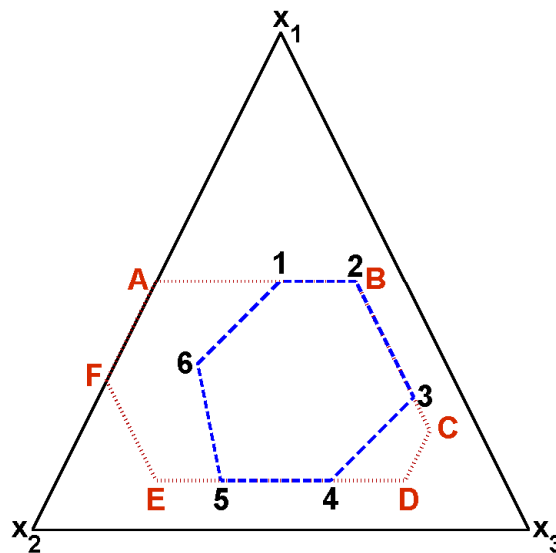


Figure 76 The three-component constrained region defined by the single component constraints $0.1 \leq x_1 \leq 0.5$, $0.1 \leq x_2 \leq 0.7$, $0.0 \leq x_3 \leq 0.7$, and multiple component constraints $0.9 \leq 0.85x_1 + 0.9x_2 + x_3 \leq 0.95$, $0.4 \leq 0.7x_1 + x_3$.

Table 38 Coordinate points for the mixture experiment of Snee (1979).

Only SCCs				SCCs and MCCs			
Vertex	x_1	x_2	x_3	Vertex	x_1	x_2	x_3
A	0.5000	0.5000	0.0000	1	0.5000	0.2500	0.2500
B	0.5000	0.1000	0.4000	2	0.5000	0.1000	0.4000
C	0.2000	0.1000	0.7000	3	0.2667	0.1000	0.6333
D	0.1000	0.2000	0.7000	4	0.1000	0.3500	0.5500
E	0.1000	0.7000	0.2000	5	0.1000	0.5700	0.3300
F	0.3000	0.7000	0.0000	6	0.3333	0.5000	0.1667

The two full models under consideration are the Scheffé quadratic and special cubic mixture models, which have six and seven unknown parameters, respectively:

$$E(y) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$

and

$$E(y) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3.$$

1. Appropriate genetic algorithm (GA) parameters for Case 3

The genetic algorithm parameters of Case 3 are investigated in this section. We would like to find appropriate values for α_i and σ as shown in Table 11. The genetic algorithm parameters are investigated by using the same eight sets of conditions as used in Case 1 and Case 2. The behavior of D_w for α_i and σ values when the model being fitted is the **Scheffé quadratic model** is presented in Figure 77. Like Cases 1 and 2, the result shows that set 8, $0.02 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.1$; $0.05 \leq \alpha_m \leq 0.2$; $0.1 \leq \sigma \leq 0.3$, is the best set of α_i and σ values because it generates the highest D_w values for the beginning GA iterations and after that it becomes very stable and is superior to other sets throughout the large number of iterations. Then, the appropriate population size is considered by changing M to 9. As seen in Figure 78, $M = 7$ chromosomes is appropriate based on the behavior of D_w and computing

time. The improvement of D_w for $M = 7$ at the beginning is slightly better than $M = 9$ and after that the D_w values for both cases are close together for set 8. The behavior of G_w with set 8 of α_i and σ values when the model being fitted is the quadratic model is presented in Figure 79. In Figures 78 and 79, we also see that there are only very slight improvements of D_w and G_w at the end of a large number of iterations. Therefore, when the model being fitted is the Scheffé quadratic model, we chose $M = 7$ as the size of the population, set 8 for the values of α_i and σ , and 5,000 as the number of iterations for the two objective functions as well. The values of α_i and σ are reset to smaller values after 250 iterations. The genetic algorithm parameters in this case are similar to those of Case 1 and 2 except for the number of iterations.

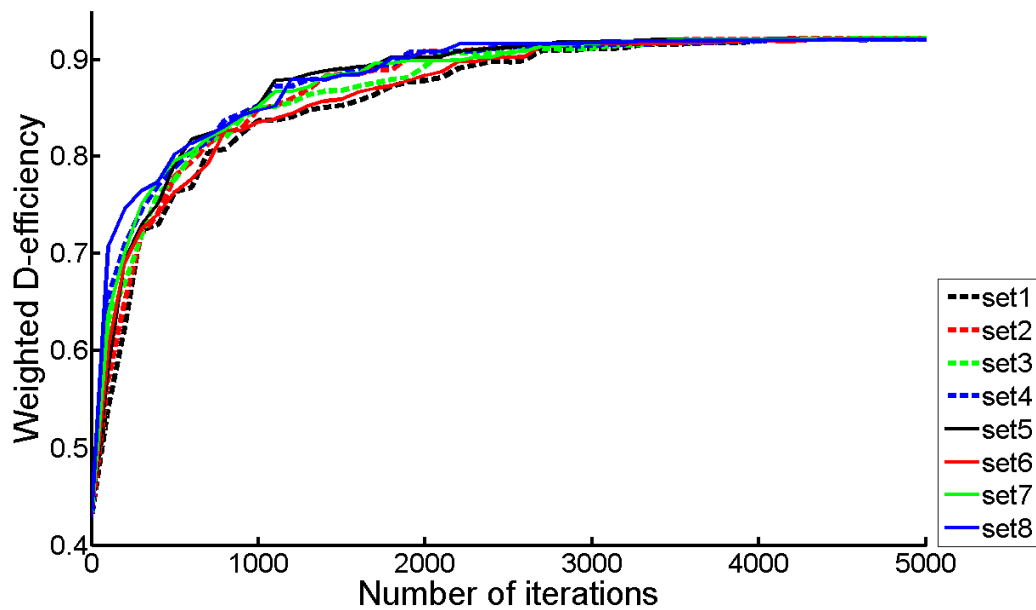


Figure 77 Progression of D_w values across eight sets of α_i and σ values assuming the Scheffé quadratic model for Snee's experiment.

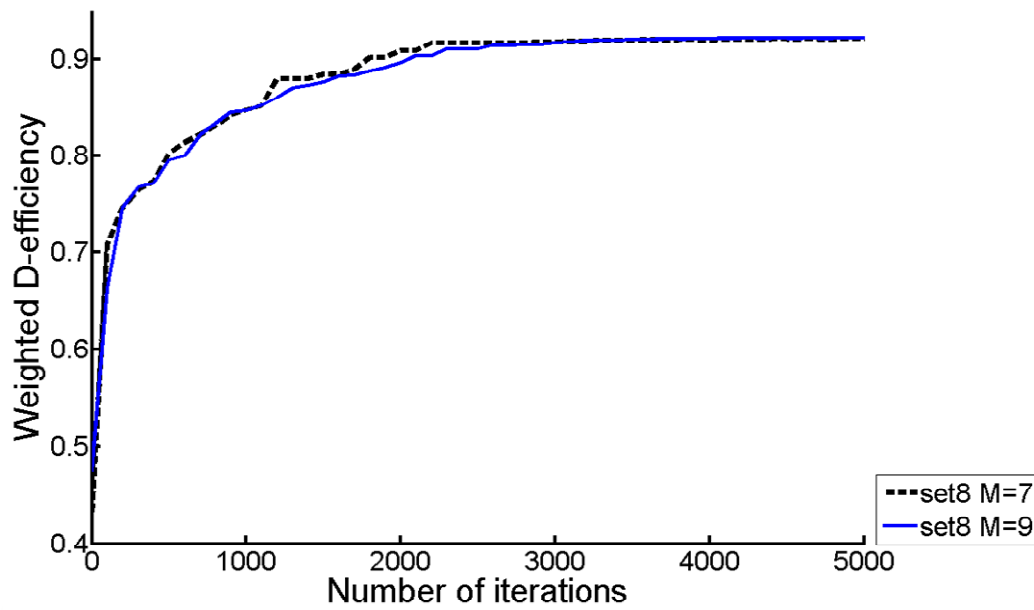


Figure 78 Behavior of D_w values of the best set of α_i and σ , with $M = 7$ and 9 , assuming the Scheffé quadratic model for Snee's experiment.



Figure 79 Progression of G_w values of the best set of α_i and σ with $M = 7$, assuming the Scheffé quadratic model for Snee's experiment.

Assuming a **Scheffé special cubic model**, $M = 7$ was determined to be the size of the population and set 8 for the values of α_i and σ for generating the mixture designs. Figures 80 and 81 show the behavior of D_w and G_w with the α_i and σ values from set 8, respectively, when the model being fitted is the special cubic model. We again notice that there are only very slight improvements of D_w and G_w values at the end of a large number of iterations. Therefore, assuming the special cubic model, the decision was to use $M = 7$ as the size of the population, set 8 for the values of α_i and σ , 5,000 as the number of iterations for two objective functions. The values of α_i and σ are reduced to smaller values after 250 iterations. Notice that the genetic parameters for the case of the special cubic model are identical with the case of the quadratic model.

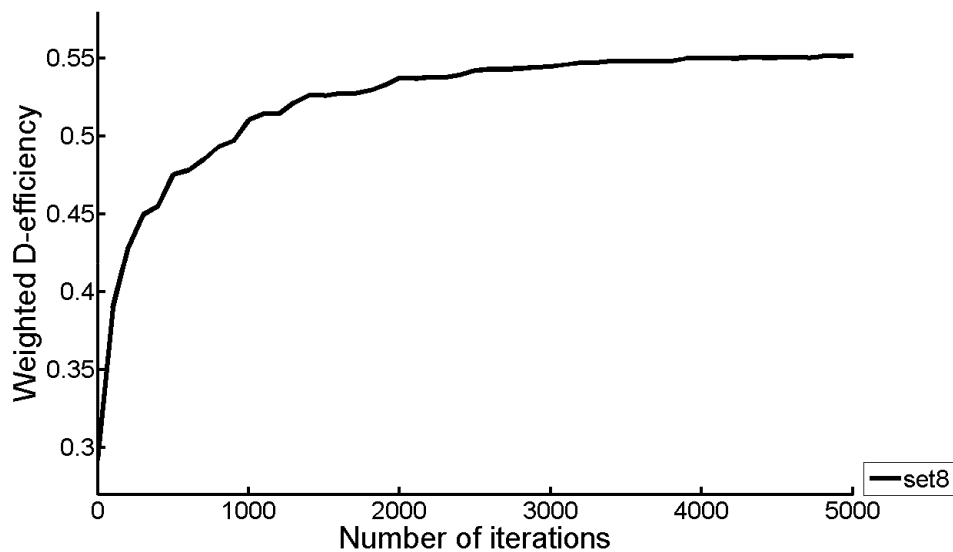


Figure 80 Behavior of D_w values with the best set of α_i and σ values and $M = 7$ assuming the full Scheffé special cubic model for Snee's experiment.

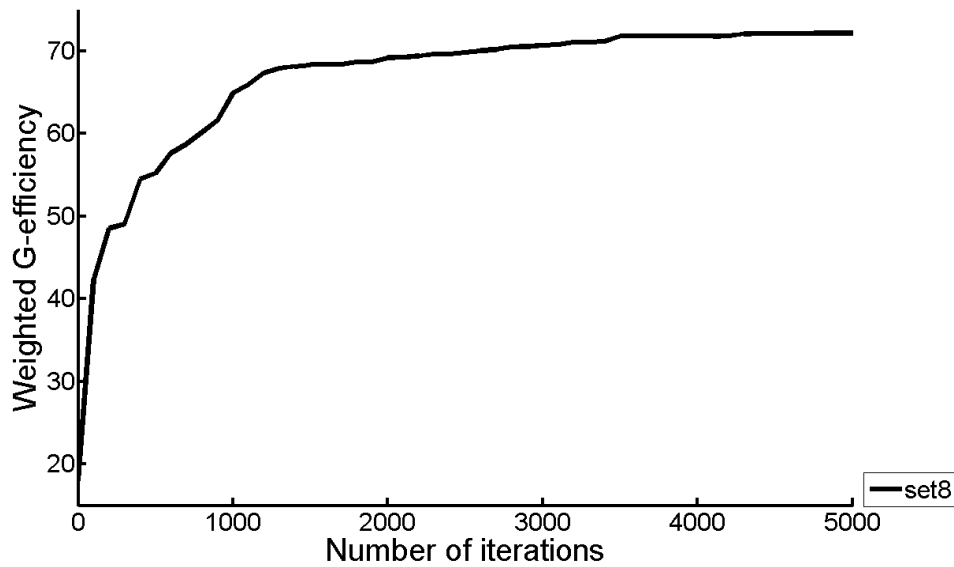


Figure 81 Progression of G_w values with the best set of α_i and σ , with $M = 7$ assuming the full Scheffé special cubic model for Snee's experiment.

2. Generating optimal exact design for Case 3

To generate model robust designs that fit all possible reduced models as efficiently as possible under D - and G -criteria for Case 3 are presented in this section. The most fit designs created using the GA and the optimal exact designs resulting from the local grid search for Case 3 are given in Appendix C. We first consider the mixture design created using the GA when the fitted model is **the Scheffé quadratic model**. There are 8 reduced models under SH and WH as shown in Table 4. We focus on two cases that vary in terms of weighted design optimal criteria as follows:

- For D_w , the GA generated designs and the optimal exact design having 7 to 12 points assuming the quadratic model are shown in Appendix Table C1 to C6.
- For G_w , the GA generated designs and the optimal exact design having 7 to 12 points assuming the quadratic model are given in Appendix Table C7 to C12.

In addition to the Scheffé quadratic model, we consider **the Scheffé special cubic model** as the fitting model. Assuming the Scheffé special cubic model, there are 9 SH models and 15 WH models as shown in Tables 6 and 7, respectively. The following our cases are examined that vary in terms of weighted design optimal criteria and heredity concept:

- For D_w with SH, the GA generated designs and the optimal exact design having 8 to 13 points are given in Appendix Tables C13 to C18.
- For D_w with WH, the GA generated designs and the optimal exact design having 8 to 13 points are given in Appendix Tables C19 to C24.
- For G_w with SH, the GA generated designs and the optimal exact design having 8 to 13 points are given in Appendix Tables C25 to C30.
- For G_w with WH, the GA generated designs and the optimal exact design having 8 to 13 points are given in Appendix Tables C31 to C36.

When the fitted model is the quadratic model, the following twelve optimal exact designs were generated:

(1) 7-point design with D_w (7MQ-D)	(7) 7-point design with G_w (7MQ-G)
(2) 9-point design with D_w (8MQ-D)	(8) 8-point design with G_w (8MQ-G)
(3) 10-point design with D_w (9MQ-D)	(9) 9-point design with G_w (9MQ-G)
(4) 11-point design with D_w (10MQ-D)	(10) 10-point design with G_w (10MQ-G)
(5) 12-point design with D_w (11MQ-D)	(11) 11-point design with G_w (11MQ-G)
(6) 13-point design with D_w (12MQ-D)	(12) 12-point design with G_w (12MQ-G)

When the fitted model is the special cubic model, 24 optimal exact designs were generated. There are six designs for D_w with SH, six designs for D_w with WH, six designs for G_w with SH and six designs for G_w with WH. The design sizes range from 8 to 13 for each group of six designs. The 24 designs with their abbreviated notation in parentheses are given below.

(1) 8-points/ SH / D_w	(8SC-S-D)	(13) 8-points/ SH / G_w	(8SC-W-G)
(2) 9-points/ SH / D_w	(9SC-S-D)	(14) 9-points/ SH / G_w	(9SC-W-G)
(3) 10-points/ SH / D_w	(10SC-S-D)	(15) 10-points/ SH / G_w	(10SC-W-G)
(4) 11-points/ SH / D_w	(11SC-S-D)	(16) 11-points/ SH / G_w	(11SC-W-G)
(5) 12-points/ SH / D_w	(12SC-S-D)	(17) 12-points/ SH / G_w	(12SC-W-G)
(6) 13-points/ SH / D_w	(13SC-S-D)	(18) 13-points/ SH / G_w	(13SC-W-G)
(7) 8-points/ WH / D_w	(8SC-W-D)	(19) 8-points/ WH / G_w	(8SC-W-G)
(8) 9-points/ WH / D_w	(9SC-W-D)	(20) 9-points/ WH / G_w	(9SC-W-G)
(9) 10-points/ WH / D_w	(10SC-W-D)	(21) 10-points/ WH / G_w	(10SC-W-G)
(10) 11-points/ WH / D_w	(11SC-W-D)	(22) 11-points/ WH / G_w	(11SC-W-G)
(11) 12-points/ WH / D_w	(12SC-W-D)	(23) 12-points/ WH / G_w	(12SC-W-G)
(12) 13-points/ WH / D_w	(13SC-W-D)	(24) 13-points/ WH / G_w	(13SC-W-G)

Tables 39 and 40 highlight the percentage increase in the value of the objective function when the fitted models are the quadratic and the special cubic models, respectively. Because some D_w values increase in the sixth and eighth decimal places, seven and nine decimal place accuracies were presented for a proper comparison of the percentage increases in D_w values for the quadratic and special cubic models, respectively. In contrast, only four decimal place accuracy is required to compare G_w values. It is clear that the percentage changes in D_w values are less than those of G_w values. As seen in Table 39, the maximum improvement for D_w and G_w values occurs for the 9-point design, while the minimum improvement for D_w and G_w values occurs for the 8-point design. As seen in Table 40, for D_w under SH and WH, the smallest percentage increase occurs for the 9-point design, while the 13-point design has the largest percentage increase. For G_w with SH, the smallest percentage increase occurs for the 10-point design, while the 13-point design has the largest percentage increase. For G_w with WH, the 11-point design has the largest percentage increase, while the smallest percentage increase occurs for the 8-point design.

Table 39 Percentage increase in the objective function when the quadratic model is the model being fitted in Snee's experiment.

Objective function	Run	Most fit designs via GA	Optimal exact design	Percentage increase (%)
D_w	7	0.8981948	0.8981999	0.00056
	8	0.8901976	0.8901980	0.00004
	9	0.8920954	0.8937718	0.18791
	10	0.9004166	0.9004436	0.00299
	11	0.9089636	0.9089689	0.00058
	12	0.9206811	0.9211973	0.05607
G_w	7	78.5896	82.6408	5.1548
	8	75.4964	76.5576	1.4057
	9	69.5982	75.9125	9.0726
	10	68.4367	72.6225	6.1163
	11	72.7577	74.6707	2.6293
	12	69.6073	73.9863	6.2911

Table 40 Percentage increase in the objective function when the special cubic model is the model being fitted in Snee's experiment.

Objective function	Heredity	Run	Most fit designs via GA	Optimal exact design	Percentage increase (%)
D_w	SH	8	0.602107345	0.602150602	0.00718
		9	0.603461386	0.603461588	0.00003
		10	0.607148091	0.607168093	0.00329
		11	0.612070104	0.612132487	0.01019
		12	0.620571647	0.620700608	0.02078
		13	0.619980945	0.620704388	0.11669
	WH	8	0.537881608	0.537882549	0.00018
		9	0.538742013	0.538742034	0.00001
		10	0.541496617	0.541671312	0.03226
		11	0.546358497	0.546625985	0.04896
		12	0.552722283	0.552750315	0.00507
		13	0.551603242	0.551986477	0.06948
G_w	SH	8	79.3815	81.0604	2.1150
		9	76.2080	77.8030	2.0930
		10	75.0934	76.2648	1.5598
		11	73.7378	76.9449	4.3493
		12	73.5677	75.0697	2.0415
		13	72.0109	75.6236	5.0168
	WH	8	79.4627	80.2259	0.9604
		9	73.8722	75.9254	2.7795
		10	75.2897	76.6085	1.7517
		11	72.1812	75.6349	4.7848
		12	71.6280	73.0826	2.0308
		13	72.1486	75.3223	4.3988

The points for the optimal exact design assuming the quadratic and special cubic models are given in Table 41. The set of points appearing in any of the 36 designs is given in Table 42. In Figure 76, the boundary formed by the SCCs and MCCs is indicated by the dashed line inside the simplex that has six vertices (labeled 1 to 6) and six edge centroids. The differences in the distributional patterns of points of the optimal exact designs assuming the quadratic model based on D_w and G_w are shown in Figure 82. The distributional patterns of points of the optimal exact designs for the special cubic model based on D_w and G_w are presented in Figure 83 and 84, respectively.

For the quadratic model with D_w , there are obvious distributional patterns of points. The points lie on all vertices with varying replication and contain near overall centroids. The larger designs contain the points of the smaller designs plus replicated vertices. For the quadratic model with G_w , seven points lie on either vertices or near vertices and a near overall centroid. The remaining points lie on either a near edge centroid or face of the polyhedron. There are no replicated points for these designs. For $n \geq 8$ with G_w , there are points in the interior of the polyhedron.

For the special cubic model with D_w , the distributional patterns of points under SH and WH are quite similar. The twelve designs contain all six vertices with varying replication and a near overall centroid. The larger designs contain the points from the smaller designs plus replicated vertices. Assuming the special cubic model with the G_w under SH and WH, the distributional patterns of points under SH and WH are quite similar. The points of the twelve designs lie on either vertices or near vertices plus a near overall centroid. The remaining points lie on near edge centroids and/or on faces of the polyhedron.

Table 41 Summary of points and replications that appearing in each of the 36 designs for Snee's mixture experiment.

Design	V ₁	V ₂	V ₃	V ₄	V ₅	V ₆	Other points
7MQ-D	1	1	1	1	1	1	G ₁
7MQ-G		1	1	1	1		G ₂ to G ₄
8MQ-D	1	1	2	1	1	1	G ₅
8MQ-G	1		1	1		1	G ₆ to G ₉
9MQ-D	1	1	2	1	2	1	G ₁₀
9MQ-G	1	1	1	1	1		G ₁₁ to G ₁₄
10MQ-D	1	1	2	1	2	2	G ₁₅
10MQ-G	1			1		1	G ₁₆ to G ₂₂
11MQ-D	1	1	2	2	2	2	G ₂₃
11MQ-G	1	1	1	1	1	1	G ₂₄ to G ₂₈
12MQ-D	2	1	2	2	2	2	G ₂₉
12MQ-G	1	1	1	1	1		G ₃₀ to G ₃₆
8MC-S-D	1	1	2	1	1	1	G ₃₇
8MC-W-D	1	1	2	1	1	1	G ₃₈
8MC-S-G	1		1	1	1		G ₃₉ to G ₄₂
8MC-W-G		1			1	1	G ₄₃ to G ₄₇
9MC-S-D	1	1	2	1	2	1	G ₄₈
9MC-W-D	1	1	2	1	2	1	G ₄₉
9MC-S-G				1		1	G ₅₀ to G ₅₆
9MC-W-G	1		1		1		G ₅₇ to G ₆₁
10MC-S-D	1	1	2	1	2	2	G ₆₂
10MC-W-D	1	1	2	1	2	2	G ₆₃
10MC-S-G	1	1		1	1		G ₆₄ to G ₆₉
10MC-W-G	1	1	1		1		G ₇₀ to G ₇₅
11MC-S-D	2	1	2	1	2	2	G ₇₆
11MC-W-D	2	1	2	1	2	2	G ₇₇
11MC-S-G	1	1	1		1	1	G ₇₈ to G ₈₃
11MC-W-G	1	1	1			1	G ₈₄ to G ₉₀
12MC-S-D	2	1	2	2	2	2	G ₉₁
12MC-W-D	2	1	2	2	2	2	G ₉₂
12MC-S-G		1	1	1			G ₉₃ to G ₁₀₁
12MC-W-G	1		1	1	1		G ₁₀₂ to G ₁₀₉
13MC-S-D	2	2	2	2	2	2	G ₁₁₀
13MC-W-D	2	2	2	2	2	2	G ₁₁₁
13MC-S-G	1	1	1	1	1	1	G ₁₁₂ to G ₁₁₈
13MC-W-G		1	1	1	1	1	G ₁₁₉ to G ₁₂₆

Table 42 List of points appearing in the 36 designs for Snee's mixture experiment.

Label	x_1	x_2	x_3	Label	x_1	x_2	x_3
Vertices				Other points			
V ₁	0.5000	0.1000	0.4000	G ₂₆	0.3444	0.1000	0.5556
V ₂	0.5000	0.2500	0.2500	G ₂₇	0.1384	0.5154	0.3462
V ₃	0.2667	0.1	0.6333	G ₂₈	0.3292	0.4457	0.2251
V ₄	0.1000	0.3500	0.5500	G ₂₉	0.2943	0.3099	0.3958
V ₅	0.1000	0.57	0.3300	G ₃₀	0.3142	0.5058	0.1800
V ₆	0.3333	0.5000	0.1667	G ₃₁	0.2968	0.3114	0.3918
Edge centroid				G ₃₂	0.2229	0.1657	0.6114
E ₁	0.1000	0.4600	0.4400	G ₃₃	0.3858	0.4153	0.1989
E ₂	0.5000	0.1750	0.3250	G ₃₄	0.4023	0.1272	0.4705
E ₃	0.3833	0.1000	0.5167	G ₃₅	0.1575	0.3517	0.4908
E ₄	0.4167	0.375	0.2083	G ₃₆	0.156	0.5415	0.3025
E ₅	0.1833	0.225	0.5917	G ₃₇	0.2885	0.3221	0.3894
E ₆	0.2167	0.535	0.2483	G ₃₈	0.2900	0.3215	0.3885
Overall centroid				G ₃₉	0.4058	0.1000	0.4942
C	0.3	0.3117	0.3883	G ₄₀	0.2883	0.3054	0.4063
Other Points				G ₄₁	0.3315	0.5000	0.1685
G ₁	0.2878	0.3109	0.4013	G ₄₂	0.4884	0.2673	0.2443
G ₂	0.4747	0.1000	0.4253	G ₄₃	0.2775	0.1000	0.6225
G ₃	0.322	0.5033	0.1747	G ₄₄	0.1000	0.3687	0.5313
G ₄	0.2885	0.317	0.3945	G ₄₅	0.4743	0.1000	0.4257
G ₅	0.2868	0.3257	0.3875	G ₄₆	0.1913	0.2264	0.5823
G ₆	0.1279	0.4458	0.4263	G ₄₇	0.2910	0.3235	0.3855
G ₇	0.3121	0.2657	0.4222	G ₄₈	0.2964	0.3115	0.3921
G ₈	0.1000	0.5678	0.3322	G ₄₉	0.2964	0.3136	0.3900
G ₉	0.5000	0.2463	0.2537	G ₅₀	0.5000	0.1115	0.3885
G ₁₀	0.2975	0.3118	0.3907	G ₅₁	0.2548	0.1178	0.6274
G ₁₁	0.2918	0.3218	0.3864	G ₅₂	0.4826	0.2761	0.2413
G ₁₂	0.231	0.5307	0.2383	G ₅₃	0.2973	0.3165	0.3862
G ₁₃	0.3143	0.5057	0.1800	G ₅₄	0.1060	0.5682	0.3258
G ₁₄	0.2369	0.1991	0.5640	G ₅₅	0.3666	0.1000	0.5334
G ₁₅	0.2963	0.3000	0.4037	G ₅₆	0.1240	0.4563	0.4197
G ₁₆	0.4908	0.2638	0.2454	G ₅₇	0.3570	0.1000	0.5430
G ₁₇	0.2424	0.1364	0.6212	G ₅₈	0.4913	0.2630	0.2457
G ₁₈	0.375	0.1554	0.4696	G ₅₉	0.3521	0.4718	0.1761
G ₁₉	0.1000	0.5488	0.3512	G ₆₀	0.2885	0.3047	0.4068
G ₂₀	0.2716	0.3243	0.4041	G ₆₁	0.2500	0.5160	0.2340
G ₂₁	0.1777	0.5466	0.2757	G ₆₂	0.2953	0.3027	0.4020
G ₂₂	0.2358	0.1464	0.6178	G ₆₃	0.2949	0.3077	0.3974
G ₂₃	0.3088	0.2926	0.3986	G ₆₄	0.2860	0.5142	0.1998
G ₂₄	0.3032	0.3041	0.3927	G ₆₅	0.1450	0.4468	0.4082
G ₂₅	0.174	0.2827	0.5433	G ₆₆	0.3083	0.2890	0.4027

Table 42 (Continued)

Label	x_1	x_2	x_3	Label	x_1	x_2	x_3
Other points				Other points			
G ₆₇	0.2466	0.1300	0.6234	G ₉₇	0.1918	0.3222	0.4860
G ₆₈	0.3704	0.4444	0.1852	G ₉₈	0.3240	0.2798	0.3962
G ₆₉	0.3262	0.1000	0.5738	G ₉₉	0.2129	0.1807	0.6064
G ₇₀	0.1000	0.3765	0.5235	G ₁₀₀	0.3426	0.4861	0.1713
G ₇₁	0.3378	0.4933	0.1689	G ₁₀₁	0.1000	0.5118	0.3882
G ₇₂	0.2485	0.5254	0.2261	G ₁₀₂	0.1644	0.4091	0.4265
G ₇₃	0.3470	0.1000	0.5530	G ₁₀₃	0.3190	0.5043	0.1767
G ₇₄	0.1710	0.2765	0.5525	G ₁₀₄	0.1990	0.5400	0.2610
G ₇₅	0.3099	0.2983	0.3918	G ₁₀₅	0.3972	0.4042	0.1986
G ₇₆	0.2852	0.3125	0.4023	G ₁₀₆	0.3600	0.1000	0.5400
G ₇₇	0.2897	0.3124	0.3979	G ₁₀₇	0.3250	0.2878	0.3872
G ₇₈	0.3546	0.4115	0.2339	G ₁₀₈	0.5000	0.2510	0.2490
G ₇₉	0.3524	0.1000	0.5476	G ₁₀₉	0.1754	0.2369	0.5877
G ₈₀	0.1000	0.4060	0.4940	G ₁₁₀	0.2905	0.3110	0.3985
G ₈₁	0.3050	0.2950	0.4000	G ₁₁₁	0.2910	0.3120	0.3970
G ₈₂	0.1724	0.5176	0.3100	G ₁₁₂	0.3678	0.1000	0.5322
G ₈₃	0.1400	0.2900	0.5700	G ₁₁₃	0.4294	0.2357	0.3349
G ₈₄	0.1000	0.5575	0.3425	G ₁₁₄	0.2885	0.3135	0.3980
G ₈₅	0.2978	0.3058	0.3964	G ₁₁₅	0.4079	0.3881	0.2040
G ₈₆	0.1571	0.2645	0.5784	G ₁₁₆	0.1165	0.4625	0.4210
G ₈₇	0.1836	0.5369	0.2795	G ₁₁₇	0.1866	0.2200	0.5934
G ₈₈	0.3877	0.3858	0.2265	G ₁₁₈	0.2085	0.5367	0.2548
G ₈₉	0.1000	0.3655	0.5345	G ₁₁₉	0.4000	0.4000	0.2000
G ₉₀	0.3529	0.1010	0.5461	G ₁₂₀	0.4347	0.2392	0.3261
G ₉₁	0.2941	0.3100	0.3959	G ₁₂₁	0.1984	0.2024	0.5992
G ₉₂	0.2960	0.3115	0.3925	G ₁₂₂	0.2036	0.5301	0.2663
G ₉₃	0.4243	0.1000	0.4757	G ₁₂₃	0.1000	0.4765	0.4235
G ₉₄	0.2750	0.5175	0.2075	G ₁₂₄	0.3827	0.1000	0.5173
G ₉₅	0.1116	0.5665	0.3219	G ₁₂₅	0.5000	0.1038	0.3962
G ₉₆	0.5000	0.1362	0.3638	G ₁₂₆	0.2835	0.3143	0.4022

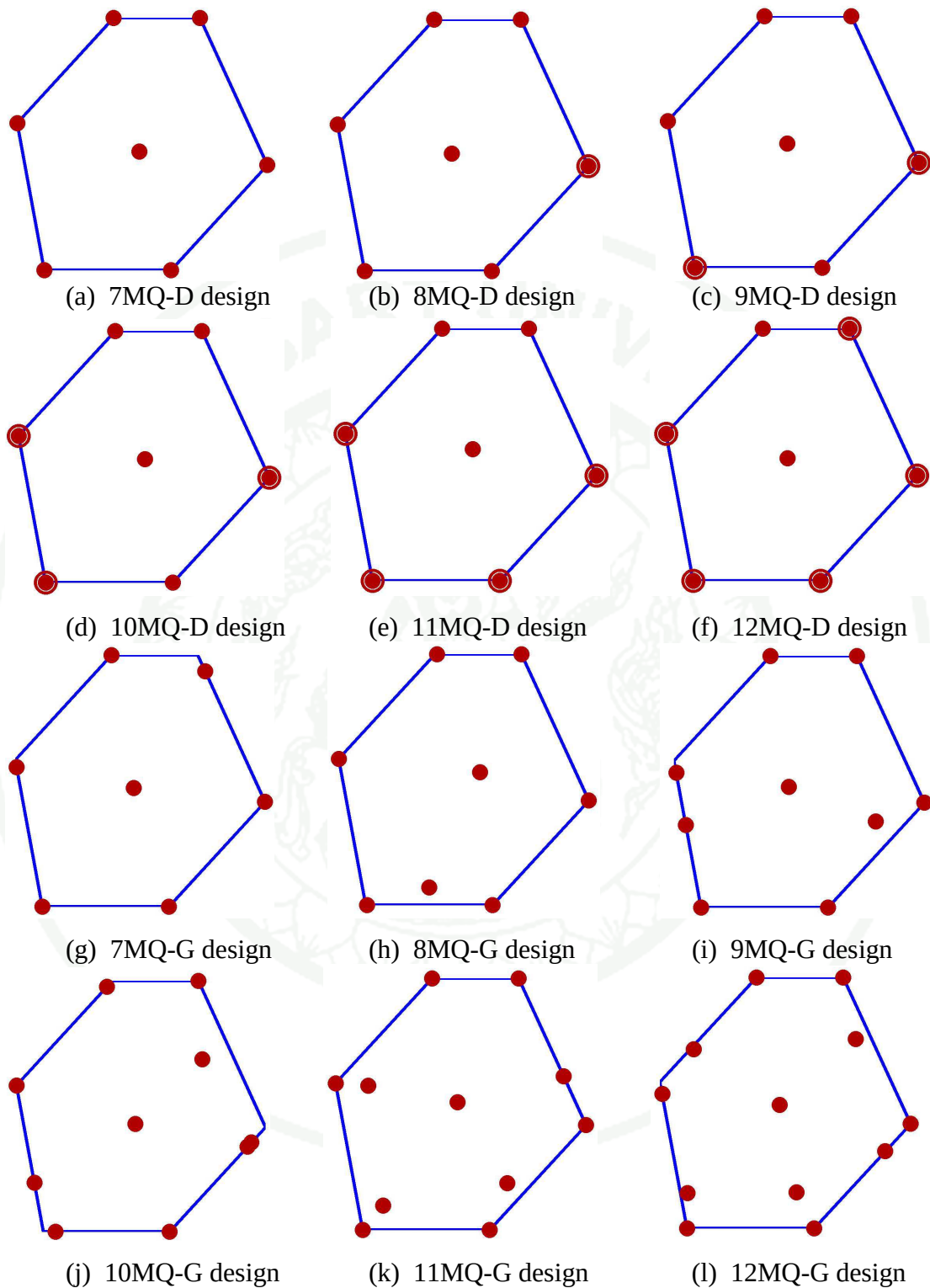


Figure 82 The optimal exact designs based on D_w and G_w assuming the Scheffé quadratic model for Snee's experiment. $\bullet$ and $\odot$ represent 1 and 2 replicates of that design point, respectively.

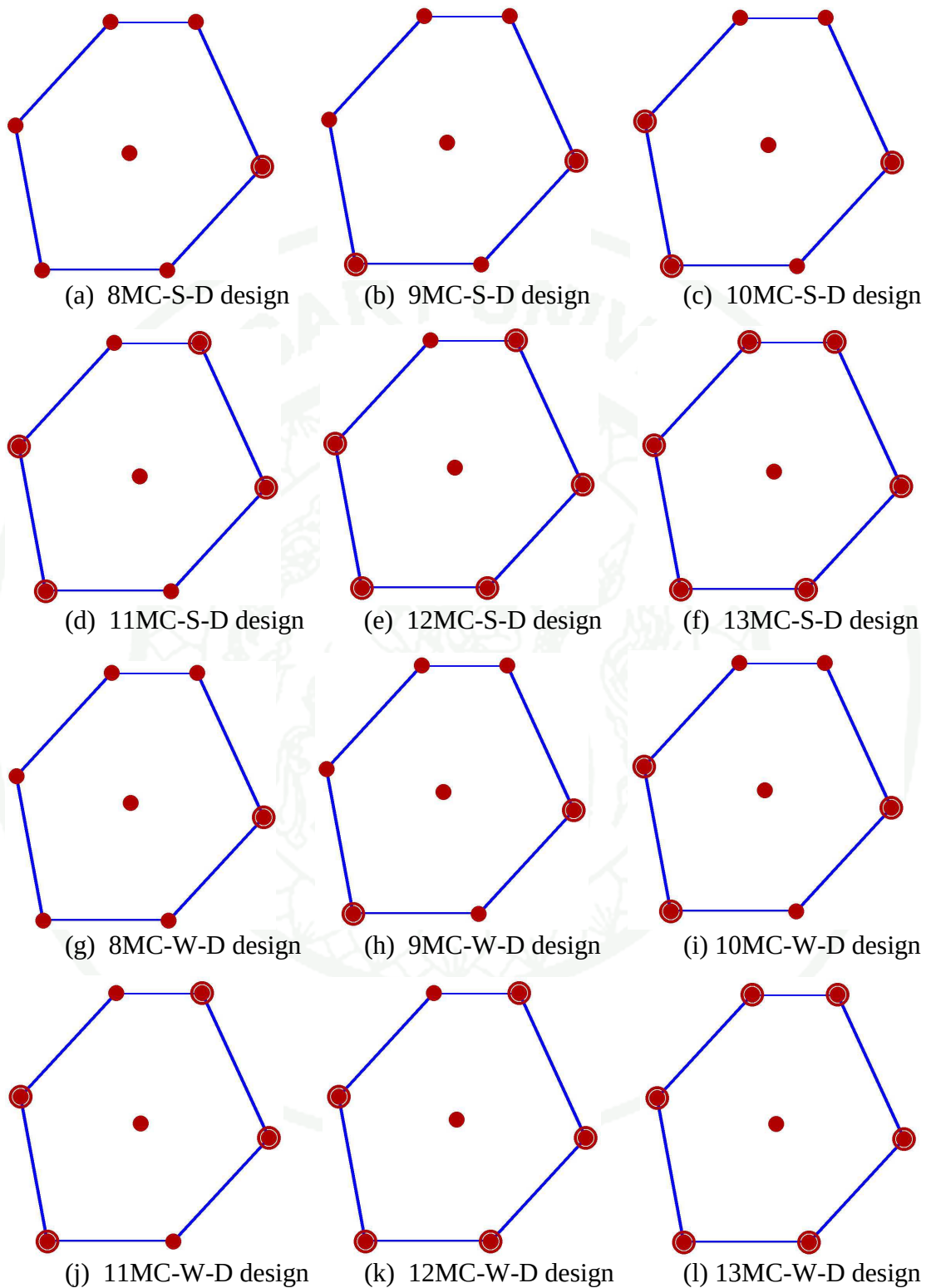


Figure 83 The optimal exact designs based on D_w for the Scheffé special cubic model for Snee's experiment. ● and ⊙ represent 1 and 2 replicates of that design point, respectively.

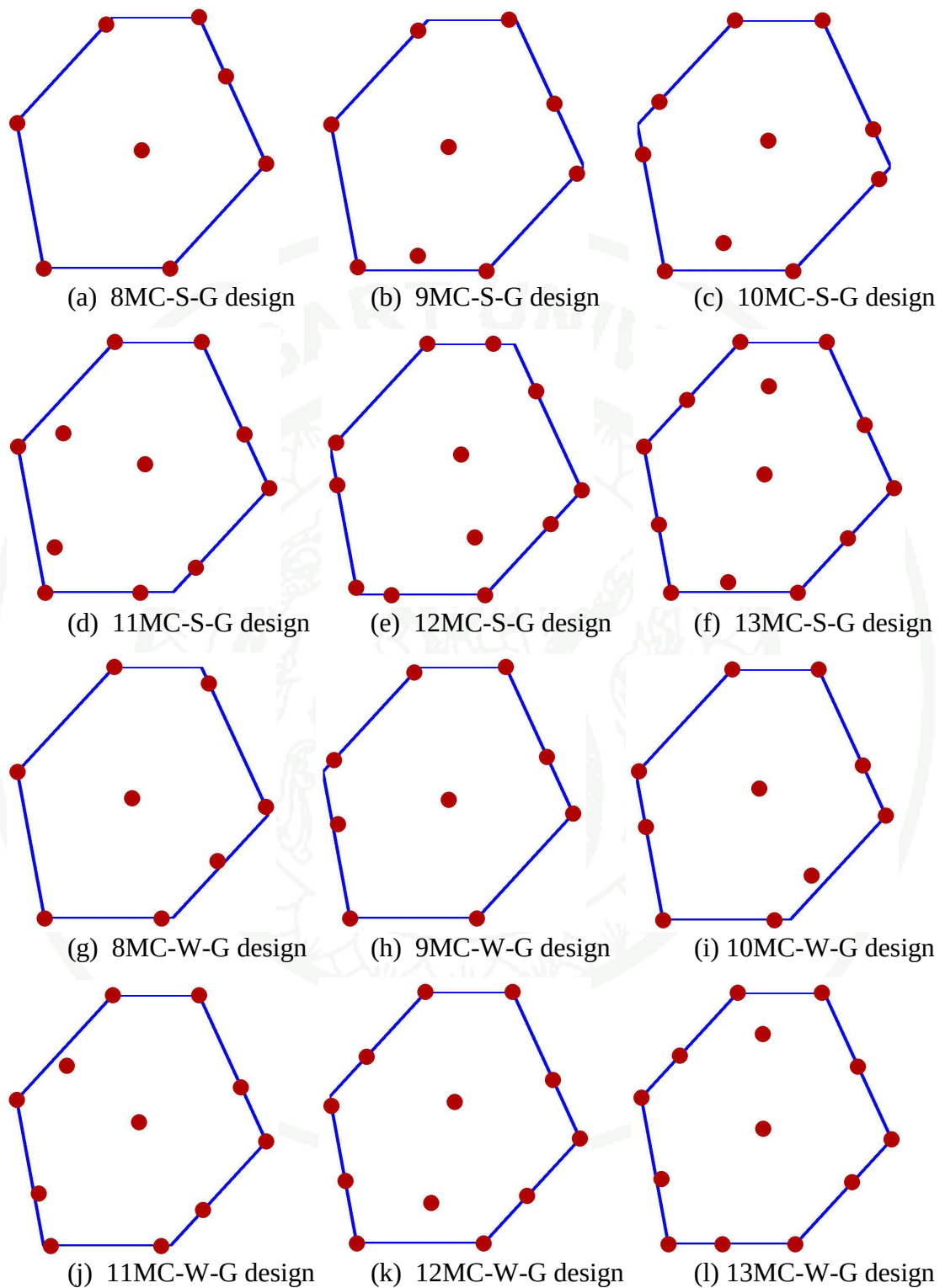


Figure 84 The optimal exact designs based on G_W for the Scheffé special cubic model for Snee's experiment. ● represent 1 replicates of that design point.

For the quadratic model, (1) the designs based on D_w are different than the designs based on G_w in that although they both contain all vertices, there is varying replication and (2) the designs based on D_w are similar to the designs based on G_w in that they both contain a point that lies near the overall centroid. Note that the designs based on G_w have a second point on the face except for $n = 7$. For the special cubic model, (1) the designs based on D_w are different than the designs based on the G_w in that they both contain all vertices but with varying replication, (2) the designs based on D_w are similar to the designs based on G_w in that there is a point that lies near the overall centroid, and (3) the distributional patterns of points under SH are quite similar to the patterns of points under WH for both D_w and G_w . Like the quadratic model, the geometries of the points based on the D_w and G_w are different. Note that all designs in this case have points that lie on either vertices or near vertices and near an overall centroid.

3. Evaluating designs for Case 3

Single-number criteria such as D - and G -efficiency are especially relevant when evaluating the proposed design. The experimenter has to address the question “which one should be chosen?” Objective function values from the GA are used to calculate the relative design efficiencies for the optimal exact designs. Relative design efficiencies are considered when the experimenter would like to know about how good his/her n -point designs are relative to all possible n -point designs based on any optimality criterion. By definition, an optimal exact design has 100% relative efficiency for its corresponding criterion. Tables 43 and 45 summarize the objective function values and the relative design efficiencies of designs for Snee’s experiment assuming the quadratic model and special cubic model, respectively.

In Table 43, assuming the quadratic model, the weighted D -optimal exact designs yield high G_w values, while the weighted G -optimal exact designs yield high

D_w values. The efficiencies of weighted D - and G -optimal exact designs are greater than 82% for both criteria. As the number of design points increase, the objective function values of the weighted D -optimal designs increase except when $n=8$ and 9. The additional design points have no impact on the objective function values of the weighted G -optimal designs.

Table 43 Performance comparison of objective function values and relative efficiencies of optimal exact designs assuming the quadratic model for Snee's experiment.

Design points	Design	Objective function values		Relative efficiencies (%)	
		D_w	G_w	D_w^{eff}	G_w^{eff}
7	7MQ-D	0.8982	80.7528	100	97.72
	7MQ-G	0.8768	82.6408	97.61	100
8	8MQ-D	0.8902	72.2707	100	94.40
	8MQ-G	0.8443	76.5576	94.84	0.00
9	9MQ-D	0.8938	66.3012	100	87.34
	9MQ-G	0.8118	75.9125	90.83	100
10	10MQ-D	0.9004	62.3158	100	85.81
	10MQ-G	0.7838	72.6225	87.05	100
11	11MQ-D	0.9090	61.5197	100	82.39
	11MQ-G	0.7968	74.6707	87.65	100
12	12MQ-D	0.9212	64.8044	100	87.59
	12MQ-G	0.7882	73.9863	85.56	100

*Boldface indicates optimal exact value D_w^{opt} and G_w^{opt} .

Although single-number criteria such as D - and G -efficiencies can be useful for evaluating proposed designs, the experimenter has to address the question “which one should be chosen *when two designs have the same efficiency values or values that are very close?*”. In this case, the experimenter needs additional information to help in the design selection process. Graphical approaches, such as a variance dispersion graph (VDG), a fraction of design space (FDS) plot and a componentwise variance dispersion graph (CVDG) can provide additional information regarding the prediction variance across the design region to assist in evaluation of competing designs.

VDGs, FDS plots and CVDGs of the weighted D -optimal exact designs and weighted G -optimal exact designs assuming the quadratic model for Snee's experiment are presented in Figures 85, 86 and 87, respectively. The minimum and maximum of the SPV for shrinkage levels between 0 and 1 are shown in the VDG. The fraction of the design space at or below any SPV value is shown in the FDS plots. The maximum of the SPV for allowable mixtures with $x_i = a$ where $L_i \leq a \leq U_i$ are shown in the CVDGs. In Table 44, the maximum SPVs are presented for the weighted D -optimal and weighted G -optimal exact designs for Snee's experiment. Figure 88 displays the VDGs, FDS plots, and CVDGs for the weighted D -optimal and weighted G -optimal exact designs for Snee's experiment. Solid and dashed lines correspond to the weighted D -optimal and the weighted G -optimal exact designs, respectively.

In Figures 85 and 88(a), the VDGs are similar for all of the weighted G -optimal exact designs, while the VDGs are quite different for all of the weighted D -optimal designs. The weighted D -optimal designs have different values at the center of the design space but seem to converge at the edges of the design space, whereas the weighted G -optimal designs have similar values at the center of the design space and tend to converge at the edges of the design space. The 7MQ-D design shows a clear advantage throughout the entire design space for all of the weighted D -optimal exact designs, while the 7MQ-G design shows a clear advantage throughout the entire design space for all of the weighted G -optimal exact designs. The weighted G -optimal exact designs show an advantage with a lower maximum SPV for shrinkage levels between 0 and 1. However, the 7MQ-D and 7MQ-G designs are quite comparable throughout the design space.

In Figures 86 and 88(b), the FDS plots provide additional evidence that the weighted D -optimal exact designs have inferior prediction variance properties compared to the weighted G -optimal exact designs. The 7MQ-D design is superior to other weighted D -optimal exact designs, while the 7MQ-G design is superior to other weighted G -optimal exact designs. The 7MQ-D and 7MQ-G designs are quite comparable throughout the design space. The values of SPV for the worse case of the weighted D -optimal exact designs (the 12MQ-D design) and weighted G -optimal

exact designs (the 10MQ-G design) are less than 6 (the G-optimal bound) for approximately 52% and 80% of the design region, respectively, while the best case of the weighted D -optimal exact designs (the 7MQ-D design) and weighted G-optimal exact designs (the 7MQ-G design) are less than 6 for approximately 90% of the design region.

In Figure 87 and 88(c), the CVDGs provide information about the variability throughout the entire mixture design space. The original lower and upper bounds of x_2 and x_3 are changed because of the MCCs. Like the VGDs and FDS plots, the weighted G-optimal exact designs perform well when compared to the weighted D -optimal designs. The 7MQ-D and 7MQ-G designs have similar profiles for all components. The maximum SPV for a weighted D -optimal and weighted G-optimal exact designs occurs at that mixture (x_1, x_2, x_3) shown in the last column of Table 44. The points (x_1, x_2, x_3) at which the maximum of SPV occurs for the weighted D - and G-optimal exact designs are similar.

Based on the VGDs, FDS plots, and CVDGs, we see that the weighted G-optimal exact designs are superior to the weighted D -optimal exact designs. The 7MQ-D design performs well throughout the design region, while the 12MQ-D design performs poorly throughout most of the design space. The 7MQ-G design performs well throughout the design region, while the 10MQ-G design performs poorly for most of the design space. The 7MQ-D design and 7MQ-G designs are quite comparable throughout the design space.

As shown in Table 44, the weighted G-optimal exact designs outperform the weighted D -optimal exact designs with respect to the maximum SPV. The 7MQ-D design and 7MQ-G designs are quite comparable with respect to the maximum SPV as well. In comparison to the weighted D -optimal exact designs, the 7MQ-D design outperforms all of the weighted D -optimal designs with respect to the maximum SPV, while the 12MQ-D design performs poorly with respect to the maximum SPV. Similarly, in comparison to the weighted G-optimal exact designs, the 7MQ-G design

outperforms all of the weighted G -optimal designs with respect to the maximum SPV, while the 10MQ-G design performs poorly with respect to the maximum SPV, however, all of the weighted G -optimal design are quite comparable.

As shown in Figure 82, the 7MQ-D design has no replicated vertices, while the 12MQ-D design has the maximum number of replicated vertices. The 7MQ-G design has only one near overall centroid point, while the other designs have points other than the near overall centroid on the face, whereas the 10MQ-G design has two points that are near vertices. The 7MQ-D and 7MQ-G designs have similar distribution patterns of points. We note that the additional points do not lead to any significant improvement in the SPV.

Assuming the quadratic model, we conclude that (1) the weighted G -optimal exact designs have better prediction properties than the weighted D -optimal exact designs throughout most of the design region, (2) the maximum SPVs for the weighted D -optimal exact designs are larger than those of the weighted G -optimal exact designs, and (3) the additional design points do not lead to better prediction variance properties for both the weighted D - and G -optimal exact designs.

Table 44 The maximum SPV for Snee's experiment assuming the quadratic model.

Design	Design points	Max SPV	Max SPV occurs that (x_1, x_2, x_3)
7MQ-D	7	6.94	(0.295, 0.31, 0.395)
8MQ-D	8	7.98	(0.295, 0.305, 0.4)
9MQ-D	9	8.93	(0.29, 0.31, 0.4)
10MQ-D	10	9.91	(0.29, 0.31, 0.4)
11MQ-D	11	11.00	(0.29, 0.31, 0.4)
12MQ-D	12	11.83	(0.29, 0.31, 0.4)
7MQ-G	7	6.74	(0.285, 0.315, 0.4)
8MQ-G	8	7.25	(0.3, 0.31, 0.39)
9MQ-G	9	7.11	(0.295, 0.305, 0.4)
10MQ-G	10	7.48	(0.29, 0.325, 0.385)
11MQ-G	11	7.22	(0.3, 0.305, 0.395)
12MQ-G	12	7.31	(0.295, 0.31, 0.395)

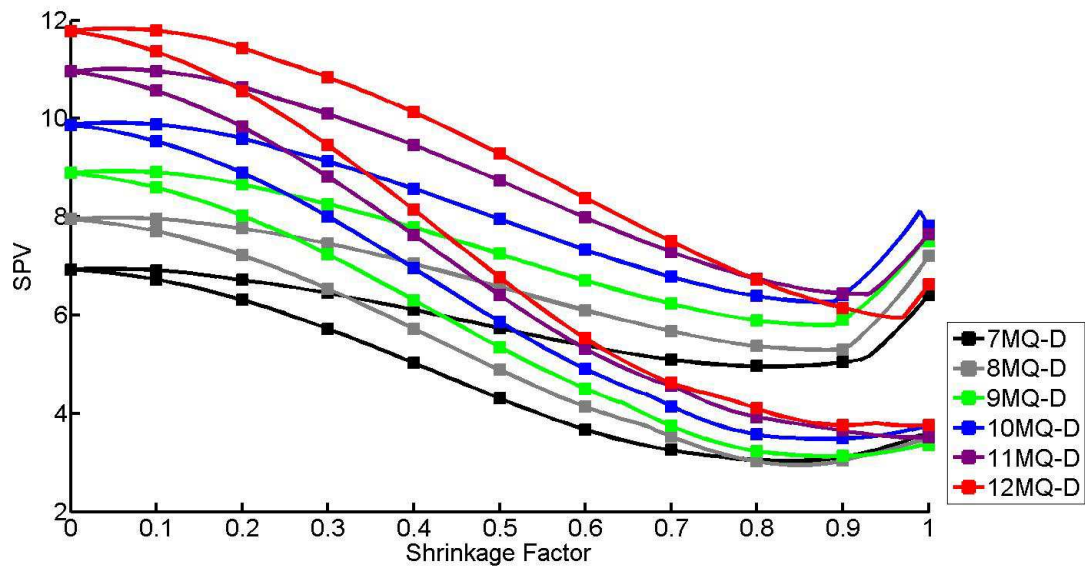
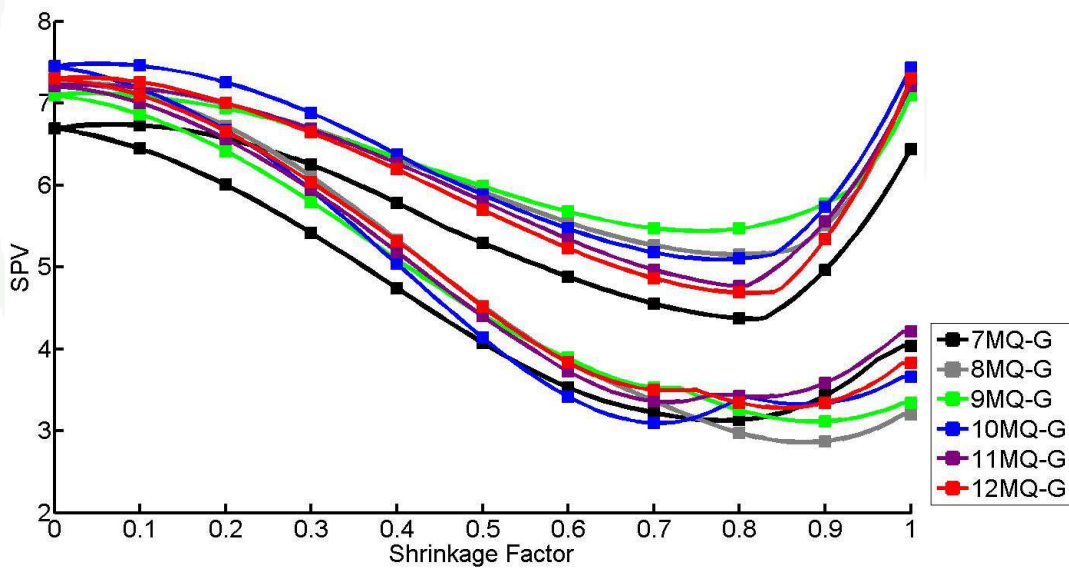
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 85 VDGs for the weighted optimal exact designs assuming the quadratic model for Snee's experiment.

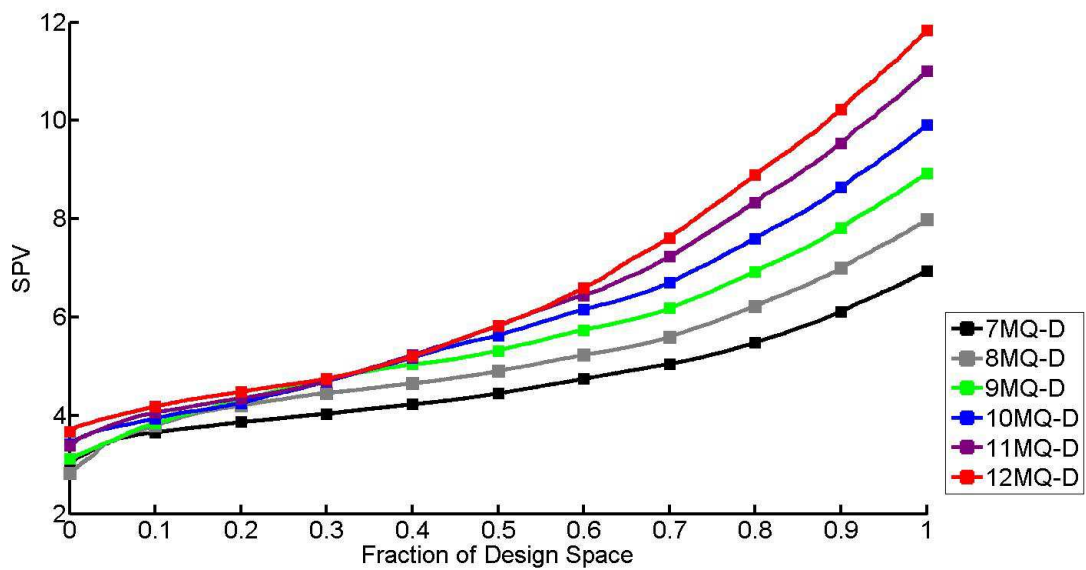
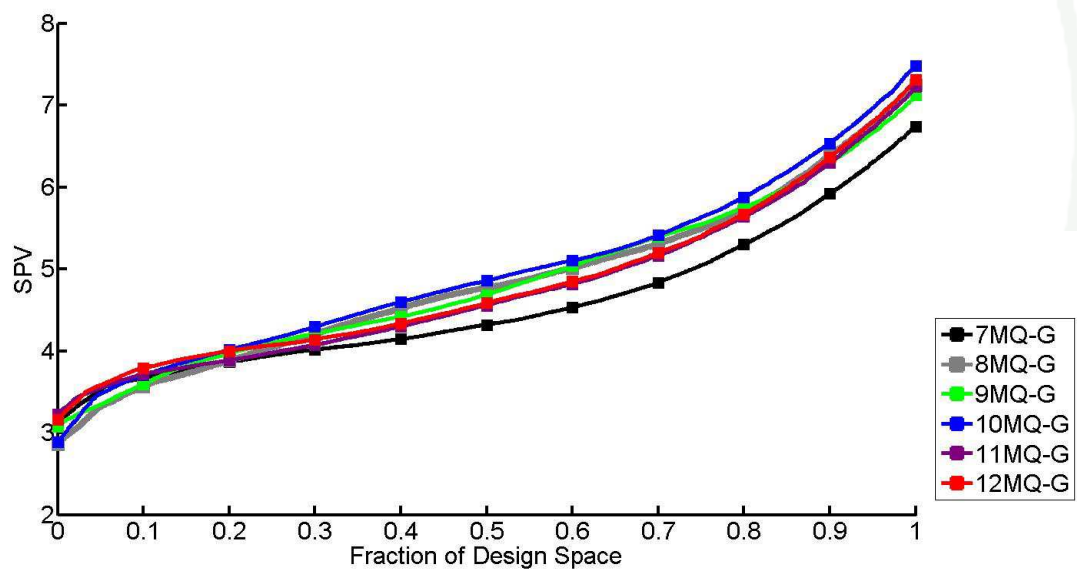
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 86 FDS plots for the weighted optimal exact designs assuming the quadratic model for Snee's experiment.

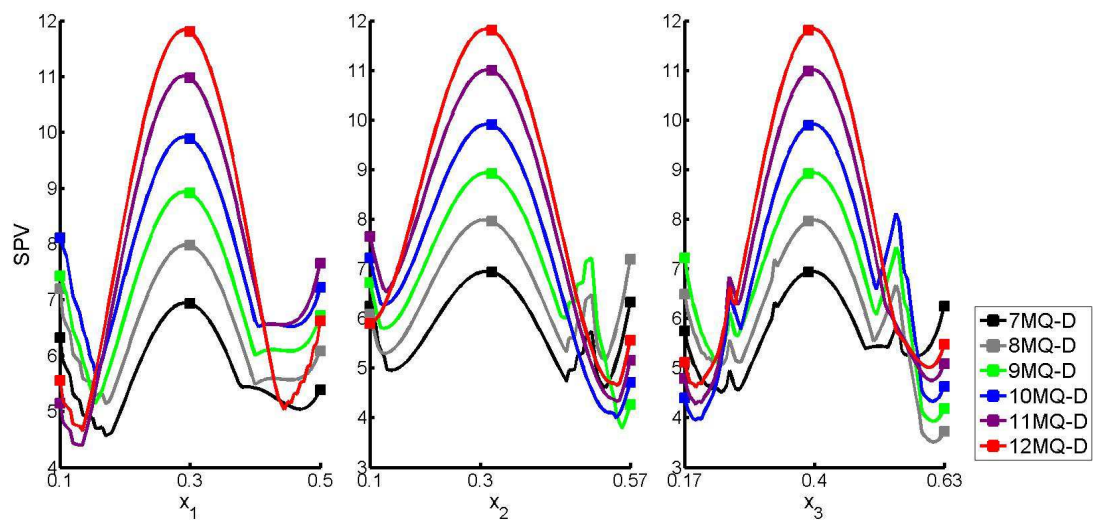
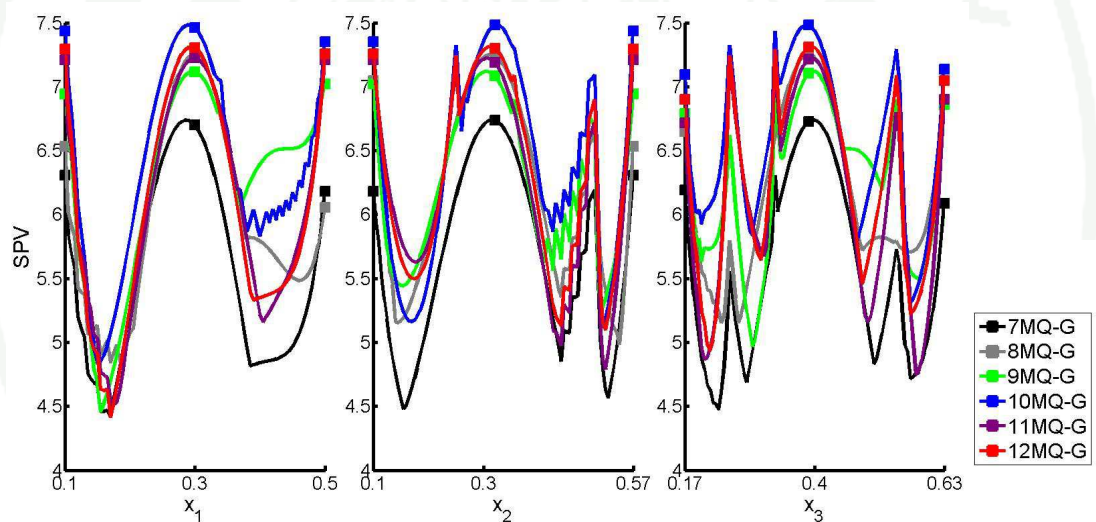
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 87 CVDGs for the weighted optimal exact designs assuming the quadratic model for Snee's experiment.

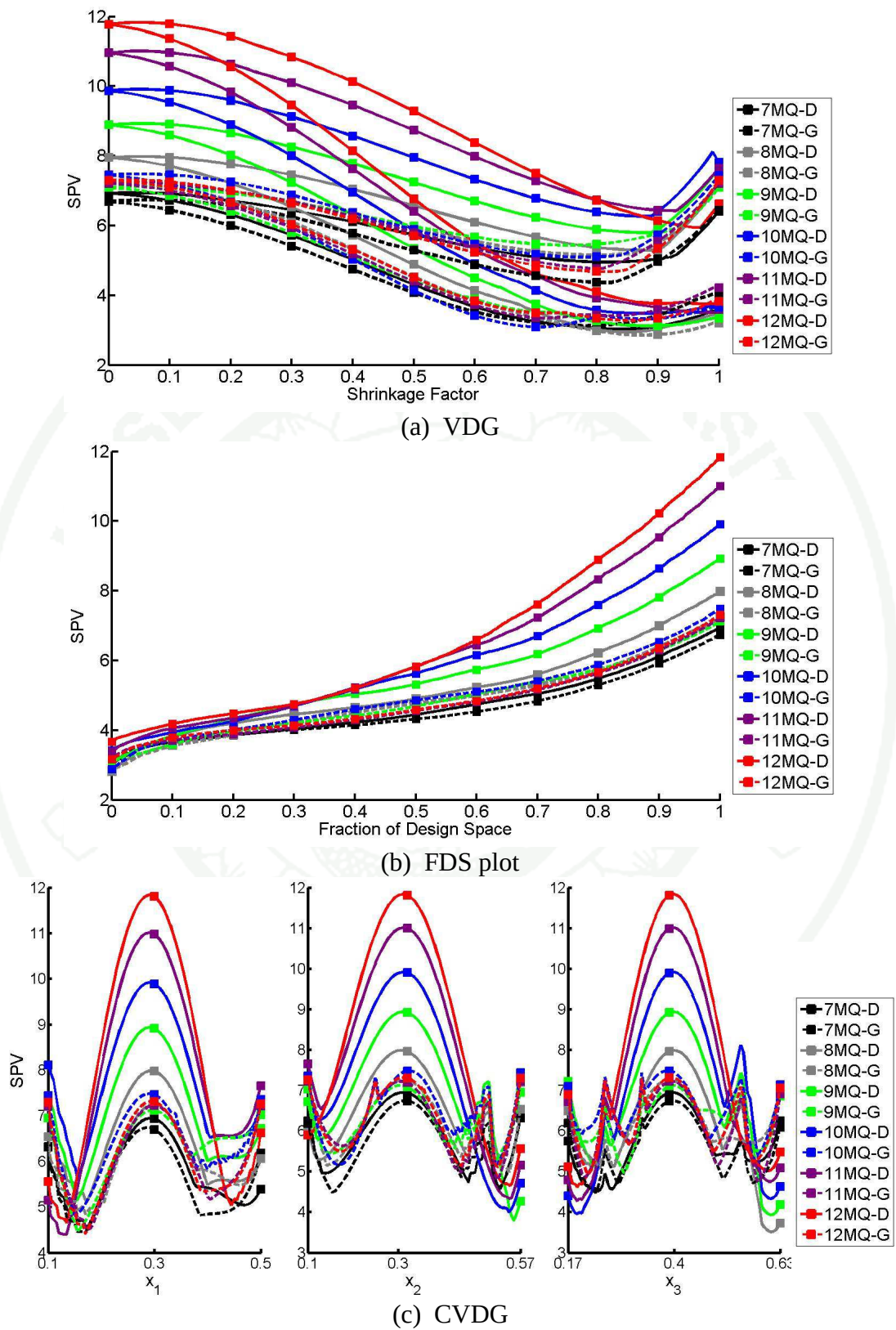


Figure 88 Graphical approaches for comparing 12 mixture designs assuming the quadratic model for Snee's experiment.

As shown in Table 45, $D_w - S$, $D_w - W$, $G_w - S$ and $G_w - W$ represent the weighted D -optimality criteria based on SH and WH, and the weighted G -optimality criteria based on SH and WH, respectively. The weighted D -optimal exact designs under SH and WH have large $D_w - S$ and $D_w - W$ values and rather small $G_w - S$ and $G_w - W$ values. The weighted G -optimal exact designs under SH and WH have high $G_w - S$ and $G_w - W$ values as well as quite low $D_w - S$ and $D_w - W$ value. We observe that the weighted G -optimal exact designs under SH having $n = 10$ and 12 points are identical to the weighted G -optimal exact designs under WH or have relative efficiencies very close to 100%. Theoretically, the relative efficiencies should be 100%, but the GA terminated before finding the true weighted optimal exact designs under SH or WH. The weighted D -optimal exact designs under SH and WH have relative efficiencies greater than 99% for the D -criterion and greater than 73% for the G -criterion, while the weighted G -optimal exact designs under SH and WH have efficiencies greater than 85% for all criteria. As the number of design points increases, the objective function values of the weighted optimal exact designs increase accordingly for the weighted D -optimal exact designs based on SH and WH except when $n = 13$. As the number of design points increase, the objective function values of the weighted G -optimal exact designs based on SH and WH do not show a significant improvement in the maximum SPV.

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Table 45 Performance comparison of objective function values and relative efficiencies based on the D - and G -criteria for optimal exact designs assuming the special cubic model for Snee's experiment.

n	Design	Objective function values				Relative efficiencies (%)			
		D_w -S	D_w -W	G_w -S	G_w -W	D_w^{eff} -S	D_w^{eff} -W	G_w^{eff} -S	G_w^{eff} -W
8	8MC-S-D	0.6022	0.5378	66.0555	66.1731	100	99.98	81.49	82.48
	8MC-W-D	0.6021	0.5379	66.0580	66.1830	99.99	100	81.49	82.50
	8MC-S-G	0.5846	0.5218	81.0604	79.7389	97.08	97.00	100	99.39
	8MC-W-G	0.5645	0.5063	80.0897	80.2259	93.75	94.13	98.80	100
9	9MC-S-D	0.6035	0.5387	60.3417	60.1498	100	99.99	78.67	79.22
	9MC-W-D	0.6034	0.5388	60.3045	60.1186	99.99	100	77.51	79.18
	9MC-S-G	0.5485	0.4895	77.8030	75.7612	90.90	90.85	100	99.78
	9MC-W-G	0.5628	0.5025	76.7007	75.9254	93.26	93.27	98.58	100
10	10MC-S-D	0.6072	0.5416	56.4677	55.9439	100	99.99	74.02	73.03
	10MC-W-D	0.6071	0.5417	56.4195	55.9271	99.99	100	73.96	73.00
	10MC-S-G	0.5409	0.4825	76.2648	74.8928	89.08	89.08	99.97	97.76
	10MC-W-G	0.5532	0.4952	76.2852	76.6085	91.11	91.43	100	100
11	11MC-S-D	0.6122	0.5465	60.3386	59.5580	100	99.98	78.42	78.74
	11MC-W-D	0.6121	0.5466	60.2805	59.5534	99.98	100	78.34	78.74
	11MC-S-G	0.5385	0.4815	76.9449	74.9006	87.96	88.08	100	99.03
	11MC-W-G	0.5450	0.4875	75.3575	75.6349	89.02	89.17	97.94	100
12	12MC-S-D	0.6207	0.5527	61.2338	58.3776	100	99.99	81.57	79.58
	12MC-W-D	0.6206	0.5528	61.1759	58.3393	99.98	100	81.49	79.53
	12MC-S-G	0.5316	0.4752	75.0697	73.3561	85.64	85.97	100	100
	12MC-W-G	0.5385	0.4806	73.3508	73.0826	86.76	86.94	97.71	99.63
13	13MC-S-D	0.6207	0.5519	60.1639	56.9847	100	99.98	79.56	75.65
	13MC-W-D	0.6206	0.5520	60.1720	56.9968	99.98	100	79.57	75.67
	13MC-S-G	0.5331	0.4779	75.6236	74.9519	85.89	86.57	100	99.51
	13MC-W-G	0.5357	0.4807	74.9997	75.3223	86.30	87.08	99.18	100

*Boldface indicates optimal exact value of D_w^{opt} and G_w^{opt} .

Figure 89 presents the VDGs of the weighted D -optimal and weighted G -optimal exact designs assuming the special cubic model for Snee's experiment. Figure 90 displays the FDS plots of the weighted D -optimal and weighted G -optimal exact designs assuming the special cubic model for Snee's experiment. Figure 91 presents the CVDGs of the weighted D -optimal and weighted G -optimal exact designs for the special cubic model for Snee's experiment. Table 46 presents the maximum SPV for the weighted D -optimal and weighted G -optimal exact designs assuming the special cubic model for Snee's experiment.

Figure 89 shows the minimum and maximum of the SPV for shrinkage levels between 0 and 1. The VDGs for the weighted D -optimal exact designs under SH and WH for each design size n display identical profiles, while the VDGs for all of the weighted G -optimal exact designs have similar profiles. The SPVs for the weighted D -optimal exact designs (except when $n=8$) are greater than that of the weighted G -optimal exact designs most of the design space. The SPVs for the 8MC-S-D and 8MC-W-D designs are comparable to those of the weighted G -optimal designs. The weighted G -optimal exact designs are superior with a lower maximum SPV for shrinkage levels between 0 and 1.

Figure 90 shows the fraction of the design space at or below any SPV value. The weighted D -optimal exact designs under SH and WH for each design size n are identical, while the weighted G -optimal exact designs under SH and WH are comparable. The weighted G -optimal exact designs are superior to the weighted D -optimal exact designs. At the design center, the weighted D -optimal exact design and weighted G -optimal exact designs are also quite similar. However, the weighted D -optimal exact designs are no longer competitive at the boundary of the region for each design. The SPVs for 8MC-S-D and 8MC-W-D designs are competitive with those of the weighted G -optimal designs for most of the design space except at the boundary. The SPVs of weighted D - and G -optimal exact designs begin to increase sharply at near the boundary of the design space except for the 13MC-S-D and 13MC-W-D designs. The values of SPV for the worse case of the weighted D -optimal exact designs (the 13MC-S-D and 13MC-W-D designs) are less than 7 (the G -optimal

bound) for approximately 55% of the design region, while the best case of the weighted D -optimal exact designs (the 8MC-S-D and 8MC-W-D designs) are less than 7 for approximately 85% of the design region. For the weighted G -optimal exact designs, the SPVs for the 8MC-W-G design are less than 7 for approximate 95% of the design region, while the SPVs for the remaining designs are less than 7 for more than 85% of the design region. It is clear that the weighted G -optimal exact designs have much flatter and lower FDS curves throughout the design region, indicating a more desirable SPV distribution.

Figure 91 shows the variability over the entire mixture design space and the maximum SPV for allowable mixtures with $x_i = a$ where $L_i \leq a \leq U_i$. The SPVs of the weighted D -optimal exact designs under SH and WH for each design size n are identical for three components and exhibit similar patterns of SPV values, while the SPV of the weighted G -optimal exact designs under SH and WH show otherwise. The weighted G -optimal exact designs perform well with respect to the weighted D -optimal designs. The last column of Table 46 presents the mixture (x_1, x_2, x_3) at which the maximum SPV occurs for the weighted D -optimal and weighted G -optimal exact designs. The mixtures (x_1, x_2, x_3) at which the maximum SPV occurs for the weighted D -optimal designs are quite similar except for the 13MC-S-D and 13MC-W-D designs, whereas the mixtures (x_1, x_2, x_3) at which the maximum SPV occurs for the weighted G -optimal designs occurs are quite different for each design.

In Figures 89 through 91, the VDGs, FDS plots, and CVDGs for the weighted D -optimal exact designs based on SH and WH are identical, while the VDGs, FDS plots, and CVDGs for the weighted G -optimal exact designs based on SH and WH have similar profiles. The patterns shown in each of the graphical approach for the weighted D -optimal exact designs differs from those of the weighted G -optimal exact designs. The weighted G -optimal exact designs are superior to most of the weighted D -optimal designs; however, the 8MC-S-D and 8MS-W-D designs compete with the weighted G -optimal designs. As shown in Table 46, the maximum SPVs for the weighted D -optimal exact designs under SH and WH are quite comparable. Similarly,

the SPVs for the weighted G -optimal exact designs under SH and WH are quite comparable. The weighted D -optimal exact designs are incomparable with the weighted G -optimal exact designs based on the maximum SPV. The 11MC-S-D design is the best having a smaller maximum SPV for the weighted D -optimal exact designs, while the 8MC-S-G design is the best with smaller maximum SPVs for the weighted G -optimal exact designs. The 8MC-S-G design is the best with smaller maximum SPVs for all of the weighted optimal exact designs. Assuming the special cubic model, the additional design points do not yield a significant improvement in the SPV as displayed in Figures 89 to Figure 91.

For the special cubic model, we conclude that (1) the weighted G -optimal exact designs have better prediction variance properties than the weighted D -optimal exact designs throughout the design region, (2) the weighted G -optimal exact designs under SH and WH have similar profiles, whereas the weighted D -optimal exact designs under SH and WH show identical profiles, (3) the maximum SPVs for the weighted D -optimal exact designs results in higher values than those of the weighted G -optimal exact designs in all cases, (4) the maximum SPVs for the weighted D -optimal exact designs under SH and WH are quite similar, and the maximum SPVs for the weighted G -optimal exact designs under SH and WH are also similar, and (5) as the design size increases, the weighted D -optimal designs display poorer prediction variance properties, whereas the weighted G -optimal designs do not indicate better prediction properties.

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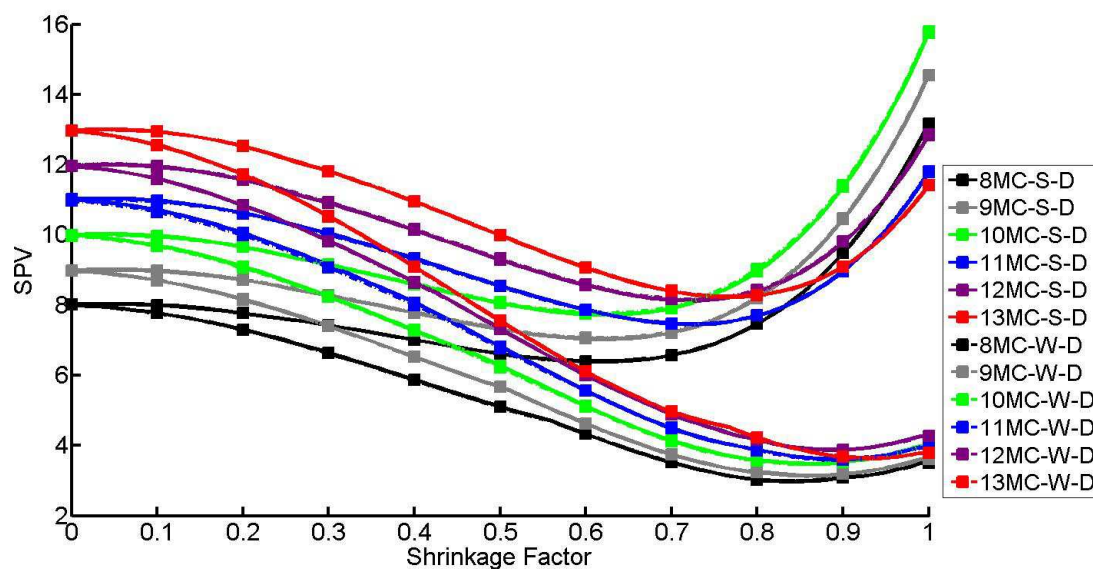
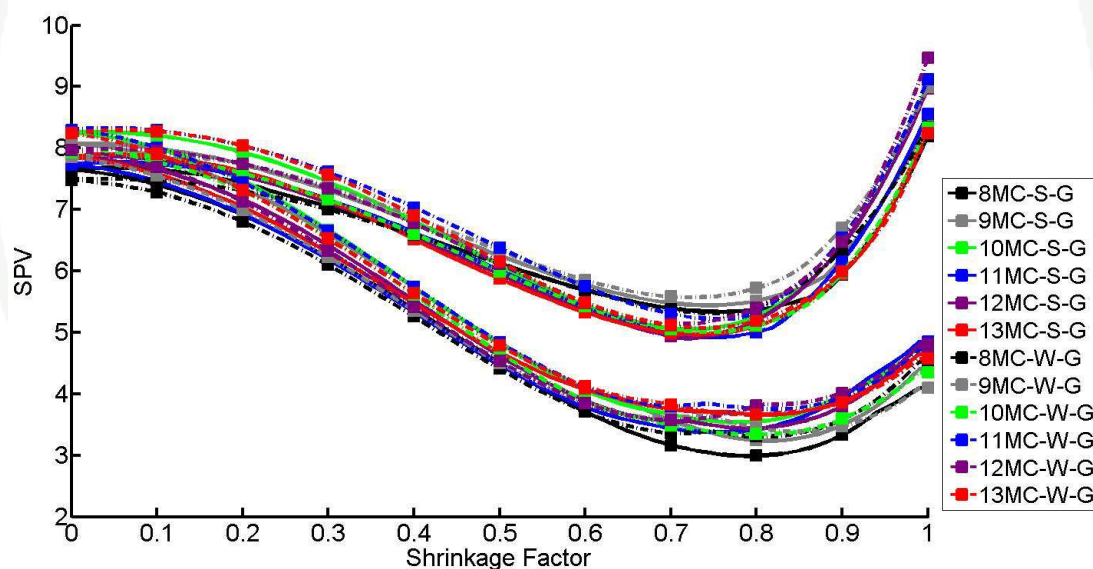
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 89 VDGs for the weighted optimal exact designs assuming the special cubic model for Snee's experiment.

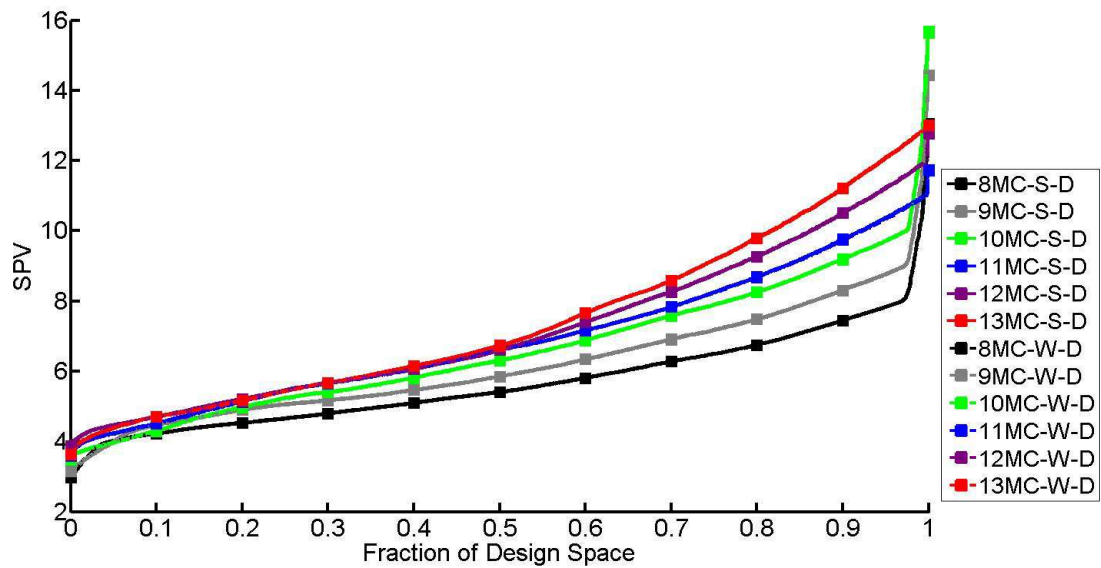
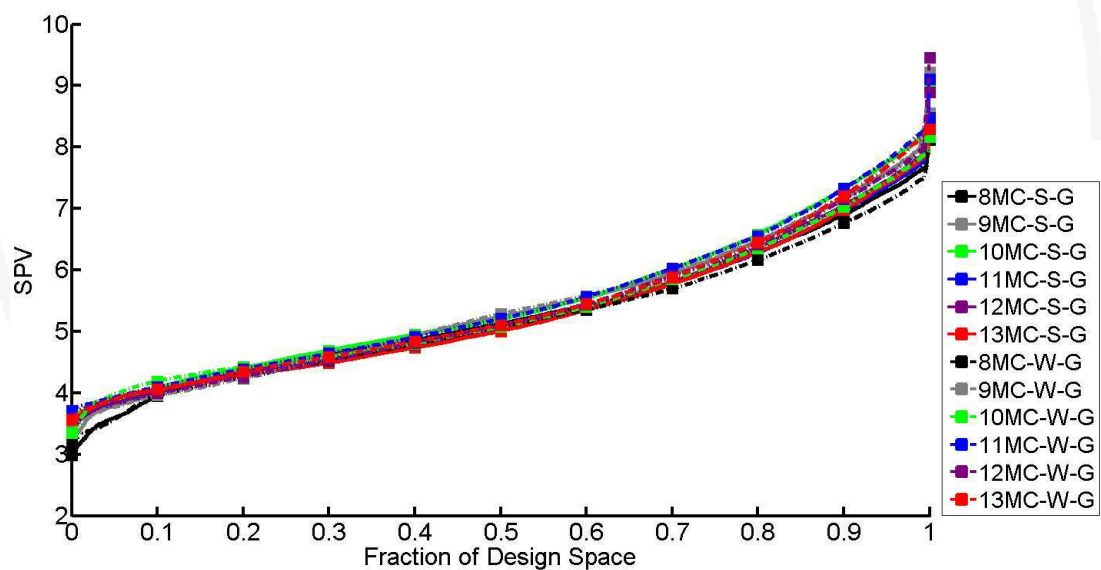
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 90 FDS plots for the weighted optimal exact design assuming the special cubic model for Snee's experiment.

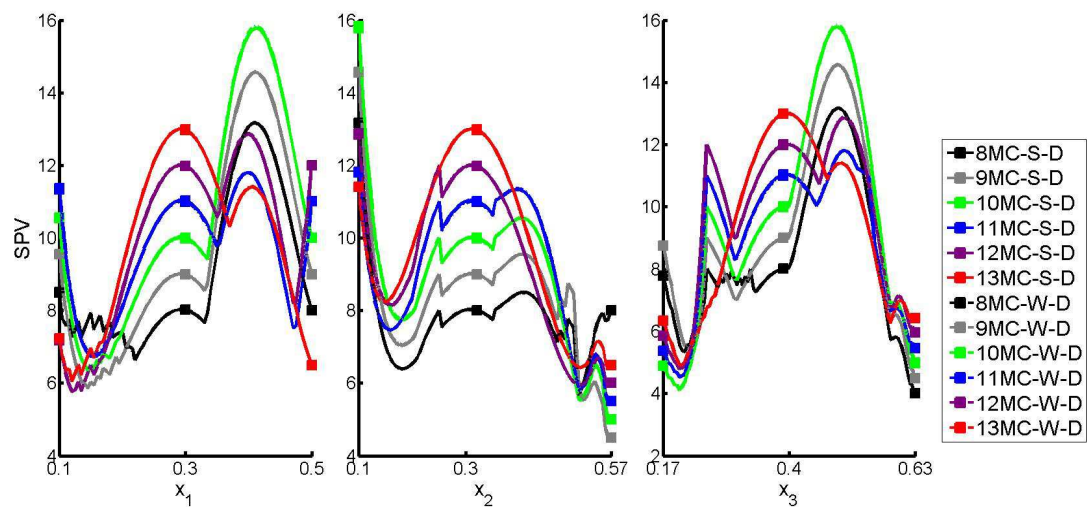
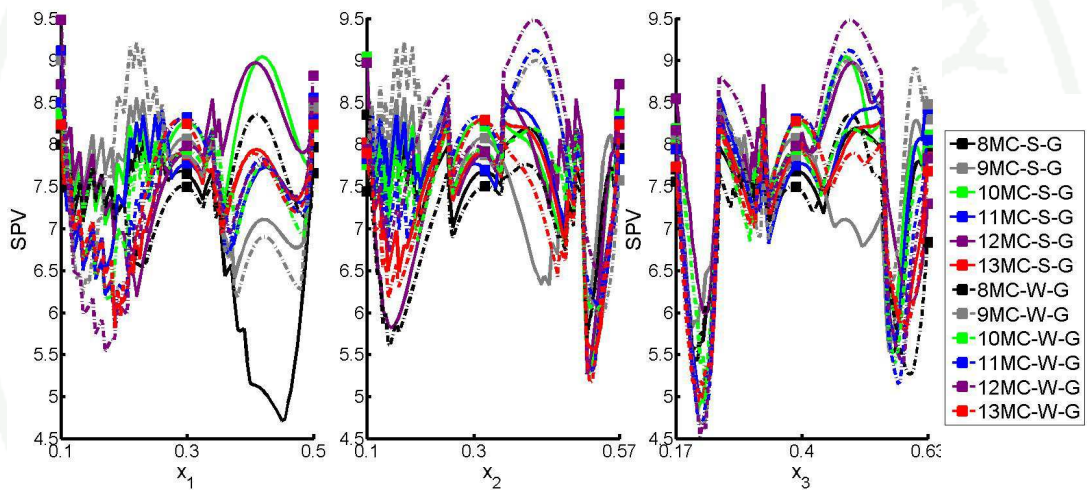
(a) The weighted D -optimal exact designs(b) The weighted G -optimal exact designs

Figure 91 CVDGs for the weighted optimal exact designs assuming the special cubic model for Snee's experiment.

Table 46 The maximum SPV values assuming the special cubic model for Snee's experiment.

	Design	Max SPV	Max SPV occurs that (x_1, x_2, x_3)
The weighted <i>D</i> -optimal exact designs based on SH	8MC-S-D	13.17	(0.41, 0.1, 0.49)
	9MC-S-D	14.55	(0.41, 0.1, 0.49)
	10MC-S-D	15.77	(0.41, 0.1, 0.49)
	11MC-S-D	11.79	(0.4, 0.1, 0.5)
	12MC-S-D	12.85	(0.4, 0.1, 0.5)
	13MC-S-D	13.00	(0.295, 0.31, 0.395)
The weighted <i>D</i> -optimal exact designs based on WH	8MC-W-D	13.16	(0.41, 0.1, 0.49)
	9MC-W-D	14.57	(0.41, 0.1, 0.49)
	10MC-W-D	15.82	(0.41, 0.1, 0.49)
	11MC-W-D	11.81	(0.4, 0.1, 0.5)
	12MC-W-D	12.87	(0.4, 0.1, 0.5)
	13MC-W-D	12.99	(0.295, 0.31, 0.395)
The weighted <i>G</i> -optimal exact designs based on SH	8MC-S-G	8.19	(0.1, 0.4, 0.5)
	9MC-S-G	8.56	(0.22, 0.17, 0.61)
	10MC-S-G	9.04	(0.42, 0.1, 0.48)
	11MC-S-G	8.55	(0.5, 0.25, 0.25)
	12MC-S-G	8.97	(0.41, 0.1, 0.49)
	13MC-S-G	8.31	(0.5, 0.25, 0.25)
The weighted <i>G</i> -optimal exact designs based on WH	8MC-W-G	8.35	(0.41, 0.1, 0.49)
	9MC-W-G	9.22	(0.22, 0.17, 0.61)
	10MC-W-G	8.32	(0.1, 0.57, 0.33)
	11MC-W-G	9.11	(0.1, 0.415, 0.485)
	12MC-W-G	9.47	(0.1, 0.41, 0.49)
	13MC-W-G	8.29	(0.29, 0.315, 0.395)

4. Examining model robustness for Case 3

The experimenter would like a design that will generate data that are adequate for fitting a model. However, the form of the final model that will be adopted for prediction and determination of optimum conditions is rarely known in advance. If some terms in the starting for “full” model are insignificant after the data are collected, then the design may no longer have desirable prediction variance properties. The experimenter would like a design that allows model modification for a class of specific models. Thus, model robustness is very important for addressing this problem. We use the FDS plots to study if a design is model robust.

Suppose **the quadratic model** corresponds to the most complex “full” model that the experimenter might need to adequately model the data. Then, there are 8 models nested within the full model for $q = 3$. Table 47 presents a number of possible nested models for the quadratic model which might be of interest when examining mixture designs. The last column of Table 47 presents the maximum SPV values for each model of the 7MQ-D design, and the corresponding FDS curves are shown in Figure 92. We note that (1) the quadratic and linear models are wrapped around the other models considered, (2) the plots for Model A to Model F are located between the plots for the quadratic and linear models, (3) the models having the same number of model parameters have similar FDS curve profiles, and (4) the FDS curve for any model will be at or below a model that it is nested within. The FDS curve for the quadratic model has a rather different slope from those of the remaining curves. Therefore, the addition of quadratic terms has a much larger affect on the stability of the SPV values.

Comparing a design’s SPV properties for sets of models to the SPV properties of the quadratic model and the linear model gives a manageable summary of that design’s prediction variance performance. Therefore, only the quadratic model and the linear model will be considered for assessment of model robustness for a design.

Table 47 Summary information for the set of possible reduced models assuming a quadratic model for Snee's experiment.

Type of model	Term in model	p	Max SPV
Quadratic	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3$	6	6.94
Model A	$x_1, x_2, x_3, x_1x_3, x_2x_3$	5	6.16
Model B	$x_1, x_2, x_3, x_1x_2, x_2x_3$	5	6.14
Model C	$x_1, x_2, x_3, x_1x_2, x_1x_3$	5	6.02
Model D	x_1, x_2, x_3, x_2x_3	4	6.13
Model E	x_1, x_2, x_3, x_1x_3	4	5.37
Model F	x_1, x_2, x_3, x_1x_2	4	5.75
Linear	x_1, x_2, x_3	3	3.75

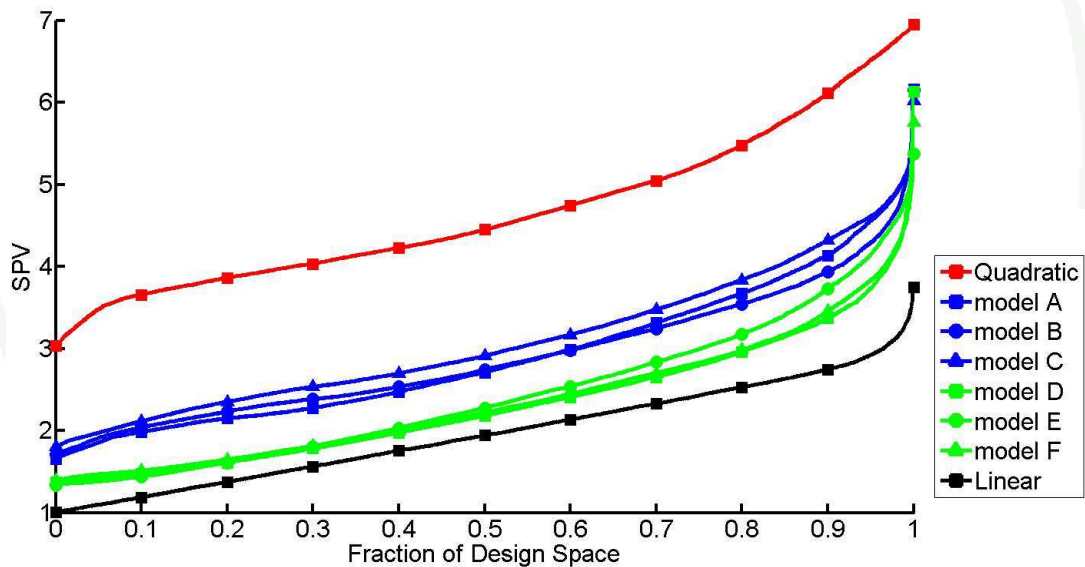


Figure 92 FDS plots of the 7MQ-D design for several models for Snee's experiment.

The comparison between the weighted D -optimal and weighted G -optimal exact designs for each design size are presented in Figure 93. The comparison for all of the weighted D -optimal and G -optimal exact designs are shown in Figures 94 and 95, respectively. Table 48 gives the G -efficiency for each design. In the previous section, the weighted G -optimal exact designs were superior to the weighted D -optimal exact designs. However, the 7MQ-D design is quite comparable to the

weighted G -optimal exact designs. That is, the curves in the VDGs, FDS plots, and CVDGs for the quadratic model for the weighted G -optimal exact designs are lower than those for the weighted D -optimal exact designs for most of the design space except for design 7MQ-D. As shown in Table 48, only the maximum SPV values for the linear model of the weighted G -optimal exact designs are larger than those of the weighted D -optimal exact designs except when $n = 7$ and 11 resulting in a lower G -efficiency, whereas the maximum SPV values for the quadratic model of the weighted G -optimal exact designs are smaller than those of the weighted D -optimal exact designs resulting in a higher G -efficiency.

Table 48 The maximum SPV values and the approximate G -efficiencies for the weighted D - and G -optimal exact designs for two model types, assuming the quadratic model for Snee's experiment.

Design	Model type	G-eff	Design	Model type	G-eff
7MQ-D	Quadratic	86.39	7MQ-G	Quadratic	89.04
	Linear	79.98		Linear	81.42
8MQ-D	Quadratic	75.15	8MQ-G	Quadratic	82.81
	Linear	73.87		Linear	73.74
9MQ-D	Quadratic	67.18	9MQ-G	Quadratic	84.28
	Linear	80.21		Linear	78.34
10MQ-D	Quadratic	60.51	10MQ-G	Quadratic	80.19
	Linear	81.51		Linear	76.35
11MQ-D	Quadratic	54.50	11MQ-G	Quadratic	83.07
	Linear	75.40		Linear	77.58
12MQ-D	Quadratic	50.71	12MQ-G	Quadratic	82.04
	Linear	90.87		Linear	78.93

In Figure 93, for the linear model, the profiles of the weighted D -optimal and weighted G -optimal exact designs are quite similar for the most of the design space. The FDS curves for the quadratic model for the weighted G -optimal designs are lower than those for the weighted D -optimal designs for most of the design space. However, for the quadratic model with $n = 7$ and 8, the weighted D -optimal and weighted G -optimal exact designs perform similarly for most of the design space. The weighted G -optimal exact designs perform best for the quadratic and linear models, maintain better stability for large values of SPV and have the best G -efficiency for both model

types. However, for both the linear model and quadratic models with $n=7$ and 8, the weighted D -optimal and weighted G -optimal exact designs have similar profiles throughout the design space.

As seen in Figures 94 and 95, the 7MQ-D design performs the best for the quadratic and linear models based on the D -criterion, while the 7MQ-G design performs the best for the quadratic and linear models based on the G -criterion since they have the best G -efficiency for both model types. For the majority of the design space, all of the weighted D -optimal and weighted G -optimal designs appear to have good robustness properties, while the weighted G -optimal designs maintain stability and are relatively flat for both models at the largest SPV values. For $n=7$ and 8, the weighted D -optimal and weighted G -optimal designs are recommended as model robust designs because the lines for both the linear and quadratic models are similar and relatively flat throughout the design space. For $9 \leq n \leq 13$, the weighted G -optimal designs are recommended for model robustness over the weighted D -optimal exact designs because (1) the curves associated with both models for the weighted G -optimal designs on the FDS plots are closer together than they are for the weighted D -optimal exact designs and (2) the weighted G -optimal designs appear to overall outperform the weighted D -optimal exact designs.

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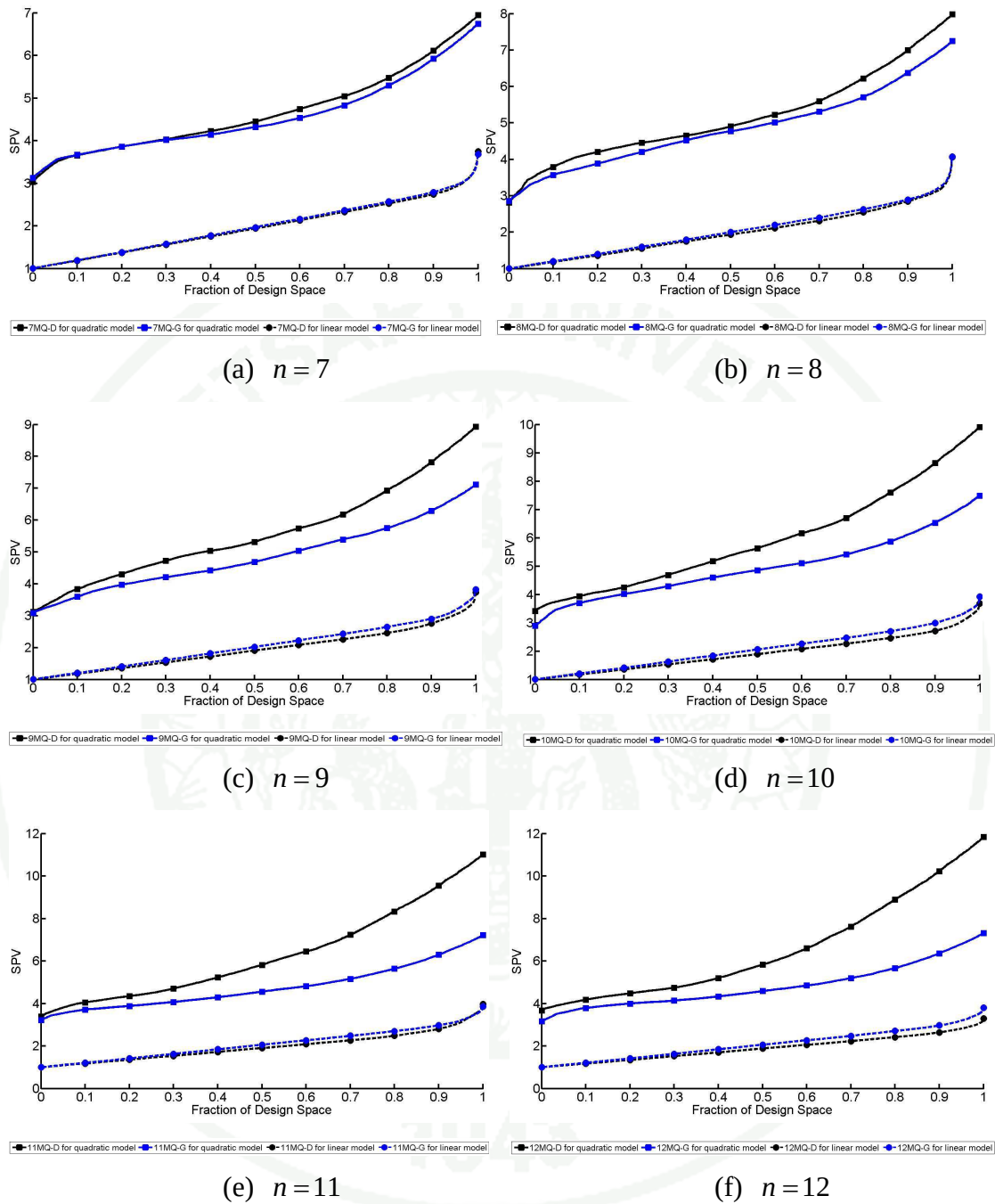


Figure 93 FDS plots for comparing the weighted D - and G -optimal exact designs for two types of models assuming the quadratic model for Snee's experiment.

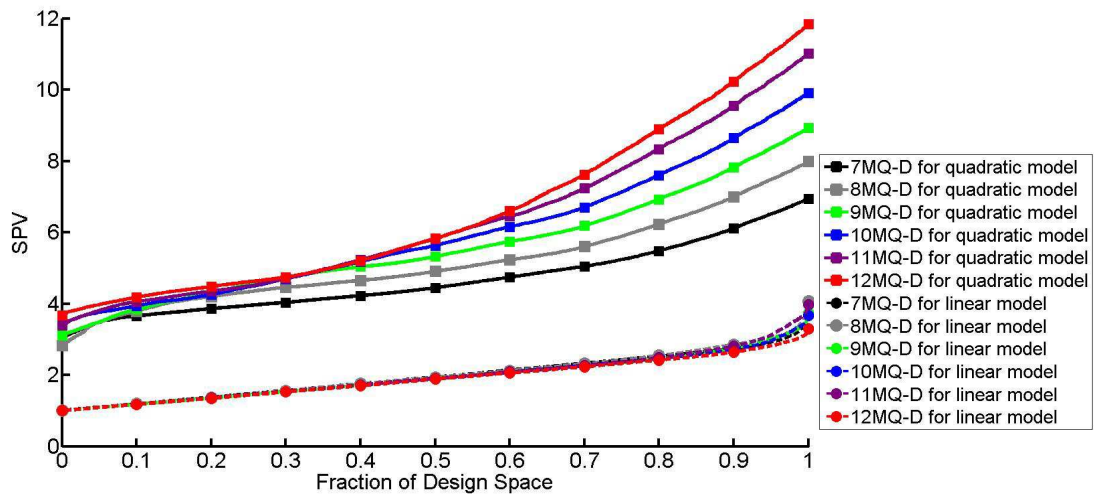


Figure 94 FDS plots for comparing the D -optimal exact designs for two types of models assuming the quadratic model for Snee's experiment.

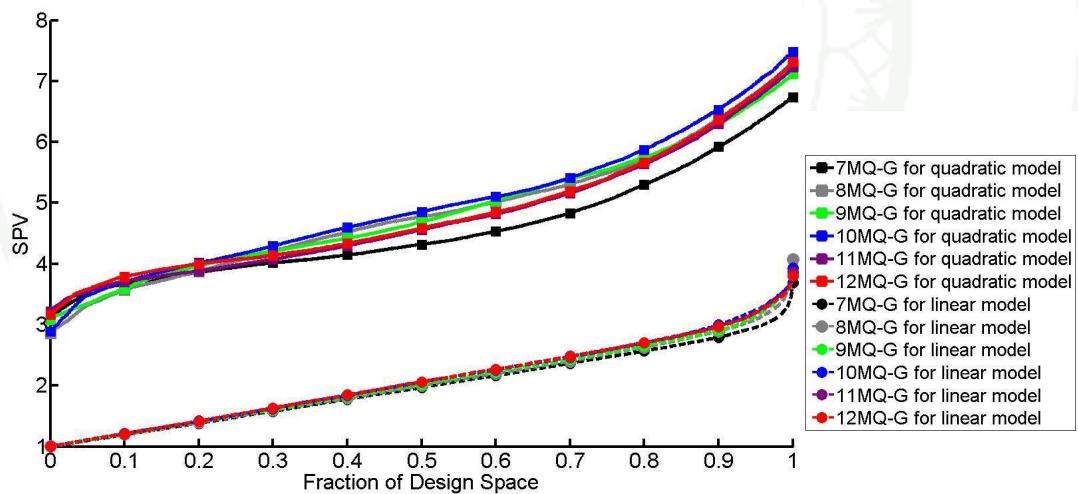


Figure 95 FDS plots for comparing the G -optimal exact designs for two types of models assuming the quadratic model for Snee's experiment.

Now suppose that **the special cubic model** corresponds to the most complex model that the experimenter might need to adequately model the experimental data. There are 9 SH models and 15 WH models that are nested within the special cubic model for mixture models with three components. Table 49 shows a number of possible nested models of the special cubic model under SH which might be of interest when studying mixture designs. Figure 96 contains the corresponding FDS curves for the 8MC-S-D design for which the full model with 7 model parameters is given by the purple curve, while the model having 6, 5, 4, and 3 model parameters are represented by the red, blue, green, and black curves, respectively. The black FDS curve represents the linear model and is below the green curves (for linear models with one quadratic term); the green FDS curves are below the blue curves (for linear models with two quadratic terms); the blue FDS curves are at or below the red curve (for the quadratic model); and the red FDS curve is at or below the purple FDS curve (for the special cubic model). The FDS curve for the quadratic and special cubic models have similar profiles except near the boundary of the design space. The FDS curve for the quadratic and special cubic models have a very different slopes than the remaining curves. Thus, the addition of cubic term has a much larger effect on the stability of the SPV values than the addition of quadratic terms.

Table 49 Summary information for the possible SH reduced models assuming the special cubic model for Snee's experiment.

Type of model	Term in model	p
Special cubic	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3, x_1x_2x_3$	7
Quadratic	$x_1, x_2, x_3, x_1x_2, x_1x_3, x_2x_3$	6
Model A	$x_1, x_2, x_3, x_1x_3, x_2x_3$	5
Model B	$x_1, x_2, x_3, x_1x_2, x_2x_3$	5
Model C	$x_1, x_2, x_3, x_1x_2, x_1x_3$	5
Model D	x_1, x_2, x_3, x_2x_3	4
Model E	x_1, x_2, x_3, x_1x_3	4
Model F	x_1, x_2, x_3, x_1x_2	4
Linear	x_1, x_2, x_3	3

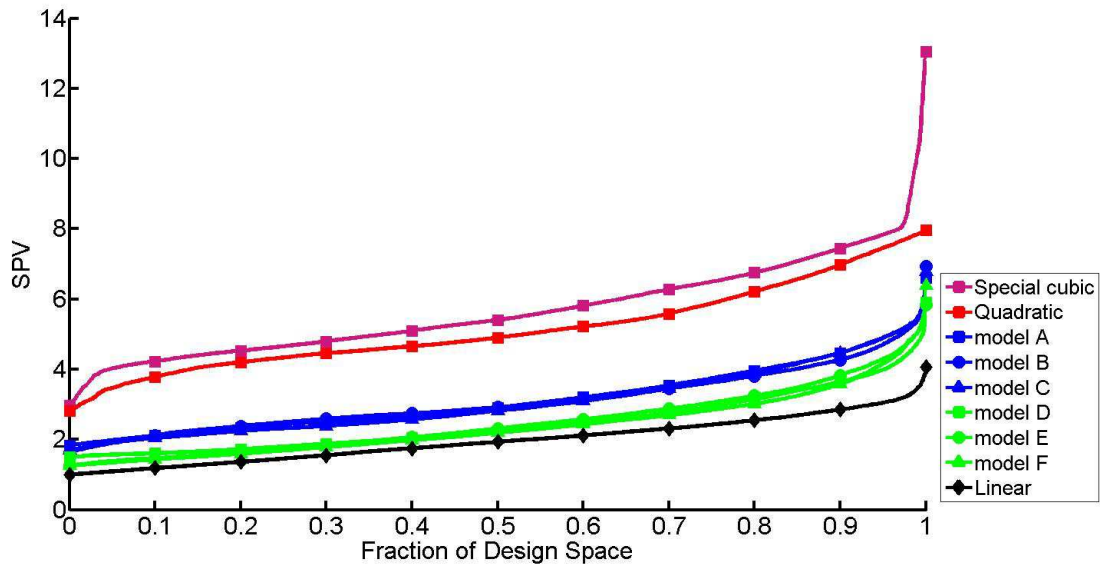


Figure 96 FDS plots for the 8MC-S-D design across several models for Snee's experiment.

We note that the curves for the special cubic, quadratic, and linear models envelop the curves for other models with the FDS curves for a larger model have at or above the curve of the nested model for all fractions of the design space. Thus, when assessing model robustness, we will restrict the study to the special cubic, quadratic, and linear models on a single FDS plot. The comparisons of the weighted D -optimal exact designs under SH and WH, and weighted G -optimal exact designs under SH and WH for each the designs are presented in Figure 97. The comparison of the weighted D -optimal exact designs under SH and WH are shown in Figure 98, and the comparison of the weighted G -optimal exact designs under SH and WH are displayed in Figure 99. The G -efficiencies of the weighted D - and G -optimal exact designs for the three model types are presented in Table 50.

In the previous section, we concluded that (1) the weighted G -optimal exact designs are superior to the weighted D -optimal exact designs; however, the 8MC-S-D and 8MS-W-D designs are competitive with the weighted G -optimal designs, (2) the weighted G -optimal exact designs under SH and WH are similarly competitive, and (3) the weighted D -optimal exact designs under SH and WH are identical.

As seen in Figure 97, for the special cubic model, for the quadratic model, and for the linear model, the weighted D -optimal exact designs under SH and WH have identical FDS curves, while the FDS curves for the weighted G -optimal exact designs under SH and WH show similar profiles. That is, the performance of the weighted D -optimal exact designs under SH and WH are comparable and the performance of the weighted G -optimal exact designs under SH and WH are comparable as well.

For the linear model, the FDS curves for the weighted D - and G -optimal exact designs are similar throughout the whole design space for $8 \leq n \leq 10$, while the FDS curves for the weighted D -optimal exact designs are lower than those for the weighted G -optimal exact designs for the part of the design space associated with the large SPV values for $11 \leq n \leq 13$. For the quadratic model, the FDS curves for the weighted G -optimal exact designs have a larger fraction of the total design space at or below the FDS curves for the weighted D -optimal exact designs. For the special cubic model, the weighted G -optimal exact designs perform better than the weighted D -optimal designs for most of the design space. At the boundary of the design space, the weighted D -optimal exact designs for the special cubic model having $8 \leq n \leq 10$ perform poorly because the SPVs increase significantly. However, for the special cubic model with $n=8$, the weighted D -optimal designs are quite competitive with the weighted G -optimal exact designs except near the boundary of the design space. For both the quadratic and special cubic models, the weighted G -optimal exact designs perform better than the weighted D -optimal designs for most of the design space because they maintain better stability for large values of SPV.

As shown in Table 50, the maximum SPVs for the weighted D -optimal exact designs under SH and WH are comparable and the maximum SPVs for the weighted G -optimal exact designs under SH and WH are quite comparable. Only the maximum SPVs for the linear model of the weighted G -optimal exact designs are higher than those of the weighted D -optimal exact designs resulting in lower G -efficiency except for $n=8$. The maximum SPVs for the quadratic and special cubic models of the weighted G -optimal exact designs are smaller than those of the weighted D -optimal exact designs, resulting in higher G -efficiency.

Figure 98 shows that the 8MC-S-D and 8MC-W-D designs have lower and flatter FDS curves for all three model types for most of the design space, while the other designs are comparable. The SPVs for the 13MC-S-D and 13MC-W-D designs do not increase sharply at the boundary. Figure 99 shows that the weighted G-optimal designs have lower and flatter FDS curves for all three model types for most of the design space. All of the weighted G-optimal exact designs are quite comparable and have good prediction variance properties.

Note that (1) the weighted *D*-optimal exact designs under SH perform as well as the weighted *D*-optimal exact designs under WH, (2) the weighted *G*-optimal exact designs under SH perform as well as the weighted *G*-optimal exact designs under WH, (3) the weighted *G*-optimal exact designs perform better than the weighted *D*-optimal exact designs for most of the design region, (4) the weighted *D*-optimal exact designs for the special cubic model having $8 \leq n \leq 10$ perform poorly at the boundary of the design space where the SPVs increase sharply, and (5) the weighted *D*-optimal and weighted *G*-optimal exact designs are quite comparable for $n=8$ for most of the design space except at the boundary of the design.

Overall, for case 3, the weighted *G*-optimal and weighted *D*-optimal exact designs appear to have good robustness properties, while the weighted *G*-optimal exact designs are more robust designs because 1) the three lines for the special cubic, quadratic, and linear models are quite similar, (2) they have much flatter and lower FDS curves for all models considered indicating a more desirable distribution of SPV values, and (3) they have good *G*-efficiencies for the special cubic model and the models nested within the special cubic model. The weighted *D*-optimal designs perform poorly for the special cubic model at the boundary of the design space; otherwise they perform well.

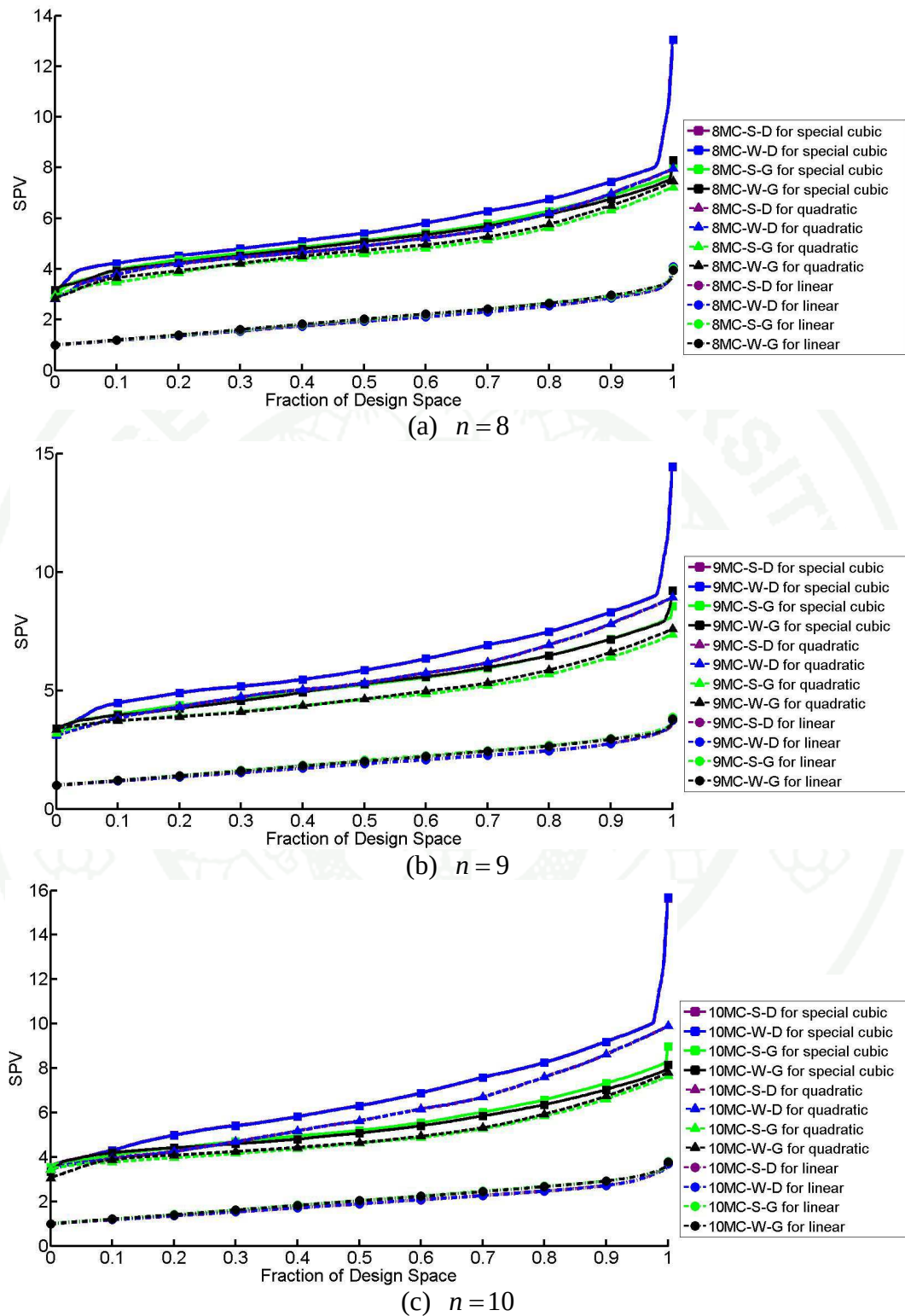


Figure 97 FDS plots for comparing the weighted D - and G -optimal exact design for three types of models assuming the special cubic model for Snee's experiment.

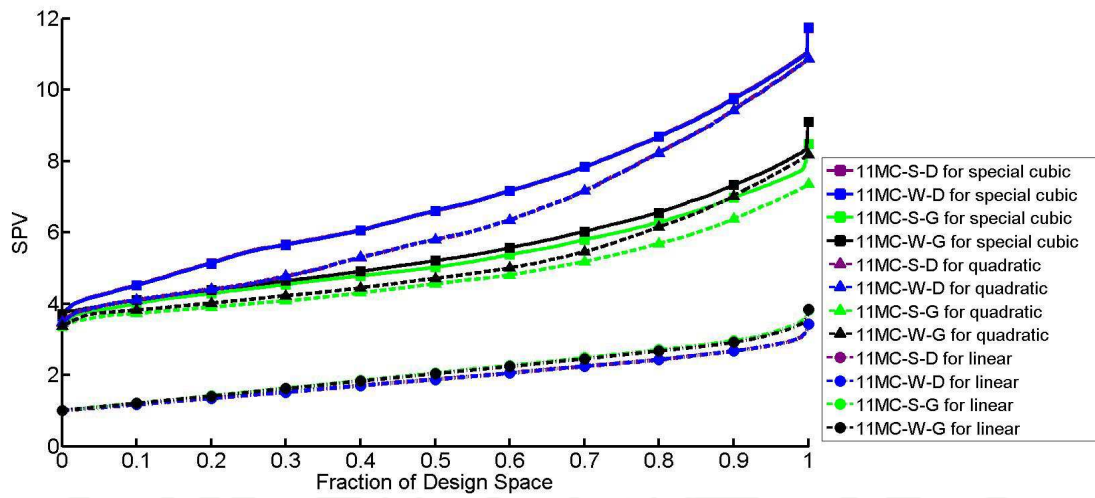
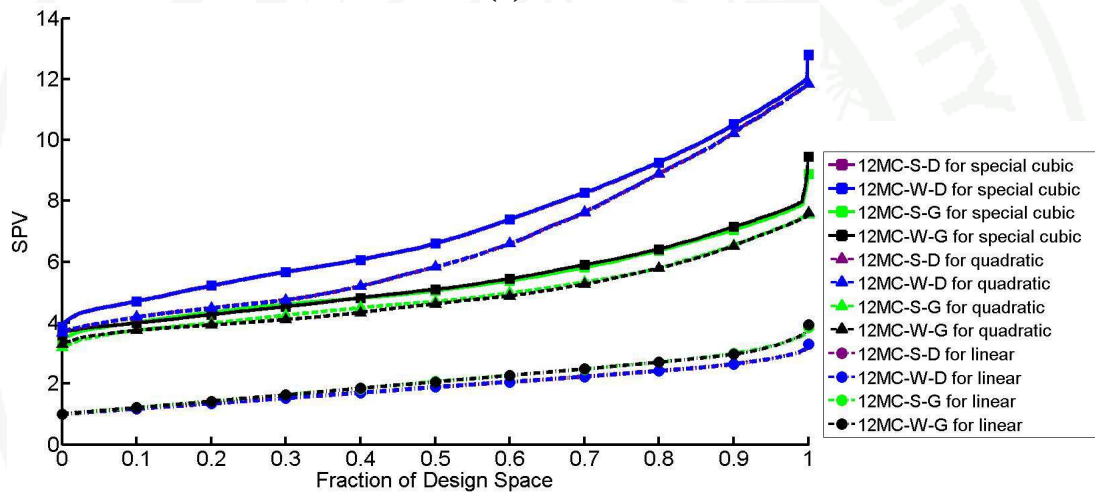
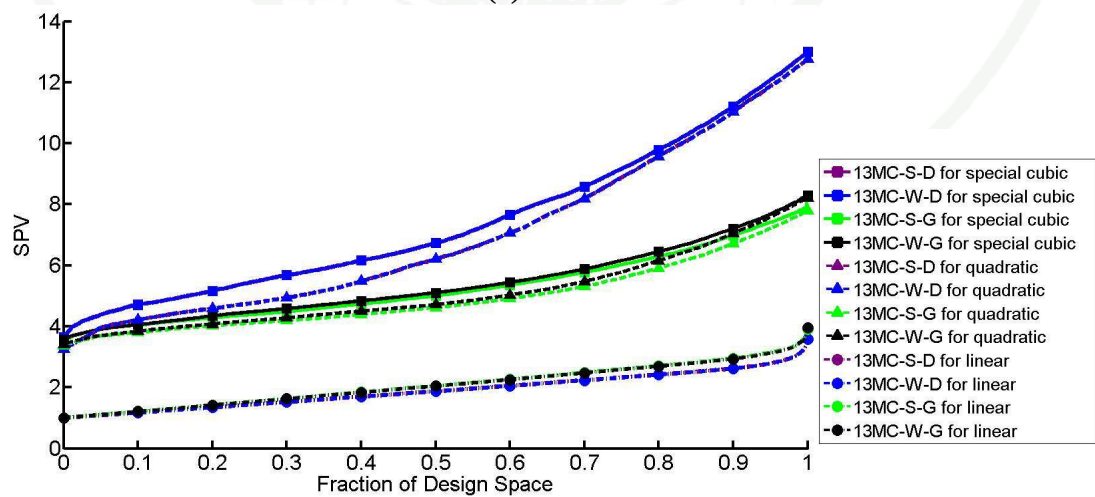
(d) $n = 11$ (e) $n = 12$ (f) $n = 13$

Figure 97 (Continued).

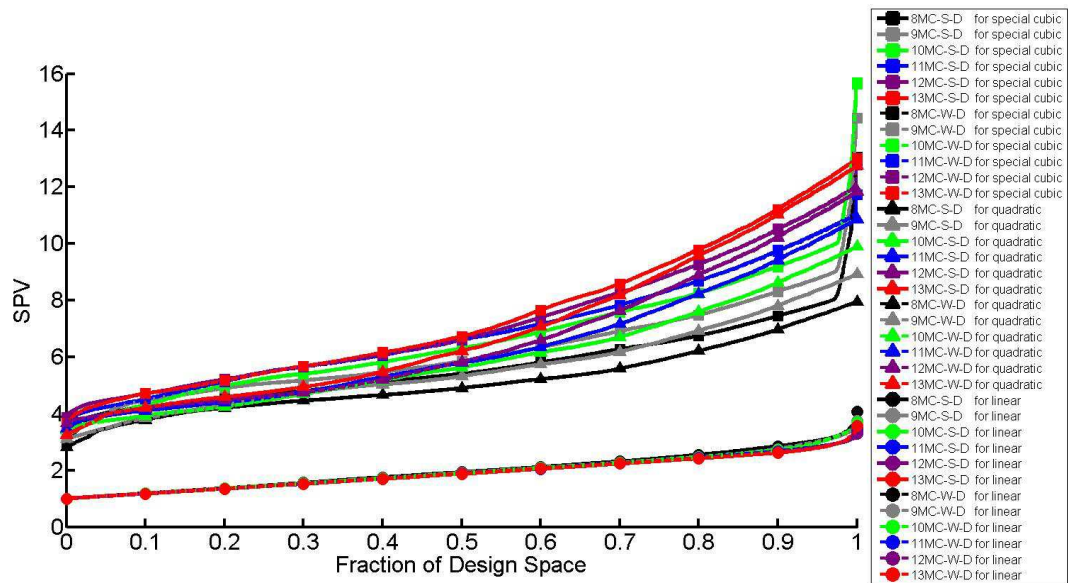


Figure 98 FDS plots for comparing the D -optimal exact designs under SH and WH for three types of models assuming the special cubic model for Snee's experiment.

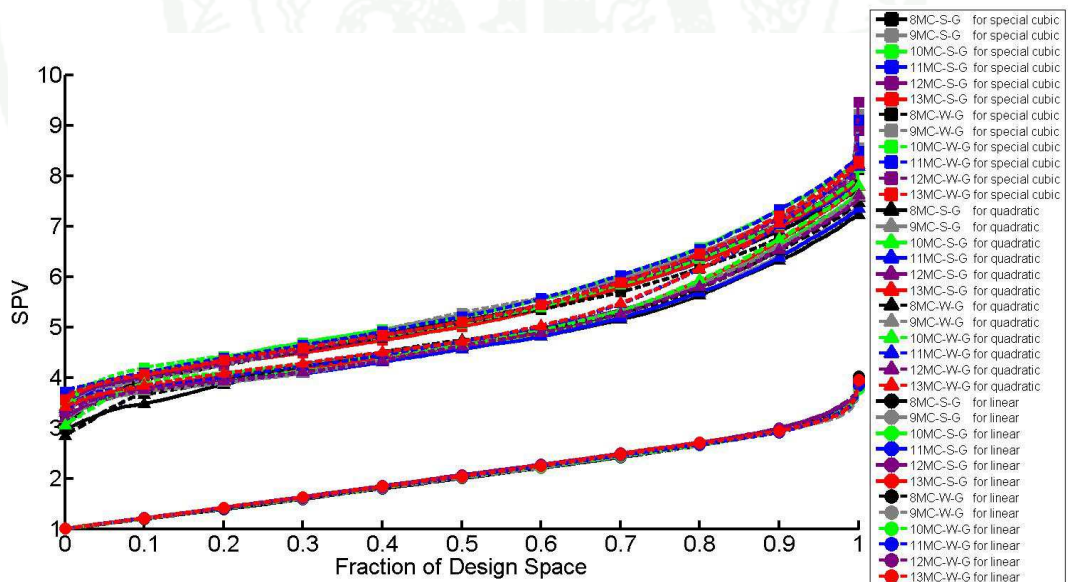


Figure 99 FDS plots for comparing the G -optimal exact designs under SH and WH for three types of models assuming the special cubic model for Snee's experiment.

Table 50 The maximum SPV values and the approximate G -efficiencies for the weighted D - and G -optimal exact designs for three model types, assuming the special cubic model for Snee's experiment.

Design	Model type	G-efficiency	Design	Model type	G-efficiency
8MC-S-D	SC	53.62	8MC-S-G	SC	86.27
	Q	75.38		Q	83.17
	L	73.66		L	74.60
9MC-S-D	SC	48.53	9MC-S-G	SC	81.80
	Q	67.25		Q	78.62
	L	80.12		L	77.51
10MC-S-D	SC	44.76	10MC-S-G	SC	78.02
	Q	60.59		Q	78.46
	L	81.41		L	79.05
11MC-S-D	SC	59.70	11MC-S-G	SC	82.55
	Q	55.17		Q	81.71
	L	87.61		L	78.53
12MC-S-D	SC	54.80	12MC-S-G	SC	78.71
	Q	50.71		Q	79.47
	L	90.87		L	77.88
13MC-S-D	SC	53.83	13MC-S-G	SC	84.96
	Q	47.01		Q	77.05
	L	83.96		L	76.59
8MC-W-D	SC	53.63	8MC-W-G	SC	84.47
	Q	75.38		Q	80.48
	L	73.59		L	76.01
9MC-W-D	SC	48.47	9MC-W-G	SC	75.97
	Q	67.18		Q	79.07
	L	80.17		L	79.02
10MC-W-D	SC	44.63	10MC-W-G	SC	85.76
	Q	60.66		Q	76.94
	L	81.30		L	79.68
11MC-W-D	SC	59.61	11MC-W-G	SC	76.92
	Q	55.26		Q	73.40
	L	87.40		L	78.23
12MC-W-D	SC	54.70	12MC-W-G	SC	74.03
	Q	50.65		Q	78.82
	L	90.74		L	76.13
13MC-W-D	SC	53.84	13MC-W-G	SC	84.42
	Q	47.02		Q	73.06
	L	83.90		L	75.96

Discussion

When an analysis of data from a mixture experiment is performed and then the initial model for which the design is chosen does not turn out to be the final model resulting from the analysis phase, the initial design may no longer have desirable prediction variance properties with respect to the final model. Therefore, the robustness of a design to model change is very critical. Model robustness means that a design performs consistently well for all possible reduced models within the largest user-specified model.

The GA presented in this dissertation is an efficient approach for the generation of highly efficient experimental designs based on weighted D - and G -optimality criteria which have desirable model-robust properties. Designs for 3 and 4 mixture component experiments are generated when the experimental region is an irregularly-shaped polyhedron. Our GA leads to the generation of near weighted D - and G -optimal exact n -point designs when using real-number encoding and well-defined genetic operators. After applying a local grid search to the points of a near weighted D - and G -optimal exact design, the weighted D - and G -optimal exact mixture designs are reported. For illustrative purposes, examples for three cases, including three and four components with only SCCs and three components with SCCs and MCCs are presented. The computations in this dissertation are performed using Matlab computational software (Matlab student version 2010a).

As in Borkowski (2003) and Atkinson *et al.* (2007), it is also assumed that (1) a design is called an *approximate* design when it is viewed as a probability measure on the design space and the number of trials for any design point is not required to be an integer and (2) the design is called an *exact* design when the number of trials for any design point is an integer. Therefore, all designs used by experimenters in practice are *exact* designs by definition. We can conclude that our algorithm produces weighted optimal *exact* n -point designs. The resulting designs are called weighted D -optimal exact designs when the designs minimize the weighted average of the volumes of the confidence ellipsoids about the model parameter estimates or,

equivalently, maximize the weighted average of the $\frac{|\mathbf{X}'\mathbf{X}|^{1/p}}{n}$ across a set of reduced models. The resulting designs are called weighted G -optimal exact designs when the designs minimize the weighted average of the maximum prediction variances throughout the design space across a set of reduced models.

The general conclusions given by Goldberg (1991), Davis (1991), Wright (1991), Michalewicz (1992), Houck *et al.* (1996) and Haupt *et al.* (2004) were that the real-value GA encoding performs well in terms of mathematical optimization problems, efficiency and quality of solutions as well as allows for the use of numerical reproduction operators. Therefore, we use the real-value encoding in this dissertation.

The values of GA parameters α_i and σ affect the speed of convergence to the optimal design and the performance of the GA. The optimal choice of α_i and σ values is in an open area and no rules currently exist for selecting those parameter values. Therefore, an appropriate choice of values of genetic parameters, such as α_i and σ , is investigated in this dissertation. We find that $0.01 \leq \alpha_b, \alpha_{bc}, \alpha_{wc} \leq 0.1$, $0.05 \leq \alpha_m \leq 0.2$, $0.1 \leq \sigma \leq 0.3$ are appropriate for all cases considered. The ranges of α_i and σ in this dissertation differ from those proposed by Borkowski (2003), Heredia-Langner *et al.* (2003, 2004), and Drain *et al.* (2004). These authors do not recommend the use of higher values of α_i and σ .

The GA presented in this dissertation generates designs by selecting points from a continuous design space. That is, the GA does not require selection of points from a user-defined candidate set of mixtures, while design-generating algorithms given by Snee and Marquardt (1974), Mitchell (1974), Snee (1979) and Cook and Nachtsheim (1980) do require selection of points from a finite subset of candidate points in the design space when generating designs. The search in a continuous design space will produce an upper bound for efficiencies that is larger than the upper bound

when the search is in a discrete design space. The computing time necessary to construct weighted D - and G -optimal exact mixture designs of the GA varies with the number of components, the number of design points, the type of model under consideration and the number of possible reduced models within the model under consideration.

For the distributional pattern of design points with the quadratic model and the special cubic model, the weighted D -optimal exact designs tend to position most design points on the design space boundary, and especially at vertices with certain vertices being replicated because the weighted average of the $\frac{|\mathbf{X}'\mathbf{X}|^{1/p}}{n}$ tends to be maximized by selection of boundary points. The weighted G -optimal exact designs, however, tend to place most design points on or near the boundary but without replication. That is, the points are scattered throughout the region because a wide distribution of points tend to minimize the weighted average of the maximum prediction variance in the design region. Note that the distribution pattern of design points for the special cubic model based on SH and WH are similar.

On the basis of prediction variance, the results imply that the weighted G -optimal exact designs are superior to the weighted D -optimal exact designs for both the quadratic model and the special cubic model, while the weighted optimal exact designs for the special cubic model under SH and WH are comparable. Weighted G -optimal exact designs include design points near the overall centroid and at interior points, while some weighted D -optimal exact designs do not include design points near the overall centroid and at interior points. These results are consistent with Smith (2005) which recommended that the designs which tend to place design points near the overall centroid and at interior points can help protect the fitted model from being underparameterized and imprecision in prediction variance.

The performance of the weighted D - and G -optimal exact designs are investigated using alphabetical optimality criteria, such as D - and G -criteria, and the prediction variance properties through the design space, such as VDGs, CVDGs and

FDS plots before examining model robustness. The results from this dissertation show that weighted optimal exact designs having design points near the overall centroid and at interior points have weighted G -efficiencies greater than 50% which can be considered as being a design with good prediction variance properties. This result corresponds to Snee (1975) who suggested that any design with G -efficiencies greater than 50% can be considered as a good design.

In this dissertation, FDS plots which show the behavior of SPV throughout the design space are adopted to study the robustness of a design to model change when the initial model does not turn out to be the final model. That is, the robust design is the model that starts with small values of SPV and remains relatively flat throughout the design space across a set of possible reduced models.

The weighted G -optimal exact designs produced by our GA tend to have better model-robust properties than the weighted D -optimal exact designs produced by our GA. The results from the quadratic model are consistent with those of the special cubic model. The weighted G -optimal exact designs, however, take more time to generate designs than the weighted D -optimal exact designs do. The weighted D -optimal exact designs are easy to obtain because they are calculated based on the determinant of information matrices which require relatively fewer computations in comparison to the weighted G -optimal exact designs which are very difficult to obtain because they involve numerical evaluation of the scaled prediction variance throughout the entire design region. Specifically, the scaled prediction variance is evaluated over the set of points from an extreme vertices design because the maximum scaled prediction variance typically occurs at one of these boundary points.

Model-robust properties of the weighted optimal exact designs under SH perform similarly to those under WH. The full models under consideration are identical and the objective functions are calculated assuming that reduced models having an equal number of model parameters receive equal weights. The weighted optimal exact designs under WH take more time to generate designs than the

weighted optimal exact designs under SH because the set of reduced models under the WH principle is larger than the set of reduced models under the SH principle.

We also find that the weighted D -optimal exact designs, which have a desirable weighted D -optimality criterion, but do not have desirable prediction variance properties, may have not model-robust properties. Therefore, we suggest that the prediction variance properties of a design should be considered before examining model robustness. It can be concluded that the best designs produced by our procedure possess good optimality criteria for their corresponding criteria, good prediction variance properties, and then good robustness properties.

CONCLUSION AND RECOMMENDATIONS

Conclusion

The research work presented in this dissertation focuses on the application of a genetic algorithm (GA) to generate model robust designs for mixture experiments having an experimental region that is an irregularly-shaped polyhedron inside a simplex. Two new versions of crossover operators and a mutation operator were developed to handle the component constraints when generating mixture designs for an irregularly-shaped polyhedron region. Additional generalizations of the weighted design optimality criteria were introduced that (1) did not require that all models should be weighted equally and (2) only models having an equal number of model parameters receive equal weight. The designs generated in this dissertation are based on optimizing the weighted D - and G -criteria over a continuous region. Several experimental situations were considered, including mixture experiments with only single component constraints (SCCs) for mixtures with three and four components, as well as mixture experiments with both SCCs and multiple component constraints (MCCs) for mixtures with three components.

The following comments and conclusions summarize this research :

1. Strategies for choosing an optimal design depend on the goal of the experimenter. The goal of the weighted D -optimal exact design is to find a set of design points for which the weighted average of the $\frac{|\mathbf{X}'\mathbf{X}|^{1/p}}{n}$ which is directly related to minimizing the average of the volumes of the confidence hyperellipsoids across all possible models is maximized, while the goal of the weighed G -optimal exact design is to find a set of design points for which the weighted average of the maximum of the prediction variance in the design region across all possible models is minimized. That is, (1) if the experimenter decides to focus on estimation of model parameters, using the weighted D -optimal exact design is the recommended choice for a design optimality criterion, or (2) if the experimenter decides to focus on precise estimation

of the mean response throughout the design space, the weighted G -optimal exact design is the recommended choice. The D - and G - weighted design optimality criteria are calculated over a subset of all possible reduced models under SH and WH principles.

2. The distributional patterns of the design points depend on many factors such as the number of components, the shape and complexity of an irregularly-shaped polyhedron region, the number of design points and the model form are employed to construct the design. From the examples presented in this dissertation, the observed distributional patterns of the design points are summarized as follows:

- For the quadratic model and special cubic model, the distributional patterns of points based on the weighted D - and G -criteria are very different. All vertices with varying replication are included for the weighted D -criterion, while the points tend to be scattered over the experimental region with unreplicated vertices for the weighted G -criterion.
- For the special cubic model, the geometries of the points under SH and WH are quite similar for the weighted D -criterion and for the weighted G -criterion.
- The majority of the design points based on the weighted D -criterion tends to be the set of all vertices but with varying replication, either edge centroid or near-edge centroids (except for Case 3), and near overall centroids (except for Case 2). Note that for weighted D -criterion and the quadratic model, when a “near edge” point appears, a “near edge” point appears for the special cubic model as well. On the other hand, if a “near edge” point does not have appear for the quadratic model, then a “near edge” point does not have appear special cubic model as well. However, the majority of design points based on the weighted G -criterion are scattered over the experimental region, including vertices or near vertices without replications, edge centroids or near edge centroids, interior points, a face or near face centroid, and a near overall centroid. Good designs based on the weighted D -criterion tend to

minimize the weighted average of the $\frac{|\mathbf{X}'\mathbf{X}|^{1/p}}{n}$, while good designs based on the weighted G -criterion tend to minimize the weighted average of the maximum prediction variance in the design region.

3. To find the weighted optimal exact designs, the objective function values are used to calculate the relative efficiency of any set of design points. By definition, for the quadratic and special cubic models, the weighted D - and G -optimal exact designs should have 100% relative efficiencies for their corresponding criterion. The weighted G -optimal exact designs are summarized as follows: (1) the weighted G -optimal exact designs under SH or WH have 100% relative efficiencies for their corresponding criterion and (2) the weighted G -optimal exact designs under SH or WH will not have 100% relative efficiencies for their corresponding criterion (that is, the weighted G -optimal exact designs under SH are identical to the weighted G -optimal exact designs under WH); however the objective function values of the weighted G -optimal exact designs under SH are very close to those under WH. Theoretically, the relative efficiencies should be 100%, but the GA terminated before finding the true weighted optimal exact designs under SH and WH.

4. As the number of design points increases, the objective function values of the weighted D -optimal exact designs also increase. However, as the number of design points increases, the objective function values of the weighted G -optimal exact designs only show an insignificant improvement. Note that if a design has no interior points, no point on the faces, and, thus no near overall centroid, then that design does not have good prediction variance properties and has a larger maximum SPV. The results from the CVDGs indicate that if a design does not have good prediction variance properties, then additional points should be included near the overall centroid, near a face centroid, or at an interior point to provide a significant improvement in the maximum prediction variance.

5. If the experimenter is concerned with protecting against the worst-case for prediction variance values, then minimizing the maximum SPV is suggested as the

criterion for consideration. For the quadratic model and special cubic model, the weighted G -optimal exact designs outperform the weighted D -optimal exact designs with respect to the maximum SPV. For the special cubic model, the weighted D -optimal exact designs under SH and WH are quite comparable with respect to the maximum SPV, while the weighted G -optimal exact designs under SH and WH are quite comparable with respect to the maximum SPV as well. When the experimenter is interested in the weighted D -optimal exact designs, the experimenter should still carefully consider the maximum SPV for a design selection. Note that if a design has no interior points, and thus, no near overall centroid, then it has a larger maximum SPV. A design having a large maximum SPV can be improved by adding the mixture $(x_1, x_2, \dots, x_q)$ at the location where the maximum SPV occurs. This location corresponds to the mixture proportions that are located at the peaks in the CVDG .

6. To evaluate designs with respect to an alphabetic optimality criterion, the weighted D - and G - optimality criteria are considered in this dissertation. Recall that large weighted D - and G -efficiencies are desirable. For the quadratic model and special cubic model, the weighted D -efficiency for the weighted D -optimal exact designs is larger than it is for the weighted G -optimal exact designs, while the weighted G -efficiency for the weighted G -optimal exact designs is larger than it is for the weighted D -optimal exact designs. For the special cubic model, the weighted D -efficiency under SH and WH are quite comparable for weighted D -optimal exact designs, while the weighted G -efficiency under SH and WH are quite comparable for weighted G -optimal exact designs as well. Note that a design that is generated based on one criterion always performs well when evaluated by that criterion.

7. Recall that larger is better for D_w , $D_w - S$, $D_w - W$, G_w , $G_w - S$ and $G_w - W$. For the quadratic model, the weighted D -optimal exact designs which include a near overall centroid and points on the faces have high G_w values, while the weighted G -optimal exact designs have high D_w values. For the special cubic model, the weighted D -optimal exact designs under SH have high $D_w - W$ values but quite

low $G_w - S$ and $G_w - W$ values, while the weighted D -optimal exact designs under WH have high $D_w - S$ values but quite low $G_w - S$ and $G_w - W$ values. On the other hand, the weighted G -optimal exact designs under SH have high $G_w - W$, $D_w - S$ and $D_w - W$ values, whereas the weighted G -optimal exact designs under WH have large $G_w - S$, $D_w - S$ and $D_w - W$ values. Note that the designs which are generated based on one optimality criterion may perform poorly when evaluated by another criterion. Therefore, the experimenter should be aware that the choice of design may be dependent on the choice of an evaluation criterion.

8. To evaluate designs with respect to prediction variance properties, graphical approaches (specifically the VDGs, FDS plots, and CVDGs), were used. The designs having no interior points, no points on the faces, and thus, no near overall centroid have poorer prediction variance properties. For the quadratic model and special cubic model, the weighted G -optimal exact designs have better prediction variance properties than the weighted D -optimal exact designs. The weighted D - and G -optimal exact designs are quite comparable at the design center; however the weighted D -optimal exact designs are no longer competitive at the boundary of the region. That is, the weighted G -optimal designs outperform the weighted D -optimal exact designs near the boundary. For the special cubic model, excluding the worst-case designs, the weighted optimal exact designs under SH and WH are comparable with respect to prediction variance properties. The worst-case designs with respect to the maximum SPV come from only the weighted D -optimal exact designs. Note that the worst-case designs for Case 1 have no near overall centroid, while the worst-case designs for Case 2 have two points near one vertex and no near overall centroid. As the number of design points increases, there is no significant improvement in the prediction variance properties. From the CVDGs, the worst cases of the weighted D -optimal exact designs have the maximum SPV near the overall centroid, or on a face or near a face centroid. Therefore, if the experimenter would like to improve the design, the experimenter should add the mixture $(x_1, x_2, \dots, x_q)$ at which the maximum SPV occurs.

9. When comparing model robustness with the special cubic model, the weighted *D*-optimal exact designs under SH and WH are quite comparable, while the weighted *G*-optimal exact designs under SH and WH are quite comparable as well. When comparing model robustness with the quadratic model and special cubic model, the weighted *D*- and *G*-optimal exact designs, excluding the worst-case designs with respect to the maximum SPV, appear to have good robustness properties. However, the weighted *G*-optimal exact designs are recommended for model robustness over the weighted *D*-optimal exact designs. Note that the designs that have good prediction variance properties and lower the maximum SPV possess good robustness properties. Therefore, the performance of a design with respect to prediction variance properties should also be investigated when examining model robustness. If the experimenter believes that the initial model will not turn out to be the final model after analysis of the experimental data, and the weighted *D*-optimal exact design is considered, then the experimenter should be very cautious when choosing a design. However, if the initial model does not turn out to be the final model, then the weighted *G*-optimal exact designs are suggested because it protects against having a final model with poor prediction variance properties.

Recommendations

The work described in this dissertation has the following potential extensions in several directions for future research:

1. The GA which is presented in this dissertation can be extended to generate designs with more than four components where the experimental region is an irregularly-shaped polyhedral region. The computation time may be dramatically increased because the number of reduced models and dimension of $\mathbf{X}'\mathbf{X}$ increase. Therefore, developing a more time-efficient algorithm for higher dimensional problems can be explored when an experiment requires a larger number of mixture components.

2. Our GA can be extended to consider other objective functions, such as weighted A- and IV-optimality criteria. The GA would produce weighted A- or IV-optimal exact mixture designs. The goal of weighted A-optimality is to minimize the weighted average of the sum of the variances of the model parameter estimates over a set of reduced models which is equivalent to minimizing the weighted average of the trace $\left[(\mathbf{X}'\mathbf{X})^{-1} \right]$ across a set of reduced models, while the goal of weighted IV-optimality is to minimize the weighted average of the average prediction variance in the design region across a set of reduced models which is equivalent to minimizing the weighted average of the average of the scaled prediction variance $\left(n\mathbf{x}_m' (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_m \right)$ over the design region across a set of reduced models. We then modify the GA to generate model robust design with respect to these criteria.

3. In many industrial processes, the response may not only depend on the proportion of the mixture components but also on experimental conditions related to process variables. Common process variables are temperature, processing time, mixing time, and other settings of equipment used in the process, which can be set independently of the component proportions in the mixture but can affect the blending properties of the mixture. The GA that is presented in this dissertation can be extended to generate mixture designs which include both mixture components and process variables. Therefore, the GA can be extended to consider robust mixture designs that include process variables.

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APPENDICES

The seal of Kasetsart University is a large, light green circular emblem in the background. It features the university's name in Thai script at the top, a central figure of a deity or royal figure, and the year 1943 at the bottom.

Appendix A

The most fit designs via GA and the optimal exact designs for the poultry experiment.

Appendix Table A1 The most fit designs via GA and the optimal exact design with 7-points based on D -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.0000	0.2000	0.8000	0.2000	0.0000
0.8000	0.2000	0.0000	0.7000	0.3000	0.0000
0.3000	0.2000	0.5000	0.8000	0.0000	0.2000
0.3000	0.3000	0.4000	0.3000	0.2000	0.5000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.7000	0.3000	0.0000	0.3000	0.3000	0.4000
$D_w = 0.910121$			$D_w = 0.910121$		

Appendix Table A2 The most fit designs via GA and the optimal exact design with 8-points based on D -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
$D_w = 0.908224$			$D_w = 0.908224$		

Appendix Table A3 The most fit designs via GA and the optimal exact design with 9-points based on D -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5050	0.3000	0.1950	0.5000	0.3000	0.2000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$D_w = 0.917581$			$D_w = 0.917644$		

Appendix Table A4 The most fit designs via GA and the optimal exact design with 10-points based on D -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5658	0.1632	0.2710	0.5680	0.1641	0.2679
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$D_w = 0.918343$			$D_w = 0.918352$		

Appendix Table A5 The most fit designs via GA and the optimal exact design with 11-points based on D -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.5400	0.3000	0.1600	0.5388	0.3000	0.1612
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.5700	0.1600	0.2700	0.5695	0.1614	0.2691
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
$D_w = 0.919214$			$D_w = 0.919218$		

Appendix Table A6 The most fit designs via GA and the optimal exact design with 12-points based on D -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5700	0.1600	0.2700	0.5713	0.1573	0.2714
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$D_w = 0.924121$			$D_w = 0.924131$		

Appendix Table A7 The most fit designs via GA and the optimal exact design with 7-points based on G -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3293	0.3000	0.3707	0.3215	0.3000	0.3785
0.3196	0.1804	0.5000	0.3300	0.1700	0.5000
0.5800	0.1500	0.2700	0.5719	0.1611	0.2670
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.6555	0.3000	0.0445	0.6566	0.3000	0.0434
$G_w = 79.7656$			$G_w = 80.2307$		

Appendix Table A8 The most fit designs via GA and the optimal exact design with 8-points based on G -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.6236	0.1069	0.2695	0.6168	0.0664	0.3168
0.6900	0.3000	0.0100	0.7000	0.3000	0.0000
0.3500	0.1500	0.5000	0.3357	0.1643	0.5000
0.5373	0.2927	0.1700	0.5199	0.2602	0.2199
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.1800	0.0200	0.8000	0.1643	0.0357
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
$G_w = 77.9279$			$G_w = 81.0509$		

Appendix Table A9 The most fit designs via GA and the optimal exact design with 9-points based on G -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.8000	0.1866	0.0134	0.8000	0.1766	0.0234
0.4304	0.3000	0.2696	0.5000	0.3000	0.2000
0.5861	0.1632	0.2507	0.5841	0.1464	0.2695
0.3000	0.2900	0.4100	0.3000	0.3000	0.4000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.3384	0.1616	0.5000	0.3243	0.1757	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.6734	0.0046	0.3220	0.6500	0.0000	0.3500
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$G_w=77.5300$			$G_w=80.4382$		

Appendix Table A10 The most fit designs via GA and the optimal exact design with 10-points based on G -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.4451	0.0600	0.4949	0.4619	0.0567	0.4814
0.5700	0.1500	0.2800	0.5763	0.1596	0.2641
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.4867	0.2828	0.2305	0.4838	0.2894	0.2268
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.7793	0.2185	0.0022	0.7837	0.2163	0.0000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.0700	0.1300	0.8000	0.0642	0.1358
$G_w=79.3559$			$G_w=80.9403$		

Appendix Table A11 The most fit designs via GA and the optimal exact design with 11-points based on G -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.6742	0.0100	0.3158	0.6822	0.0000	0.3178
0.7965	0.0929	0.1106	0.7564	0.1079	0.1357
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5500	0.2900	0.1600	0.5512	0.3000	0.1488
0.4157	0.0843	0.5000	0.4192	0.0808	0.5000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.3000	0.2358	0.4642	0.3000	0.2349	0.4651
0.5500	0.1600	0.2900	0.5462	0.1659	0.2879
$G_w = 76.1713$			$G_w = 78.4854$		

Appendix Table A12 The most fit designs via GA and the optimal exact design with 12-points based on G -criterion assuming the quadratic model for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.6799	0.2467	0.0734	0.6689	0.2586	0.0725
0.3600	0.1800	0.4600	0.4029	0.1734	0.4237
0.7997	0.0405	0.1598	0.8000	0.0360	0.1640
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5600	0.1600	0.2800	0.5852	0.1493	0.2655
0.5300	0.0100	0.4600	0.4693	0.0307	0.5000
0.7100	0.2900	0.0000	0.7000	0.3000	0.0000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.7893	0.2107	0.0000	0.8000	0.2000	0.0000
0.4675	0.3000	0.2325	0.4208	0.3000	0.2792
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$G_w = 73.5764$			$G_w = 76.9692$		

Appendix Table A13 The most fit designs via GA and the optimal exact design with 8-points based on D -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5900	0.1200	0.2900	0.5911	0.1177	0.2912
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
$D_w = 0.603485$			$D_w = 0.603490$		

Appendix Table A14 The most fit designs via GA and the optimal exact design with 9-points based on D -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5972	0.1328	0.2700	0.5957	0.1329	0.2714
$D_w = 0.605693$			$D_w = 0.605695$		

Appendix Table A15 The most fit designs via GA and the optimal exact design with 10-points based on D -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.5754	0.1478	0.2768	0.5765	0.1470	0.2765
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$D_w = 0.614326$			$D_w = 0.614327$		

Appendix Table A16 The most fit designs via GA and the optimal exact design with 11-points based on D -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5228	0.3000	0.1772	0.5247	0.3000	0.1753
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5789	0.1461	0.2750	0.5785	0.1445	0.2770
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
$D_w = 0.614187$			$D_w = 0.614196$		

Appendix Table A17 The most fit designs via GA and the optimal exact design with 12-points based on D -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5800	0.1400	0.2800	0.5792	0.1416	0.2792
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
$D_w = 0.617569$			$D_w = 0.617572$		

Appendix Table A18 The most fit designs via GA and the optimal exact design with 13-points based on D -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5700	0.1400	0.2900	0.5773	0.1400	0.2827
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.4900	0.3000	0.2100	0.5025	0.3000	0.1975
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$D_w = 0.615383$			$D_w = 0.615610$		

Appendix Table A19 The most fit designs via GA and the optimal exact design with 8-points based on D -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5879	0.1321	0.2800	0.5873	0.1312	0.2815
$D_w = 0.545553$			$D_w = 0.545554$		

Appendix Table A20 The most fit designs via GA and the optimal exact design with 9-points based on D -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5900	0.1400	0.2700	0.5905	0.1456	0.2639
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
$D_w = 0.548367$			$D_w = 0.548413$		

Appendix Table A21 The most fit designs via GA and the optimal exact design with 10-points based on D -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5700	0.1600	0.2700	0.5698	0.1608	0.2694
$D_w = 0.556032$			$D_w = 0.556033$		

Appendix Table A22 The most fit designs via GA and the optimal exact design with 11-points based on D -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.4800	0.3000	0.2200	0.4794	0.3000	0.2206
0.5700	0.1600	0.2700	0.5703	0.1585	0.2712
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
$D_w = 0.557230$			$D_w = 0.557233$		

Appendix Table A23 The most fit designs via GA and the optimal exact design with 12-points based on D -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5748	0.1574	0.2678	0.5735	0.1550	0.2715
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
$D_w = 0.560806$			$D_w = 0.560818$		

Appendix Table A24 The most fit designs via GA and the optimal exact design with 13-points based on D -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5739	0.1556	0.2705	0.5773	0.1542	0.2685
0.4966	0.3000	0.2034	0.4982	0.3000	0.2018
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
$D_w = 0.557857$			$D_w = 0.557868$		

Appendix Table A25 The most fit designs via GA and the optimal exact design with 8-points based on G -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5400	0.1300	0.3300	0.5538	0.1137	0.3325
0.5300	0.3000	0.1700	0.5470	0.3000	0.1530
0.8000	0.1000	0.1000	0.8000	0.1000	0.1000
0.3600	0.1500	0.4900	0.3408	0.1592	0.5000
0.7500	0.0000	0.2500	0.7571	0.0000	0.2429
0.5094	0.0000	0.4906	0.5154	0.0000	0.4846
0.3002	0.2998	0.4000	0.3000	0.3000	0.4000
0.7300	0.2700	0.0000	0.7260	0.2740	0.0000
$G_w = 70.6078$			$G_w = 72.7775$		

Appendix Table A26 The most fit designs via GA and the optimal exact design with 9-points based on G -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.4879	0.3000	0.2121	0.5000	0.3000	0.2000
0.6400	0.0000	0.3600	0.6500	0.0000	0.3500
0.4926	0.0074	0.5000	0.5000	0.0000	0.5000
0.5700	0.1470	0.2830	0.5599	0.1786	0.2615
0.3045	0.1955	0.5000	0.3227	0.1773	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.8000	0.1700	0.0300	0.8000	0.1772	0.0228
0.3100	0.3000	0.3900	0.3000	0.3000	0.4000
$G_w = 81.1388$			$G_w = 85.3896$		

Appendix Table A27 The most fit designs via GA and the optimal exact design with 10-points based on G -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.4900	0.3000	0.2100	0.4865	0.3000	0.2135
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7994	0.1124	0.0882	0.7976	0.1124	0.0900
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.6300	0.0000	0.3700	0.6309	0.0000	0.3691
0.5779	0.1789	0.2432	0.5841	0.1732	0.2427
0.3193	0.1807	0.5000	0.3193	0.1807	0.5000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$G_w = 79.6723$			$G_w = 79.8722$		

Appendix Table A28 The most fit designs via GA and the optimal exact design with 11-points based on G -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.4900	0.0500	0.4600	0.4936	0.0593	0.4471
0.6995	0.3000	0.0005	0.7000	0.3000	0.0000
0.4900	0.0100	0.5000	0.5000	0.0000	0.5000
0.4924	0.3000	0.2076	0.5045	0.3000	0.1955
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.3000	0.2015	0.4985	0.3000	0.2034	0.4966
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.6495	0.0000	0.3505	0.6600	0.0000	0.3400
0.5793	0.1795	0.2412	0.5384	0.1946	0.2670
0.8000	0.0700	0.1300	0.8000	0.0738	0.1262
$G_w = 76.2473$			$G_w = 78.2705$		

Appendix Table A29 The most fit designs via GA and the optimal exact design with 12-points based on G -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2200	0.4800	0.3000	0.2319	0.4681
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.5300	0.3000	0.1700	0.5380	0.3000	0.1620
0.5908	0.1092	0.3000	0.6020	0.0980	0.3000
0.4126	0.0875	0.4999	0.4137	0.0863	0.5000
0.6343	0.0000	0.3657	0.6454	0.0000	0.3546
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.0399	0.1601	0.8000	0.0800	0.1200
0.7927	0.2073	0.0000	0.7816	0.2184	0.0000
0.5124	0.2560	0.2316	0.4928	0.2544	0.2528
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$G_w = 77.4266$			$G_w = 80.5527$		

Appendix Table A30 The most fit designs via GA and the optimal exact design with 13-points based on G -criterion assuming the special cubic model under SH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.4271	0.2958	0.2771	0.4248	0.3000	0.2752
0.4200	0.0800	0.5000	0.4029	0.0971	0.5000
0.5631	0.1591	0.2778	0.5744	0.1666	0.2590
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.6034	0.0023	0.3943	0.6041	0.0000	0.3959
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.5764	0.2994	0.1242	0.6029	0.3000	0.0971
0.7200	0.0400	0.2400	0.6698	0.0550	0.2752
0.7869	0.0940	0.1191	0.8000	0.0627	0.1373
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3000	0.2100	0.4900	0.3000	0.2237	0.4763
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
$G_w = 75.9085$			$G_w = 79.5852$		

Appendix Table A31 The most fit designs via GA and the optimal exact design with 8-points based on G -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.7334	0.2666	0.0000	0.7032	0.2968	0.0000
0.3388	0.1795	0.4817	0.3531	0.1469	0.5000
0.7391	0.0000	0.2609	0.7780	0.0000	0.2220
0.5217	0.1458	0.3325	0.6028	0.0928	0.3044
0.5523	0.3000	0.1477	0.5048	0.3000	0.1952
0.8000	0.0900	0.1100	0.8000	0.1444	0.0556
0.3076	0.2998	0.3926	0.3000	0.3000	0.4000
0.5084	0.0027	0.4889	0.5209	0.0000	0.4791
$G_w = 68.5531$			$G_w = 76.4169$		

Appendix Table A32 The most fit designs via GA and the optimal exact design with 9-points based on G -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5155	0.3000	0.1845	0.5030	0.3000	0.1970
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.6500	0.0000	0.3500	0.6500	0.0000	0.3500
0.5600	0.1800	0.2600	0.5659	0.1657	0.2684
0.3200	0.1800	0.5000	0.3173	0.1827	0.5000
0.8000	0.1789	0.0211	0.8000	0.1826	0.0174
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
$G_w = 83.1989$			$G_w = 83.4761$		

Appendix Table A33 The most fit designs via GA and the optimal exact design with 10-points based on G -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.5865	0.1535	0.2600	0.5678	0.1637	0.2685
0.8000	0.2000	0.0000	0.8000	0.2000	0.0000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.8000	0.1200	0.0800	0.8000	0.1089	0.0911
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.3170	0.1830	0.5000	0.3168	0.1832	0.5000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.4976	0.0024	0.5000	0.4964	0.0036	0.5000
0.6300	0.0000	0.3700	0.6166	0.0000	0.3834
$G_w = 77.6776$			$G_w = 78.0611$		

Appendix Table A34 The most fit designs via GA and the optimal exact design with 11-points based on G -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.6700	0.0000	0.3300	0.6583	0.0000	0.3417
0.4100	0.1000	0.4900	0.4193	0.1000	0.4807
0.5000	0.3000	0.2000	0.5000	0.3000	0.2000
0.6900	0.3000	0.0100	0.6755	0.3000	0.0245
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5437	0.1828	0.2735	0.5522	0.1828	0.2650
0.7545	0.2455	0.0000	0.7379	0.2621	0.0000
0.3000	0.2298	0.4702	0.3000	0.2220	0.4780
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.8000	0.1200	0.0800	0.8000	0.1384	0.0616
$G_w = 77.3873$			$G_w = 77.9426$		

Appendix Table A35 The most fit designs via GA and the optimal exact design with 12-points based on G -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3000	0.2000	0.5000	0.3000	0.2000	0.5000
0.6600	0.0000	0.3400	0.6656	0.0000	0.3344
0.4590	0.0410	0.5000	0.4258	0.0742	0.5000
0.7600	0.2400	0.0000	0.7615	0.2385	0.0000
0.4800	0.2600	0.2600	0.5347	0.2642	0.2011
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.8000	0.1000	0.1000	0.8000	0.1000	0.1000
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
0.4387	0.3000	0.2613	0.4303	0.3000	0.2697
0.5847	0.1127	0.3026	0.5884	0.1087	0.3029
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
$G_w = 76.9225$			$G_w = 78.8811$		

Appendix Table A36 The most fit designs via GA and the optimal exact design with 13-points based on G -criterion assuming the special cubic model under WH for the poultry experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.6100	0.0300	0.3600	0.5955	0.0450	0.3595
0.5700	0.1600	0.2700	0.5654	0.1587	0.2759
0.4100	0.0900	0.5000	0.4326	0.0674	0.5000
0.4048	0.3000	0.2952	0.4093	0.3000	0.2907
0.7946	0.0844	0.1210	0.8000	0.0784	0.1216
0.6595	0.0000	0.3405	0.6737	0.0000	0.3263
0.3000	0.3000	0.4000	0.3000	0.3000	0.4000
0.5593	0.3000	0.1407	0.5851	0.3000	0.1149
0.8000	0.0000	0.2000	0.8000	0.0000	0.2000
0.3006	0.2127	0.4867	0.3000	0.2137	0.4863
0.5000	0.0000	0.5000	0.5000	0.0000	0.5000
0.7700	0.2300	0.0000	0.7800	0.2200	0.0000
0.7000	0.3000	0.0000	0.7000	0.3000	0.0000
$G_w = 75.6435$			$G_w = 78.3922$		

The seal of Kasetsart University is a large, light green circular emblem in the background. It features the university's name in Thai script at the top, a central figure of a deity or royal figure, and the year 1943 at the bottom.

Appendix B

The most fit designs via GA and the optimal exact designs for the flare experiment.

Appendix Table B1 The most fit designs via GA and the optimal exact design with 11-points based on D -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.1000	0.4300	0.0700	0.4000	0.1000	0.4307	0.0693
0.4000	0.2816	0.2884	0.0300	0.4000	0.2843	0.2857	0.0300
0.6000	0.2175	0.1030	0.0795	0.6000	0.2200	0.1000	0.0800
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.5046	0.3654	0.1000	0.0300	0.5104	0.3596	0.1000	0.0300
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
$D_w=0.080514$				$D_w=0.080757$			

Appendix Table B2 The most fit designs via GA and the optimal exact design with 12-points based on D -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2200	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.5969	0.1000	0.2231	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.4196	0.1004	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.2889	0.2811	0.0300	0.4000	0.2836	0.2864	0.0300
0.4000	0.1000	0.4569	0.0431	0.4000	0.1000	0.4312	0.0688
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.5200	0.3500	0.1000	0.0300	0.5127	0.3573	0.1000	0.0300
$D_w=0.080663$				$D_w=0.080990$			

Appendix Table B3 The most fit designs via GA and the optimal exact design with 13-points based on D -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.5500	0.1000	0.3100	0.0400	0.5386	0.1000	0.3176	0.0438
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.2800	0.2900	0.0300	0.4000	0.2834	0.2866	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.5997	0.1000	0.2203	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.4153	0.1047	0.0800	0.4000	0.4200	0.1000	0.0800
0.5998	0.2202	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.5236	0.3464	0.1000	0.0300	0.5189	0.3511	0.1000	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
$D_w = 0.080828$				$D_w = 0.081060$			

Appendix Table B4 The most fit designs via GA and the optimal exact design with 14-points based on D -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.1003	0.4200	0.0797	0.4000	0.1000	0.4200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.2900	0.2800	0.0300	0.4000	0.2912	0.2788	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.5997	0.1003	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.5900	0.1000	0.2700	0.0400	0.5871	0.1000	0.2700	0.0429
0.6000	0.2204	0.1000	0.0796	0.6000	0.2200	0.1000	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.4198	0.1002	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5082	0.3618	0.1000	0.0300	0.5120	0.3580	0.1000	0.0300
$D_w = 0.081396$				$D_w = 0.081560$			

Appendix Table B5 The most fit designs via GA and the optimal exact design with 15-points based on D -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5999	0.2191	0.1010	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2600	0.1000	0.0400	0.6000	0.2563	0.1000	0.0437
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4023	0.4177	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.5213	0.1000	0.3487	0.0300	0.5243	0.1000	0.3457	0.0300
0.4000	0.2899	0.2801	0.0300	0.4000	0.2859	0.2841	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
$D_w = 0.081952$				$D_w = 0.082119$			

Appendix Table B6 The most fit designs via GA and the optimal exact design with 16-points based on D -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.5999	0.1000	0.2201	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.2984	0.2716	0.0300	0.4000	0.2864	0.2836	0.0300
0.4000	0.2706	0.2766	0.0528	0.4000	0.2728	0.2721	0.0551
0.5989	0.2211	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.4192	0.1008	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.5250	0.1000	0.3450	0.0300	0.5232	0.1000	0.3468	0.0300
0.4011	0.1000	0.4189	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
$D_w = 0.082394$				$D_w = 0.082530$			

Appendix Table B7 The most fit designs via GA and the optimal exact design with 11-points based on G -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.5998	0.1500	0.1702	0.0800	0.6000	0.1467	0.1733	0.0800
0.4280	0.3800	0.1120	0.0800	0.4374	0.3826	0.1000	0.0800
0.4008	0.1100	0.4092	0.0800	0.4000	0.1000	0.4200	0.0800
0.5357	0.3326	0.1017	0.0300	0.5452	0.3248	0.1000	0.0300
0.4026	0.2875	0.2799	0.0300	0.4000	0.2760	0.2940	0.0300
0.6000	0.2500	0.1000	0.0500	0.6000	0.2450	0.1000	0.0550
0.5100	0.1000	0.3300	0.0600	0.5067	0.1000	0.3291	0.0642
0.5974	0.1000	0.2726	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.4654	0.1006	0.0340	0.4000	0.4685	0.1000	0.0315
0.4003	0.1000	0.4697	0.0300	0.4000	0.1000	0.4700	0.0300
0.4079	0.3380	0.1853	0.0688	0.4000	0.3726	0.1584	0.0690
$G_w = 64.6127$				$G_w = 71.7332$			

Appendix Table B8 The most fit designs via GA and the optimal exact design with 12-points based on G -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.3126	0.2574	0.0300	0.4000	0.2867	0.2833	0.0300
0.4591	0.3609	0.1000	0.0800	0.5028	0.3172	0.1000	0.0800
0.5475	0.1000	0.2725	0.0800	0.5880	0.1000	0.2320	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2178	0.1100	0.0722	0.6000	0.2345	0.1000	0.0655
0.4000	0.1265	0.3935	0.0800	0.4000	0.1000	0.4200	0.0800
0.4006	0.3352	0.1843	0.0799	0.4000	0.3883	0.1317	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.5600	0.3100	0.1000	0.0300	0.5716	0.2984	0.1000	0.0300
0.4300	0.4074	0.1057	0.0569	0.4000	0.3887	0.1532	0.0581
0.4600	0.1448	0.3400	0.0552	0.4892	0.1190	0.3438	0.0480
$G_w = 60.8486$				$G_w = 73.2223$			

Appendix Table B9 The most fit designs via GA and the optimal exact design with 13-points based on G -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.4400	0.1017	0.0583	0.4000	0.4500	0.1000	0.0500
0.4000	0.3102	0.2597	0.0301	0.4000	0.2884	0.2816	0.0300
0.6000	0.1127	0.2077	0.0796	0.6000	0.1000	0.2230	0.0770
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4323	0.3877	0.1000	0.0800	0.4077	0.4123	0.1000	0.0800
0.4108	0.1023	0.4569	0.0300	0.4192	0.1000	0.4508	0.0300
0.4000	0.1000	0.4400	0.0600	0.4000	0.1000	0.4444	0.0556
0.5194	0.1947	0.2335	0.0524	0.5045	0.2289	0.2187	0.0479
0.4909	0.1000	0.3291	0.0800	0.4932	0.1000	0.3268	0.0800
0.4200	0.4489	0.1010	0.0301	0.4228	0.4472	0.1000	0.0300
0.6000	0.2679	0.1021	0.0300	0.6000	0.2700	0.1000	0.0300
0.4026	0.1827	0.3347	0.0800	0.4000	0.1564	0.3636	0.0800
0.5615	0.2585	0.1000	0.0800	0.5838	0.2362	0.1000	0.0800
$G_w = 62.8829$				$G_w = 68.7614$			

Appendix Table B10 The most fit designs via GA and the optimal exact design with 14-points based on G -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4001	0.3156	0.2543	0.0300	0.4000	0.2955	0.2745	0.0300
0.5989	0.2211	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4106	0.4094	0.1000	0.0800	0.4025	0.4175	0.1000	0.0800
0.4000	0.1016	0.4621	0.0363	0.4000	0.1000	0.4610	0.0390
0.4000	0.2952	0.2248	0.0800	0.4000	0.2779	0.2421	0.0800
0.5300	0.1038	0.2862	0.0800	0.5348	0.1000	0.2852	0.0800
0.4608	0.1000	0.4092	0.0300	0.4529	0.1000	0.4171	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4996	0.2695	0.1808	0.0501	0.5000	0.2371	0.2090	0.0539
0.6000	0.1000	0.2400	0.0600	0.6000	0.1000	0.2420	0.0580
0.5954	0.2746	0.1000	0.0300	0.5917	0.2783	0.1000	0.0300
0.4500	0.3995	0.1001	0.0504	0.4623	0.3895	0.1000	0.0482
0.4000	0.1100	0.4100	0.0800	0.4000	0.1000	0.4200	0.0800
0.5812	0.1000	0.2888	0.0300	0.6000	0.1000	0.2700	0.0300
$G_w = 68.0784$				$G_w = 71.5466$			

Appendix Table B11 The most fit designs via GA and the optimal exact design with 15-points based on G -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.1500	0.3700	0.0800	0.4000	0.1453	0.3747	0.0800
0.4000	0.2900	0.2800	0.0300	0.4000	0.3205	0.2495	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4770	0.3430	0.1000	0.0800	0.4695	0.3505	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.5100	0.2606	0.1994	0.0300	0.5165	0.2535	0.2000	0.0300
0.5915	0.1010	0.2775	0.0300	0.5925	0.1000	0.2775	0.0300
0.5988	0.1000	0.2312	0.0700	0.6000	0.1000	0.2326	0.0674
0.4000	0.3900	0.1300	0.0800	0.4000	0.3807	0.1393	0.0800
0.4200	0.4190	0.1010	0.0600	0.4230	0.4200	0.1000	0.0570
0.4800	0.2145	0.2558	0.0497	0.4607	0.2216	0.2700	0.0477
0.4800	0.1000	0.3400	0.0800	0.4915	0.1000	0.3285	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.1196	0.4223	0.0581	0.4000	0.1000	0.4415	0.0585
0.5996	0.2204	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
$G_w = 66.7775$				$G_w = 68.9409$			

Appendix Table B12 The most fit designs via GA and the optimal exact design with 16-points based on G -criterion assuming the quadratic model for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4661	0.3378	0.1661	0.0300	0.4652	0.4048	0.1000	0.0300
0.4362	0.1000	0.3860	0.0778	0.4515	0.1000	0.3685	0.0800
0.6000	0.1005	0.2195	0.0800	0.6000	0.1000	0.2200	0.0800
0.4065	0.1000	0.4428	0.0507	0.4000	0.1000	0.4510	0.0490
0.6000	0.2344	0.1000	0.0656	0.6000	0.2300	0.1000	0.0700
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5100	0.3100	0.1000	0.0800	0.5015	0.3185	0.1000	0.0800
0.4500	0.2300	0.2731	0.0469	0.4479	0.2666	0.2470	0.0385
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.3871	0.1329	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.4279	0.1121	0.0600	0.4000	0.3838	0.1583	0.0579
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.2597	0.3097	0.0306	0.4000	0.2453	0.3247	0.0300
0.4000	0.1494	0.3706	0.0800	0.4000	0.1343	0.3857	0.0800
0.5274	0.1087	0.3173	0.0466	0.5293	0.1000	0.3260	0.0447
$G_w = 67.4434$				$G_w = 73.5949$			

Appendix Table B13 The most fit designs via GA and the optimal exact design with 15-points based on D -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.5974	0.1000	0.2226	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.4616	0.1000	0.0384	0.4000	0.4607	0.1000	0.0393
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.2200	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4592	0.3608	0.1000	0.0800	0.4827	0.3373	0.1000	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.2244	0.2956	0.0800	0.4000	0.2327	0.2873	0.0800
0.6000	0.1200	0.2500	0.0300	0.6000	0.1227	0.2473	0.0300
0.5730	0.2970	0.1000	0.0300	0.5521	0.3179	0.1000	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.2900	0.2800	0.0300	0.4000	0.2900	0.2800	0.0300
$D_w = 0.032547$				$D_w = 0.032623$			

Appendix Table B14 The most fit designs via GA and the optimal exact design with 16-points based on D -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4020	0.1000	0.4680	0.0300	0.4018	0.1000	0.4682	0.0300
0.6000	0.1300	0.2400	0.0300	0.6000	0.1222	0.2478	0.0300
0.4000	0.2868	0.2832	0.0300	0.4000	0.2857	0.2843	0.0300
0.4000	0.2210	0.2990	0.0800	0.4000	0.2385	0.2815	0.0800
0.5300	0.1000	0.2900	0.0800	0.4935	0.1000	0.3265	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.2200	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2600	0.1000	0.0400	0.6000	0.2577	0.1000	0.0423
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
$D_w = 0.032880$				$D_w = 0.032996$			

Appendix Table B15 The most fit designs via GA and the optimal exact design with 17-points based on D -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.6000	0.1900	0.1300	0.0800	0.6000	0.1893	0.1307	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.2611	0.2589	0.0800	0.4000	0.2600	0.2600	0.0800
0.5244	0.3456	0.1000	0.0300	0.5269	0.3431	0.1000	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4008	0.4192	0.1000	0.0800	0.4026	0.4174	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.6000	0.2200	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.2837	0.2863	0.0300	0.4000	0.2833	0.2867	0.0300
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.6000	0.1000	0.2600	0.0400	0.6000	0.1000	0.2604	0.0396
0.5918	0.1000	0.2282	0.0800	0.6000	0.1000	0.2200	0.0800
$D_w = 0.033104$				$D_w = 0.033161$			

Appendix Table B16 The most fit designs via GA and the optimal exact design with 18-points based on D -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.6000	0.1000	0.2600	0.0400	0.6000	0.1000	0.2571	0.0429
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.5996	0.1000	0.2204	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.2800	0.2900	0.0300	0.4000	0.2826	0.2874	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.5300	0.3400	0.1000	0.0300	0.5119	0.3581	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5900	0.2300	0.1000	0.0800	0.5962	0.2238	0.1000	0.0800
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.2741	0.2459	0.0800	0.4000	0.2593	0.2607	0.0800
0.6000	0.2204	0.1000	0.0796	0.6000	0.2200	0.1000	0.0800
0.6000	0.2331	0.1369	0.0300	0.6000	0.2293	0.1407	0.0300
0.4001	0.1000	0.4199	0.0800	0.4000	0.1000	0.4200	0.0800
$D_w = 0.033177$				$D_w = 0.033272$			

Appendix Table B17 The most fit designs via GA and the optimal exact design with 19-points based on D -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4001	0.1000	0.4199	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.4197	0.1003	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.6000	0.2300	0.1400	0.0300	0.6000	0.2183	0.1517	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5946	0.2249	0.1005	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.1001	0.4199	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.6000	0.2300	0.1000	0.0700	0.6000	0.2327	0.1000	0.0673
0.5142	0.3556	0.1002	0.0300	0.5204	0.3496	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.5800	0.1000	0.2400	0.0800	0.5231	0.1000	0.2969	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.2841	0.2859	0.0300	0.4000	0.2828	0.2872	0.0300
0.4000	0.2536	0.2664	0.0800	0.4000	0.2642	0.2558	0.0800
$D_w = 0.033265$				$D_w = 0.033446$			

Appendix Table B18 The most fit designs via GA and the optimal exact design with 20-points based on D -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.5993	0.1000	0.2207	0.0800	0.6000	0.1000	0.2200	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.2600	0.2600	0.0800	0.4000	0.2560	0.2640	0.0800
0.5066	0.1000	0.3634	0.0300	0.5190	0.1000	0.3510	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.5999	0.1000	0.2201	0.0800	0.6000	0.1000	0.2200	0.0800
0.6000	0.1800	0.1900	0.0300	0.6000	0.2089	0.1611	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.2903	0.2797	0.0300	0.4000	0.2866	0.2834	0.0300
0.6000	0.1000	0.2400	0.0600	0.6000	0.1000	0.2510	0.0490
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.5100	0.3100	0.1000	0.0800	0.5154	0.3046	0.1000	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2200	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
$D_w = 0.033385$				$D_w = 0.033430$			

Appendix Table B19 The most fit designs via GA and the optimal exact design with 15-points based on D -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5998	0.1000	0.2202	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.1001	0.4660	0.0339	0.4000	0.1000	0.4677	0.0323
0.5600	0.1416	0.2684	0.0300	0.5819	0.1195	0.2686	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.2700	0.2500	0.0800	0.4000	0.2750	0.2450	0.0800
0.4009	0.1000	0.4191	0.0800	0.4000	0.1000	0.4200	0.0800
0.4003	0.4697	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4667	0.3539	0.1000	0.0794	0.5022	0.3178	0.1000	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.5998	0.2202	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.2877	0.2823	0.0300	0.4000	0.2860	0.2840	0.0300
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
$D_w=0.028367$				$D_w=0.028429$			

Appendix Table B20 The most fit designs via GA and the optimal exact design with 16-points based on D -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.5965	0.2235	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.2830	0.2370	0.0800	0.4000	0.2455	0.2745	0.0800
0.4010	0.1000	0.4690	0.0300	0.4012	0.1000	0.4688	0.0300
0.4000	0.4699	0.1001	0.0300	0.4000	0.4700	0.1000	0.0300
0.5000	0.1000	0.3200	0.0800	0.5000	0.1000	0.3200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.6000	0.2605	0.1000	0.0395	0.6000	0.2648	0.1000	0.0352
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.2752	0.2948	0.0300	0.4000	0.2852	0.2848	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4004	0.4196	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.6000	0.1169	0.2531	0.0300	0.6000	0.1152	0.2548	0.0300
$D_w=0.028540$				$D_w=0.028672$			

Appendix Table B21 The most fit designs via GA and the optimal exact design with 17-points based on D -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.5400	0.2900	0.1400	0.0300	0.5411	0.2899	0.1390	0.0300
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.2800	0.2900	0.0300	0.4000	0.2829	0.2871	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2278	0.1000	0.0722	0.6000	0.2248	0.1000	0.0752
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.4198	0.1002	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2200	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.2200	0.3000	0.0800	0.4000	0.2490	0.2710	0.0800
0.5986	0.1000	0.2214	0.0800	0.6000	0.1000	0.2200	0.0800
0.4900	0.1000	0.3300	0.0800	0.4810	0.1000	0.3390	0.0800
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4007	0.4693	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
$D_w = 0.028732$				$D_w = 0.028741$			

Appendix Table B22 The most fit designs via GA and the optimal exact design with 18-points based on D -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.5984	0.1000	0.2716	0.0300	0.5975	0.1000	0.2725	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.6000	0.2300	0.1000	0.0700	0.6000	0.2258	0.1000	0.0742
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.5985	0.2216	0.1000	0.0799	0.6000	0.2200	0.1000	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.2600	0.2600	0.0800	0.4000	0.2624	0.2576	0.0800
0.4000	0.2900	0.2800	0.0300	0.4000	0.2832	0.2868	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5163	0.1000	0.3037	0.0800	0.5221	0.1000	0.2979	0.0800
0.4000	0.1013	0.4187	0.0800	0.4000	0.1000	0.4200	0.0800
0.5243	0.2700	0.1757	0.0300	0.5365	0.2798	0.1537	0.0300
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.4198	0.1002	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
$D_w = 0.028914$				$D_w = 0.028974$			

Appendix Table B23 The most fit designs via GA and the optimal exact design with 19-points based on D -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.2859	0.2841	0.0300	0.4000	0.2847	0.2853	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.2500	0.2700	0.0800	0.4000	0.2627	0.2573	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.5998	0.2252	0.1000	0.0750	0.6000	0.2250	0.1000	0.0750
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.5045	0.2264	0.2391	0.0300	0.4909	0.2412	0.2379	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.5300	0.1000	0.2900	0.0800	0.5239	0.1000	0.2961	0.0800
0.5879	0.2321	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.5943	0.2757	0.1000	0.0300	0.5951	0.2749	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
$D_w = 0.029016$				$D_w = 0.029124$			

Appendix Table B24 The most fit designs via GA and the optimal exact design with 20-points based on D -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.1001	0.2699	0.0300	0.6000	0.1000	0.2700	0.0300
0.4984	0.2370	0.2346	0.0300	0.4941	0.2409	0.2350	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2677	0.1023	0.0300	0.6000	0.2687	0.1013	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.2900	0.2800	0.0300	0.4000	0.2937	0.2763	0.0300
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.2600	0.2601	0.0799	0.4000	0.2573	0.2627	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.5091	0.3109	0.1000	0.0800	0.5242	0.2958	0.1000	0.0800
0.5991	0.2209	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.6000	0.1000	0.2228	0.0772	0.6000	0.1000	0.2249	0.0751
$D_w = 0.029043$				$D_w = 0.029087$			

Appendix Table B25 The most fit designs via GA and the optimal exact design with 15-points based on G -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.2983	0.2647	0.0370	0.4000	0.2814	0.2817	0.0369
0.5900	0.2800	0.1000	0.0300	0.5905	0.2795	0.1000	0.0300
0.4001	0.4698	0.1001	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5889	0.2311	0.1000	0.0800	0.5856	0.2344	0.1000	0.0800
0.5980	0.1000	0.2308	0.0712	0.6000	0.1000	0.2270	0.0730
0.4013	0.4187	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4600	0.2900	0.2200	0.0300	0.4567	0.2933	0.2200	0.0300
0.4997	0.1000	0.3203	0.0800	0.5000	0.1000	0.3200	0.0800
0.5474	0.2023	0.1947	0.0556	0.5442	0.1942	0.2076	0.0540
0.4871	0.1000	0.3788	0.0341	0.5425	0.1000	0.3275	0.0300
0.4000	0.1025	0.4200	0.0775	0.4000	0.1039	0.4200	0.0761
0.4087	0.2625	0.2488	0.0800	0.4122	0.2536	0.2542	0.0800
0.5200	0.3183	0.1000	0.0617	0.4937	0.3430	0.1000	0.0633
0.6000	0.1200	0.2500	0.0300	0.6000	0.1143	0.2427	0.0300
$G_w = 60.1853$				$G_w = 65.6713$			

Appendix Table B26 The most fit designs via GA and the optimal exact design with 16-points based on G -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4943	0.1502	0.2804	0.0751	0.4919	0.1869	0.2416	0.0796
0.6000	0.1135	0.2065	0.0800	0.6000	0.1061	0.2139	0.0800
0.5794	0.2906	0.1000	0.0300	0.5813	0.2887	0.1000	0.0300
0.6000	0.2200	0.1100	0.0700	0.6000	0.2200	0.1178	0.0622
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.5199	0.3000	0.1001	0.0800	0.5623	0.2577	0.1000	0.0800
0.4000	0.2500	0.2700	0.0800	0.4000	0.2500	0.2700	0.0800
0.4000	0.4142	0.1058	0.0800	0.4000	0.4200	0.1000	0.0800
0.4172	0.3700	0.1600	0.0528	0.4000	0.4264	0.1245	0.0491
0.5000	0.2400	0.2300	0.0300	0.5000	0.2611	0.2089	0.0300
0.4058	0.4642	0.1000	0.0300	0.4086	0.4614	0.1000	0.0300
0.6000	0.1200	0.2500	0.0300	0.6000	0.1159	0.2541	0.0300
0.4000	0.3100	0.2600	0.0300	0.4000	0.2641	0.3059	0.0300
0.5100	0.1000	0.3300	0.0600	0.4961	0.1000	0.3372	0.0667
0.4935	0.1000	0.3765	0.0300	0.5000	0.1000	0.3700	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
$G_w = 63.9092$				$G_w = 67.6680$			

Appendix Table B27 The most fit designs via GA and the optimal exact design with 17-points based on G -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.6000	0.2173	0.1034	0.0793	0.6000	0.2200	0.1000	0.0800
0.4981	0.2819	0.1900	0.0300	0.4923	0.2361	0.2416	0.0300
0.4400	0.2000	0.3057	0.0543	0.4155	0.1446	0.3874	0.0525
0.6000	0.1000	0.2208	0.0792	0.6000	0.1000	0.2200	0.0800
0.5600	0.1000	0.3100	0.0300	0.5650	0.1000	0.3050	0.0300
0.4017	0.2670	0.2514	0.0799	0.4000	0.2626	0.2574	0.0800
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.3995	0.1205	0.0800	0.4000	0.4200	0.1000	0.0800
0.4898	0.2900	0.1402	0.0800	0.5010	0.2718	0.1472	0.0800
0.5126	0.3455	0.1000	0.0419	0.4985	0.3715	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2600	0.1100	0.0300	0.6000	0.2603	0.1097	0.0300
0.5248	0.1000	0.2952	0.0800	0.4970	0.1000	0.3230	0.0800
0.4000	0.2800	0.2900	0.0300	0.4000	0.2755	0.2945	0.0300
0.6000	0.1400	0.2200	0.0400	0.6000	0.1418	0.2200	0.0382
0.4231	0.4090	0.1000	0.0679	0.4508	0.3942	0.1000	0.0550
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
$G_w = 64.5183$				$G_w = 69.9795$			

Appendix Table B28 The most fit designs via GA and the optimal exact design with 18-points based on G -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.5806	0.1000	0.2394	0.0800	0.5826	0.1000	0.2374	0.0800
0.5125	0.1900	0.2675	0.0300	0.5000	0.2330	0.2370	0.0300
0.4000	0.3100	0.2600	0.0300	0.4000	0.2959	0.2741	0.0300
0.6000	0.2208	0.1000	0.0792	0.6000	0.2200	0.1000	0.0800
0.4000	0.2400	0.2800	0.0800	0.4000	0.2745	0.2455	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4898	0.3302	0.1000	0.0800	0.5000	0.3200	0.1000	0.0800
0.6000	0.1029	0.2671	0.0299	0.6000	0.1000	0.2700	0.0300
0.6000	0.2388	0.1300	0.0312	0.6000	0.2332	0.1338	0.0330
0.4923	0.1000	0.3692	0.0385	0.4869	0.1000	0.3831	0.0300
0.4400	0.2500	0.2600	0.0500	0.4000	0.1628	0.3808	0.0564
0.5168	0.1543	0.2489	0.0800	0.4886	0.1444	0.2870	0.0800
0.4006	0.1000	0.4194	0.0800	0.4000	0.1000	0.4200	0.0800
0.5500	0.3200	0.1000	0.0300	0.5659	0.3041	0.1000	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.1096	0.2338	0.0566	0.6000	0.1319	0.2029	0.0652
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4500	0.3881	0.1089	0.0530	0.4400	0.4106	0.1000	0.0494
$G_w = 66.4605$				$G_w = 71.1533$			

Appendix Table B29 The most fit designs via GA and the optimal exact design with 19-points based on G -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4185	0.1036	0.4158	0.0621	0.4079	0.1000	0.4381	0.0540
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4721	0.3898	0.1081	0.0300	0.4673	0.4027	0.1000	0.0300
0.4000	0.2700	0.2600	0.0700	0.4000	0.2565	0.2774	0.0661
0.5900	0.1715	0.1885	0.0500	0.6000	0.1744	0.1756	0.0500
0.5996	0.2204	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4121	0.4100	0.1031	0.0748	0.4000	0.4236	0.1000	0.0764
0.6000	0.1121	0.2579	0.0300	0.6000	0.1049	0.2651	0.0300
0.4981	0.2521	0.2198	0.0300	0.4821	0.2457	0.2422	0.0300
0.4000	0.3900	0.1300	0.0800	0.4000	0.3642	0.1558	0.0800
0.5013	0.1036	0.3151	0.0800	0.5000	0.1000	0.3200	0.0800
0.4000	0.1119	0.4081	0.0800	0.4000	0.1000	0.4200	0.0800
0.5300	0.2900	0.1090	0.0710	0.4986	0.3293	0.1000	0.0721
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.5126	0.1000	0.3574	0.0300	0.5017	0.1000	0.3683	0.0300
0.4000	0.2800	0.2900	0.0300	0.4000	0.2862	0.2838	0.0300
0.4500	0.2369	0.2331	0.0800	0.4477	0.2327	0.2396	0.0800
0.6000	0.1000	0.2208	0.0792	0.6000	0.1000	0.2200	0.0800
$G_w = 66.1616$				$G_w = 71.3235$			

Appendix Table B30 The most fit designs via GA and the optimal exact design with 20-points based on G -criterion assuming the special cubic model under SH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.6000	0.2500	0.1200	0.0300	0.6000	0.2700	0.1000	0.0300
0.5000	0.3200	0.1000	0.0800	0.5000	0.3200	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4805	0.3895	0.1000	0.0300	0.4753	0.3947	0.1000	0.0300
0.6000	0.1000	0.2400	0.0600	0.6000	0.1000	0.2429	0.0571
0.5987	0.1718	0.1495	0.0800	0.6000	0.1131	0.2069	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4500	0.3800	0.1100	0.0600	0.4016	0.4425	0.1013	0.0546
0.4700	0.2300	0.2700	0.0300	0.4566	0.2434	0.2700	0.0300
0.6000	0.2202	0.1000	0.0798	0.6000	0.2200	0.1000	0.0800
0.4692	0.1008	0.4000	0.0300	0.4807	0.1000	0.3893	0.0300
0.6000	0.2373	0.1285	0.0342	0.6000	0.1915	0.1785	0.0300
0.6000	0.1000	0.2700	0.0300	0.6000	0.1000	0.2700	0.0300
0.4200	0.1530	0.3676	0.0594	0.4000	0.1000	0.4451	0.0549
0.5595	0.1000	0.2605	0.0800	0.5076	0.1000	0.3124	0.0800
0.4000	0.2551	0.2649	0.0800	0.4000	0.2600	0.2600	0.0800
0.4000	0.3066	0.2634	0.0300	0.4000	0.2855	0.2845	0.0300
0.5016	0.1960	0.2245	0.0779	0.4631	0.2377	0.2289	0.0703
0.4000	0.1000	0.4200	0.0800	0.4000	0.1000	0.4200	0.0800
$G_w = 65.3008$				$G_w = 70.9548$			

Appendix Table B31 The most fit designs via GA and the optimal exact design with 15-points based on G -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.3800	0.1400	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4000	0.4400	0.1000	0.0600	0.4000	0.4450	0.1000	0.0550
0.6000	0.2200	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.2703	0.2971	0.0326	0.4000	0.2700	0.3000	0.0300
0.4014	0.2300	0.2948	0.0738	0.4000	0.2592	0.2608	0.0800
0.4894	0.3000	0.1806	0.0300	0.4986	0.2968	0.1746	0.0300
0.4780	0.3333	0.1087	0.0800	0.4893	0.3200	0.1107	0.0800
0.6000	0.1400	0.2300	0.0300	0.6000	0.1370	0.2330	0.0300
0.5869	0.2807	0.1003	0.0321	0.5859	0.2817	0.1000	0.0324
0.5794	0.1000	0.2406	0.0800	0.5752	0.1000	0.2448	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4000	0.1006	0.4194	0.0800	0.4000	0.1000	0.4200	0.0800
0.5093	0.1842	0.2487	0.0578	0.5382	0.1473	0.2542	0.0603
0.5314	0.1000	0.3386	0.0300	0.5246	0.1000	0.3454	0.0300
$G_w = 59.7899$				$G_w = 63.3992$			

Appendix Table B32 The most fit designs via GA and the optimal exact design with 16-points based on G -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.5342	0.1000	0.3300	0.0358	0.5166	0.1000	0.3478	0.0356
0.5996	0.2204	0.1000	0.0800	0.6000	0.2200	0.1000	0.0800
0.4738	0.3403	0.1059	0.0800	0.4943	0.3257	0.1000	0.0800
0.4013	0.1000	0.4200	0.0787	0.4000	0.1000	0.4200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.4584	0.2958	0.1921	0.0537	0.4429	0.2752	0.2277	0.0542
0.5900	0.1000	0.2300	0.0800	0.5847	0.1000	0.2353	0.0800
0.4900	0.2900	0.1900	0.0300	0.5312	0.2511	0.1877	0.0300
0.4000	0.4200	0.1013	0.0787	0.4000	0.4200	0.1017	0.0783
0.6000	0.2542	0.1000	0.0458	0.6000	0.2493	0.1000	0.0507
0.5004	0.1800	0.2396	0.0800	0.5106	0.1629	0.2465	0.0800
0.4000	0.2829	0.2871	0.0300	0.4000	0.2912	0.2788	0.0300
0.4000	0.2400	0.2800	0.0800	0.4000	0.2682	0.2518	0.0800
0.5425	0.3269	0.1006	0.0300	0.5639	0.3061	0.1000	0.0300
0.6000	0.1444	0.2256	0.0300	0.6000	0.1221	0.2479	0.0300
$G_w = 61.7374$				$G_w = 67.1785$			

Appendix Table B33 The most fit designs via GA and the optimal exact design with 17-points based on G -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.5898	0.1000	0.2302	0.0800	0.5970	0.1000	0.2230	0.0800
0.4900	0.1009	0.3791	0.0300	0.4967	0.1000	0.3733	0.0300
0.4600	0.1202	0.3598	0.0600	0.4517	0.1074	0.3814	0.0595
0.4900	0.3265	0.1035	0.0800	0.4921	0.3279	0.1000	0.0800
0.4000	0.2800	0.2900	0.0300	0.4000	0.2836	0.2864	0.0300
0.4000	0.2400	0.2800	0.0800	0.4000	0.2531	0.2669	0.0800
0.4000	0.4194	0.1006	0.0800	0.4000	0.4200	0.1000	0.0800
0.4020	0.3768	0.1602	0.0610	0.4000	0.3929	0.1538	0.0533
0.4014	0.1000	0.4186	0.0800	0.4000	0.1000	0.4200	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2300	0.1300	0.0400	0.6000	0.2317	0.1297	0.0386
0.5970	0.2247	0.1000	0.0783	0.6000	0.2200	0.1000	0.0800
0.4900	0.2407	0.2393	0.0300	0.4996	0.2323	0.2381	0.0300
0.4907	0.1593	0.2700	0.0800	0.4975	0.1525	0.2700	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.5600	0.3100	0.1000	0.0300	0.5600	0.3100	0.1000	0.0300
0.6000	0.1100	0.2600	0.0300	0.6000	0.1075	0.2625	0.0300
$G_w=67.7739$				$G_w=70.5052$			

Appendix Table B34 The most fit designs via GA and the optimal exact design with 18-points based on G -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4000	0.2400	0.2800	0.0800	0.4000	0.2618	0.2582	0.0800
0.5100	0.1048	0.3552	0.0300	0.4970	0.1000	0.3730	0.0300
0.4158	0.4300	0.1000	0.0542	0.4000	0.4460	0.1000	0.0540
0.4100	0.1400	0.4000	0.0500	0.4000	0.1428	0.4015	0.0557
0.6000	0.2279	0.1421	0.0300	0.6000	0.2350	0.1350	0.0300
0.4906	0.2117	0.2318	0.0659	0.4791	0.2254	0.2277	0.0678
0.6000	0.1000	0.2646	0.0354	0.6000	0.1000	0.2680	0.0320
0.5999	0.1137	0.2064	0.0800	0.6000	0.1000	0.2200	0.0800
0.4014	0.1000	0.4186	0.0800	0.4000	0.1000	0.4200	0.0800
0.4786	0.2214	0.2700	0.0300	0.4749	0.2251	0.2700	0.0300
0.5470	0.3200	0.1030	0.0300	0.5500	0.3200	0.1000	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5197	0.1000	0.3003	0.0800	0.5160	0.1000	0.3040	0.0800
0.4000	0.2648	0.3052	0.0300	0.4000	0.2876	0.2824	0.0300
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.6000	0.2310	0.1000	0.0690	0.6000	0.2250	0.1000	0.0750
0.5502	0.2698	0.1000	0.0800	0.5377	0.2823	0.1000	0.0800
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
$G_w = 66.7748$				$G_w = 71.4587$			

Appendix Table B35 The most fit designs via GA and the optimal exact design with 19-points based on G -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.6000	0.1700	0.1900	0.0400	0.6000	0.1638	0.1822	0.0540
0.4400	0.1006	0.4000	0.0594	0.4116	0.1000	0.4337	0.0547
0.4600	0.2441	0.2183	0.0776	0.4659	0.2224	0.2317	0.0800
0.4480	0.3720	0.1000	0.0800	0.4613	0.3587	0.1000	0.0800
0.5700	0.3000	0.1000	0.0300	0.5987	0.2713	0.1000	0.0300
0.6000	0.1000	0.2697	0.0303	0.6000	0.1000	0.2700	0.0300
0.4000	0.3800	0.1700	0.0500	0.4000	0.4028	0.1573	0.0399
0.4000	0.2185	0.3015	0.0800	0.4000	0.2693	0.2507	0.0800
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.5955	0.2244	0.1001	0.0800	0.6000	0.2200	0.1000	0.0800
0.4000	0.4200	0.1000	0.0800	0.4000	0.4200	0.1000	0.0800
0.4000	0.1033	0.4170	0.0797	0.4000	0.1000	0.4200	0.0800
0.4788	0.2696	0.2216	0.0300	0.5150	0.2424	0.2126	0.0300
0.4000	0.2800	0.2900	0.0300	0.4000	0.2820	0.2880	0.0300
0.4900	0.1003	0.3297	0.0800	0.4930	0.1000	0.3270	0.0800
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.5000	0.1003	0.3697	0.0300	0.4953	0.1000	0.3747	0.0300
0.5545	0.3092	0.1000	0.0363	0.5088	0.3505	0.1000	0.0407
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
$G_w = 66.2622$				$G_w = 71.6545$			

Appendix Table B36 The most fit designs via GA and the optimal exact design with 20-points based on G -criterion assuming the special cubic model under WH for the flare experiment.

Most fit designs via GA				Optimal exact design			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
0.4900	0.1000	0.3800	0.0300	0.4823	0.1000	0.3877	0.0300
0.4100	0.1000	0.4300	0.0600	0.4000	0.1000	0.4423	0.0577
0.6000	0.2211	0.1002	0.0787	0.6000	0.2200	0.1000	0.0800
0.4192	0.3547	0.1769	0.0492	0.4000	0.3659	0.1907	0.0434
0.4100	0.4099	0.1001	0.0800	0.4000	0.4200	0.1000	0.0800
0.5100	0.1500	0.2600	0.0800	0.5118	0.1489	0.2593	0.0800
0.4000	0.2467	0.2735	0.0798	0.4000	0.2247	0.2953	0.0800
0.4000	0.3804	0.1396	0.0800	0.4000	0.3570	0.1630	0.0800
0.6000	0.1000	0.2200	0.0800	0.6000	0.1000	0.2200	0.0800
0.4000	0.2800	0.2900	0.0300	0.4000	0.2729	0.2971	0.0300
0.4900	0.3270	0.1030	0.0800	0.4967	0.3233	0.1000	0.0800
0.4000	0.1014	0.4186	0.0800	0.4000	0.1000	0.4200	0.0800
0.4869	0.1000	0.3520	0.0611	0.5317	0.1000	0.3061	0.0622
0.6000	0.1935	0.1520	0.0545	0.6000	0.2040	0.1488	0.0472
0.5200	0.2100	0.2400	0.0300	0.5070	0.2286	0.2344	0.0300
0.6000	0.1012	0.2688	0.0300	0.6000	0.1000	0.2700	0.0300
0.4000	0.1000	0.4700	0.0300	0.4000	0.1000	0.4700	0.0300
0.6000	0.2700	0.1000	0.0300	0.6000	0.2700	0.1000	0.0300
0.4000	0.4700	0.1000	0.0300	0.4000	0.4700	0.1000	0.0300
0.4700	0.4000	0.1000	0.0300	0.4657	0.4043	0.1000	0.0300
$G_w = 66.4675$				$G_w = 71.2817$			

The seal of Kasetsart University is a large, faint watermark in the background. It is circular, with the words "KASETSART UNIVERSITY" in an arc at the top and "1943" at the bottom. The center features a traditional Thai emblem with a central figure, possibly a deity or royal figure, surrounded by ornate patterns and two smaller floral motifs on the sides.

Appendix C

The most fit designs via GA and the optimal exact designs for Snee's experiment.

Appendix Table C1 The most fit designs via GA and the optimal exact design with 7-points based on D -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.2866	0.3133	0.4001	0.2878	0.3109	0.4013
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
$D_w = 0.8981948$			$D_w = 0.8981999$		

Appendix Table C2 The most fit designs via GA and the optimal exact design with 8-points based on D -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.2871	0.3251	0.3878	0.2868	0.3257	0.3875
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
$D_w = 0.8901976$			$D_w = 0.8901980$		

Appendix Table C3 The most fit designs via GA and the optimal exact design with 9-points based on D -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.3316	0.5005	0.1679	0.3333	0.5000	0.1667
0.2983	0.3110	0.3907	0.2975	0.3118	0.3907
0.2666	0.1001	0.6333	0.2667	0.1000	0.6333
0.4999	0.2501	0.2500	0.5000	0.2500	0.2500
0.1000	0.3501	0.5499	0.1000	0.3500	0.5500
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
$D_w = 0.8920954$			$D_w = 0.8937718$		

Appendix Table C4 The most fit designs via GA and the optimal exact design with 10-points based on D -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.2998	0.3003	0.3999	0.2963	0.3000	0.4037
$D_w = 0.9004166$			$D_w = 0.9004436$		

Appendix Table C5 The most fit designs via GA and the optimal exact design with 11-points based on D -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.3100	0.2900	0.4000	0.3088	0.2926	0.3986
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
$D_w = 0.9089636$			$D_w = 0.9089689$		

Appendix Table C6 The most fit designs via GA and the optimal exact design with 12-points based on D -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.3508	0.5492	0.1000	0.3500	0.5500
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2948	0.3095	0.3957	0.2943	0.3099	0.3958
0.1000	0.3502	0.5498	0.1000	0.3500	0.5500
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.3335	0.4998	0.1667	0.3333	0.5000	0.1667
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3333	0.4998	0.1669	0.3333	0.5000	0.1667
$D_w = 0.9206811$			$D_w = 0.9211973$		

Appendix Table C7 The most fit designs via GA and the optimal exact design with 7-points based on G -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.3601	0.5399	0.1000	0.3500	0.5500
0.4808	0.1000	0.4192	0.4747	0.1000	0.4253
0.3255	0.5007	0.1738	0.3220	0.5033	0.1747
0.1040	0.5677	0.3283	0.1000	0.5700	0.3300
0.2700	0.1000	0.6300	0.2667	0.1000	0.6333
0.3209	0.3031	0.3760	0.2885	0.3170	0.3945
0.4958	0.2563	0.2479	0.5000	0.2500	0.2500
$G_w = 78.5896$			$G_w = 82.6408$		

Appendix Table C8 The most fit designs via GA and the optimal exact design with 8-points based on G -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1172	0.4414	0.4414	0.1279	0.4458	0.4263
0.3000	0.2900	0.4100	0.3121	0.2657	0.4222
0.1000	0.3501	0.5499	0.1000	0.3500	0.5500
0.1070	0.5674	0.3256	0.1000	0.5678	0.3322
0.4995	0.2475	0.2530	0.5000	0.2463	0.2537
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3414	0.4879	0.1707	0.3333	0.5000	0.1667
$G_w = 75.4964$			$G_w = 76.5576$		

Appendix Table C9 The most fit designs via GA and the optimal exact design with 9-points based on G -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3501	0.2490	0.4009	0.2918	0.3218	0.3864
0.2634	0.5199	0.2167	0.2310	0.5307	0.2383
0.1000	0.5664	0.3336	0.1000	0.5700	0.3300
0.5000	0.2481	0.2519	0.5000	0.2500	0.2500
0.3945	0.4083	0.1972	0.3143	0.5057	0.1800
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.3600	0.5400	0.1000	0.3500	0.5500
0.2199	0.2301	0.5500	0.2369	0.1991	0.5640
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
$G_w = 69.5982$			$G_w = 75.9125$		

Appendix Table C10 The most fit designs via GA and the optimal exact design with 10-points based on G -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.4878	0.2665	0.2457	0.4908	0.2638	0.2454
0.2500	0.1300	0.6200	0.2424	0.1364	0.6212
0.3534	0.4699	0.1767	0.3333	0.5000	0.1667
0.3600	0.1365	0.5035	0.3750	0.1554	0.4696
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.5523	0.3477	0.1000	0.5488	0.3512
0.2948	0.2946	0.4106	0.2716	0.3243	0.4041
0.1000	0.3700	0.5300	0.1000	0.3500	0.5500
0.2100	0.5370	0.2530	0.1777	0.5466	0.2757
0.2271	0.1593	0.6136	0.2358	0.1464	0.6178
$G_w = 68.4367$			$G_w = 72.6225$		

Appendix Table C11 The most fit designs via GA and the optimal exact design with 11-points based on G -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3331	0.5001	0.1668	0.3333	0.5000	0.1667
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3100	0.2800	0.4100	0.3032	0.3041	0.3927
0.1000	0.5699	0.3301	0.1000	0.5700	0.3300
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1600	0.2700	0.5700	0.1740	0.2827	0.5433
0.3400	0.1050	0.5550	0.3444	0.1000	0.5556
0.4999	0.2501	0.2500	0.5000	0.2500	0.2500
0.1000	0.3799	0.5201	0.1000	0.3500	0.5500
0.1700	0.5199	0.3101	0.1384	0.5154	0.3462
0.3272	0.4408	0.2320	0.3292	0.4457	0.2251
$G_w = 72.7577$			$G_w = 74.6707$		

Appendix Table C12 The most fit designs via GA and the optimal exact design with 12-points based on G -criterion assuming the quadratic model for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3140	0.5058	0.1802	0.3142	0.5058	0.1800
0.3193	0.2810	0.3997	0.2968	0.3114	0.3918
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2229	0.1657	0.6114	0.2229	0.1657	0.6114
0.4000	0.4000	0.2000	0.3858	0.4153	0.1989
0.4587	0.1038	0.4375	0.4023	0.1272	0.4705
0.4655	0.1253	0.4092	0.5000	0.1000	0.4000
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.1576	0.3957	0.4467	0.1575	0.3517	0.4908
0.1691	0.5286	0.3023	0.1560	0.5415	0.3025
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.3504	0.5496	0.1000	0.3500	0.5500
$G_w = 69.6073$			$G_w = 73.9863$		

Appendix Table C13 The most fit designs via GA and the optimal exact design with 8-points based on D -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.2895	0.3206	0.3899	0.2885	0.3221	0.3894
0.5000	0.2499	0.2501	0.5000	0.2500	0.2500
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
$D_w = 0.602107345$			$D_w = 0.602150602$		

Appendix Table C14 The most fit designs via GA and the optimal exact design with 9-points based on D -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.2963	0.3112	0.3925	0.2964	0.3115	0.3921
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
$D_w = 0.603461386$			$D_w = 0.603461588$		

Appendix Table C15 The most fit designs via GA and the optimal exact design with 10-points based on D -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2994	0.2997	0.4009	0.2953	0.3027	0.4020
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3334	0.4999	0.1667	0.3333	0.5000	0.1667
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
$D_w = 0.607148091$			$D_w = 0.607168093$		

Appendix Table C16 The most fit designs via GA and the optimal exact design with 11-points based on D -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.2849	0.3122	0.4029	0.2852	0.3125	0.4023
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.3336	0.4996	0.1668	0.3333	0.5000	0.1667
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
$D_w = 0.612070104$			$D_w = 0.612132487$		

Appendix Table C17 The most fit designs via GA and the optimal exact design with 12-points based on D -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.2929	0.3101	0.3970	0.2941	0.3100	0.3959
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2666	0.1001	0.6333	0.2667	0.1000	0.6333
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.3330	0.5001	0.1669	0.3333	0.5000	0.1667
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
$D_w = 0.620571647$			$D_w = 0.620700608$		

Appendix Table C18 The most fit designs via GA and the optimal exact design with 13-points based on D -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.3334	0.4999	0.1667	0.3333	0.5000	0.1667
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.1000	0.3501	0.5499	0.1000	0.3500	0.5500
0.1000	0.5699	0.3301	0.1000	0.5700	0.3300
0.2901	0.3099	0.4000	0.2905	0.3110	0.3985
0.3332	0.5000	0.1668	0.3333	0.5000	0.1667
0.2666	0.1001	0.6333	0.2667	0.1000	0.6333
0.4967	0.1000	0.4033	0.5000	0.1000	0.4000
0.2669	0.1000	0.6331	0.2667	0.1000	0.6333
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.4995	0.2508	0.2497	0.5000	0.2500	0.2500
$D_w = 0.619980945$			$D_w = 0.620704388$		

Appendix Table C19 The most fit designs via GA and the optimal exact design with 8-points based on D -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2896	0.3212	0.3892	0.2900	0.3215	0.3885
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
$D_w = 0.537881608$			$D_w = 0.537882549$		

Appendix Table C20 The most fit designs via GA and the optimal exact design with 9-points based on D -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.2967	0.3133	0.3900	0.2964	0.3136	0.3900
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
$D_w = 0.538742013$			$D_w = 0.538742034$		

Appendix Table C21 The most fit designs via GA and the optimal exact design with 10-points based on D -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.4999	0.2504	0.2497	0.5000	0.2500	0.2500
0.1000	0.5699	0.3301	0.1000	0.5700	0.3300
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3334	0.4999	0.1667	0.3333	0.5000	0.1667
0.3335	0.4997	0.1668	0.3333	0.5000	0.1667
0.2945	0.3075	0.3980	0.2949	0.3077	0.3974
0.1000	0.3503	0.5497	0.1000	0.3500	0.5500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
$D_w = 0.541496617$			$D_w = 0.541671312$		

Appendix Table C22 The most fit designs via GA and the optimal exact design with 11-points based on D -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3336	0.4996	0.1668	0.3333	0.5000	0.1667
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.2981	0.3175	0.3844	0.2897	0.3124	0.3979
$D_w = 0.546358497$			$D_w = 0.546625985$		

Appendix Table C23 The most fit designs via GA and the optimal exact design with 12-points based on D -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1001	0.3498	0.5501	0.1000	0.3500	0.5500
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.2973	0.3086	0.3941	0.2960	0.3115	0.3925
0.3337	0.4994	0.1669	0.3333	0.5000	0.1667
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.5000	0.2504	0.2496	0.5000	0.2500	0.2500
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
$D_w = 0.552722283$			$D_w = 0.552750315$		

Appendix Table C24 The most fit designs via GA and the optimal exact design with 13-points based on D -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.4992	0.2512	0.2496	0.5000	0.2500	0.2500
0.1000	0.3502	0.5498	0.1000	0.3500	0.5500
0.1000	0.3505	0.5495	0.1000	0.3500	0.5500
0.2900	0.3102	0.3998	0.2910	0.3120	0.3970
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.4995	0.2507	0.2498	0.5000	0.2500	0.2500
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.3334	0.4999	0.1667	0.3333	0.5000	0.1667
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
$D_w = 0.551603242$			$D_w = 0.551986477$		

Appendix Table C25 The most fit designs via GA and the optimal exact design with 8-points based on G -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.4148	0.1163	0.4689	0.4058	0.1000	0.4942
0.1004	0.3586	0.5410	0.1000	0.3500	0.5500
0.2553	0.3614	0.3833	0.2883	0.3054	0.4063
0.4785	0.1000	0.4215	0.5000	0.1000	0.4000
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3343	0.4986	0.1671	0.3315	0.5000	0.1685
0.4966	0.2551	0.2483	0.4884	0.2673	0.2443
0.1000	0.5699	0.3301	0.1000	0.5700	0.3300
$G_w = 79.3815$			$G_w = 81.0604$		

Appendix Table C26 The most fit designs via GA and the optimal exact design with 9-points based on G -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.1200	0.3800	0.5000	0.1115	0.3885
0.2533	0.1201	0.6266	0.2548	0.1178	0.6274
0.4781	0.2826	0.2393	0.4826	0.2761	0.2413
0.1000	0.3511	0.5489	0.1000	0.3500	0.5500
0.3000	0.2900	0.4100	0.2973	0.3165	0.3862
0.3364	0.4954	0.1682	0.3333	0.5000	0.1667
0.1087	0.5672	0.3241	0.1060	0.5682	0.3258
0.3651	0.1000	0.5349	0.3666	0.1000	0.5334
0.1274	0.4548	0.4178	0.1240	0.4563	0.4197
$G_w = 76.2080$			$G_w = 77.8030$		

Appendix Table C27 The most fit designs via GA and the optimal exact design with 10-points based on G -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.5000	0.1002	0.3998	0.5000	0.1000	0.4000
0.2857	0.5133	0.2010	0.2860	0.5142	0.1998
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.1459	0.4380	0.4161	0.1450	0.4468	0.4082
0.3176	0.3039	0.3785	0.3083	0.2890	0.4027
0.2467	0.1300	0.6233	0.2466	0.1300	0.6234
0.1000	0.5700	0.3300	0.1000	0.5700	0.3300
0.3704	0.4444	0.1852	0.3704	0.4444	0.1852
0.3267	0.1000	0.5733	0.3262	0.1000	0.5738
0.1001	0.3500	0.5499	0.1000	0.3500	0.5500
$G_w = 75.0934$			$G_w = 76.2648$		

Appendix Table C28 The most fit designs via GA and the optimal exact design with 11-points based on G -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.5640	0.3360	0.1000	0.5700	0.3300
0.3284	0.4404	0.2312	0.3546	0.4115	0.2339
0.3501	0.1001	0.5498	0.3524	0.1000	0.5476
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.3398	0.4902	0.1700	0.3333	0.5000	0.1667
0.1001	0.3910	0.5089	0.1000	0.4060	0.4940
0.2688	0.1000	0.6312	0.2667	0.1000	0.6333
0.2927	0.3200	0.3873	0.3050	0.2950	0.4000
0.1742	0.5477	0.2781	0.1724	0.5176	0.3100
0.1600	0.2700	0.5700	0.1400	0.2900	0.5700
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
$G_w = 73.7378$			$G_w = 76.9449$		

Appendix Table C29 The most fit designs via GA and the optimal exact design with 12-points based on G -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.4200	0.1000	0.4800	0.4243	0.1000	0.4757
0.2722	0.5183	0.2095	0.2750	0.5175	0.2075
0.1206	0.5638	0.3156	0.1116	0.5665	0.3219
0.5000	0.1300	0.3700	0.5000	0.1362	0.3638
0.2190	0.2937	0.4873	0.1918	0.3222	0.4860
0.3554	0.3047	0.3399	0.3240	0.2798	0.3962
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.2128	0.1808	0.6064	0.2129	0.1807	0.6064
0.1000	0.3512	0.5488	0.1000	0.3500	0.5500
0.3426	0.4861	0.1713	0.3426	0.4861	0.1713
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.5123	0.3877	0.1000	0.5118	0.3882
$G_w = 73.5677$			$G_w = 75.0697$		

Appendix Table C30 The most fit designs via GA and the optimal exact design with 13-points based on G -criterion assuming the special cubic model under SH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3700	0.1000	0.5300	0.3678	0.1000	0.5322
0.1000	0.3500	0.5500	0.1000	0.3500	0.5500
0.5000	0.2499	0.2501	0.5000	0.2500	0.2500
0.4067	0.2800	0.3133	0.4294	0.2357	0.3349
0.3103	0.3300	0.3597	0.2885	0.3135	0.3980
0.3838	0.4216	0.1946	0.4079	0.3881	0.2040
0.1109	0.4731	0.4160	0.1165	0.4625	0.4210
0.1853	0.2220	0.5927	0.1866	0.2200	0.5934
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.3343	0.4985	0.1672	0.3333	0.5000	0.1667
0.2702	0.1000	0.6298	0.2667	0.1000	0.6333
0.1932	0.5202	0.2866	0.2085	0.5367	0.2548
0.1000	0.5690	0.3310	0.1000	0.5700	0.3300
$G_w = 72.0109$			$G_w = 75.6236$		

Appendix Table C31 The most fit designs via GA and the optimal exact design with 8-points based on G -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3333	0.5000	0.1667	0.3333	0.5000	0.1667
0.2690	0.1000	0.6310	0.2775	0.1000	0.6225
0.1000	0.3698	0.5302	0.1000	0.3687	0.5313
0.4686	0.1000	0.4314	0.4743	0.1000	0.4257
0.1000	0.5699	0.3301	0.1000	0.5700	0.3300
0.2893	0.3043	0.4064	0.1913	0.2264	0.5823
0.1839	0.2242	0.5919	0.2910	0.3235	0.3855
0.4996	0.2505	0.2499	0.5000	0.2500	0.2500
$G_w = 79.4627$			$G_w = 80.2259$		

Appendix Table C32 The most fit designs via GA and the optimal exact design with 9-points based on G -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.3800	0.1009	0.5191	0.3570	0.1000	0.5430
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.4882	0.2601	0.2517	0.4913	0.2630	0.2457
0.1000	0.3507	0.5493	0.1000	0.3500	0.5500
0.3466	0.4763	0.1771	0.3521	0.4718	0.1761
0.2695	0.3052	0.4253	0.2885	0.3047	0.4068
0.2433	0.5165	0.2402	0.2500	0.5160	0.2340
0.1000	0.5664	0.3336	0.1000	0.5700	0.3300
$G_w = 73.8722$			$G_w = 75.9254$		

Appendix Table C33 The most fit designs via GA and the optimal exact design with 10-points based on G -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.3900	0.5100	0.1000	0.3765	0.5235
0.3378	0.4933	0.1689	0.3378	0.4933	0.1689
0.5000	0.2500	0.2500	0.5000	0.2500	0.2500
0.2475	0.5141	0.2384	0.2485	0.5254	0.2261
0.3367	0.1000	0.5633	0.3470	0.1000	0.5530
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.1000	0.5692	0.3308	0.1000	0.5700	0.3300
0.1633	0.2700	0.5667	0.1710	0.2765	0.5525
0.3033	0.2893	0.4074	0.3099	0.2983	0.3918
$G_w = 75.2897$			$G_w = 76.6085$		

Appendix Table C34 The most fit designs via GA and the optimal exact design with 11-points based on G -criterion assuming the special cubic model under WH for Snee's experiment.

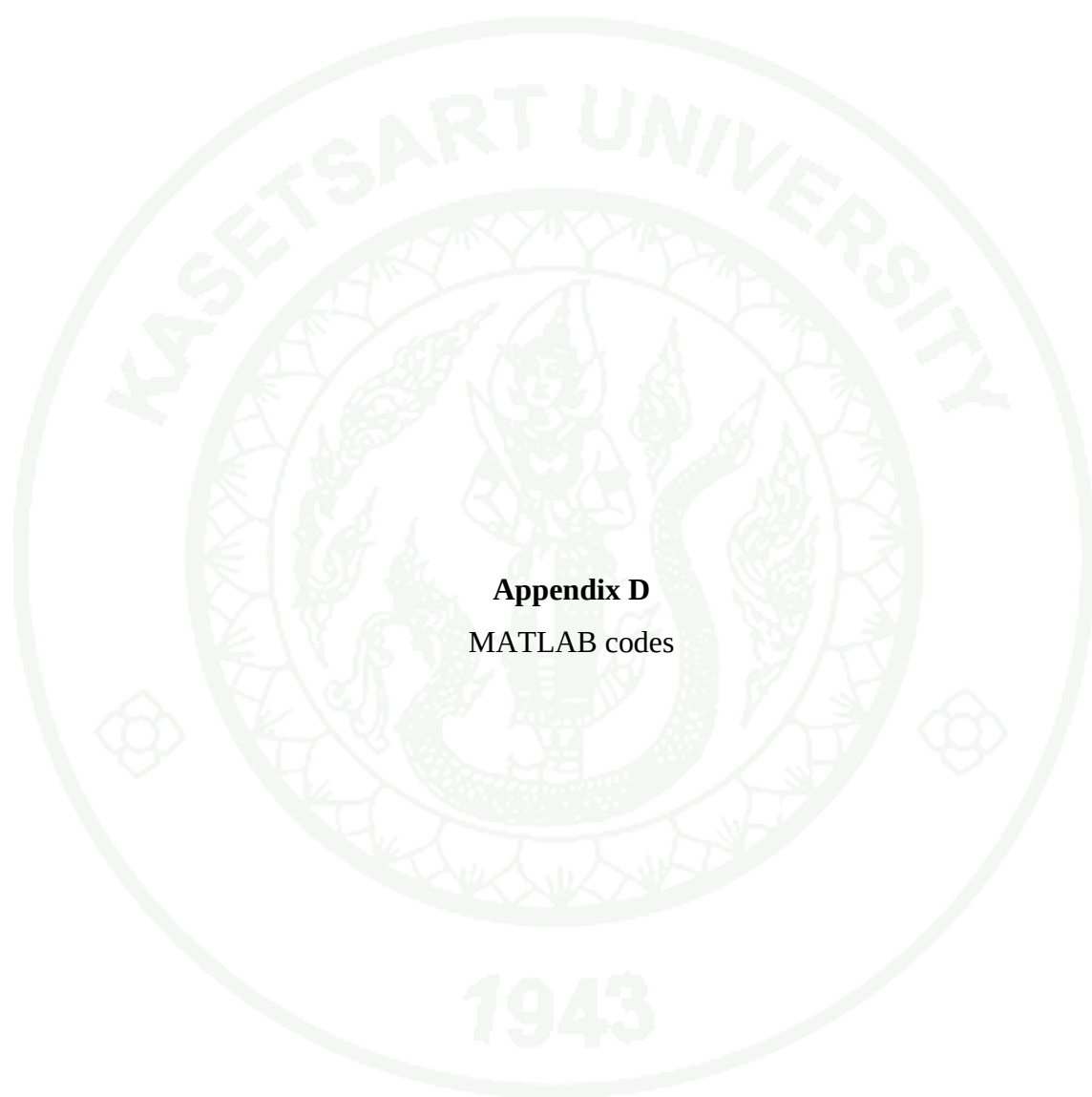
Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.5450	0.3550	0.1000	0.5575	0.3425
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.3000	0.3000	0.4000	0.2978	0.3058	0.3964
0.1609	0.2692	0.5699	0.1571	0.2645	0.5784
0.1536	0.5539	0.2925	0.1836	0.5369	0.2795
0.2667	0.1000	0.6333	0.2667	0.1000	0.6333
0.3483	0.4774	0.1743	0.3333	0.5000	0.1667
0.5000	0.2494	0.2506	0.5000	0.2500	0.2500
0.3823	0.4015	0.2162	0.3877	0.3858	0.2265
0.1000	0.3607	0.5393	0.1000	0.3655	0.5345
0.3500	0.1196	0.5304	0.3529	0.1010	0.5461
$G_w = 72.1812$			$G_w = 75.6349$		

Appendix Table C35 The most fit designs via GA and the optimal exact design with 12-points based on G -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1000	0.5689	0.3311	0.1000	0.5700	0.3300
0.5000	0.1000	0.4000	0.5000	0.1000	0.4000
0.1654	0.3774	0.4572	0.1644	0.4091	0.4265
0.3277	0.4938	0.1785	0.3190	0.5043	0.1767
0.2700	0.1001	0.6299	0.2667	0.1000	0.6333
0.2068	0.5380	0.2552	0.1990	0.5400	0.2610
0.3970	0.4044	0.1986	0.3972	0.4042	0.1986
0.1000	0.3801	0.5199	0.1000	0.3500	0.5500
0.3599	0.1000	0.5401	0.3600	0.1000	0.5400
0.3100	0.3002	0.3898	0.3250	0.2878	0.3872
0.4993	0.2510	0.2497	0.5000	0.2510	0.2490
0.1756	0.2373	0.5871	0.1754	0.2369	0.5877
$G_w = 71.6280$			$G_w = 73.0826$		

Appendix Table C36 The most fit designs via GA and the optimal exact design with 13-points based on G -criterion assuming the special cubic model under WH for Snee's experiment.

Most fit designs via GA			Optimal exact design		
x_1	x_2	x_3	x_1	x_2	x_3
0.1001	0.3594	0.5405	0.1000	0.3500	0.5500
0.2724	0.1000	0.6276	0.2667	0.1000	0.6333
0.3987	0.4019	0.1994	0.4000	0.4000	0.2000
0.4100	0.2300	0.3600	0.4347	0.2392	0.3261
0.3348	0.4978	0.1674	0.3333	0.5000	0.1667
0.1000	0.5698	0.3302	0.1000	0.5700	0.3300
0.5000	0.2439	0.2561	0.5000	0.2500	0.2500
0.1885	0.2173	0.5942	0.1984	0.2024	0.5992
0.2429	0.5271	0.2300	0.2036	0.5301	0.2663
0.1000	0.4789	0.4211	0.1000	0.4765	0.4235
0.3707	0.1000	0.5293	0.3827	0.1000	0.5173
0.5000	0.1031	0.3969	0.5000	0.1038	0.3962
0.2857	0.3500	0.3643	0.2835	0.3143	0.4022
$G_w = 72.1486$			$G_w = 75.3223$		



Appendix D
MATLAB codes

Examples of the program for calculating the objective functions based on weighted D - and G -optimality criteria for 3 components assuming the quadratic model using MATLAB student version 2010a are given.

```
%%
%% load the set of possible reduced models
%%
load Qx123.txt ;      % the full model is quadratic with q=3
vec = Qx123(:, :);
sumvec=sum(vec)';    % the number of parameters in each model
allpara=sum(sumvec); % sum of all parameter for all models
nmodel=length(vec); % the number of possible reduced models

%%
%% Calculate the values of the weighting factor where  $ic=((R-1)*W_{small})/Prange$  be
incremental values of the weighting factor,  $ws=(1/Prange)-(INCR*(Prange-1))/2$  be
the minimum of weighting factor,  $r$  be relative weighting factor, and  $pr$  be the number
of levels of the weighting factor
%%
syms ic ws r pr;
s=solve('ic=((r-1)*ws)/pr','ws=(1/pr)-((ic*(pr-1))/2)','r=100','pr=4');
ws=double(s.ws);
ic=double(s.ic);
cs = zeros(prm,1);
for ct = q:prm
    cs(ct) = length(find(sumvec==ct));
end;
for j=1:nmodel
    sv = sumvec(j);
    wvec(j)=ws+(sv-q)*ic;
    wgtvec(j)=wvec(j)/cs(sv);
end;
wgtvec=wgtvec';
```

```

%%
%% Calculate weighted D-optimality criterion
%%
objopt=[];
for i=1:ndcho
    deffopt=[];
    xtmp = y((i-1)*ndp+1:i*ndp, 1:prm); % xtmp = chromosome i
    for j =1:nmodel
        xtmpn=xtmp;
        loc=find(vec(j,)==0);
        xtmpn(:,loc)=[];
        d = det(xtmpn'*xtmpn);
        prms=sumvec(j);
        deff = 100*(d^(1/prms))/ndp;
        wgt=wtgvec(j);
        wdeff = wgt*deff;
        deffopt =[deffopt; wdeff ];
    end
    objdeff = sum(deffopt(1:nmodel,1));
    objopt = [objopt; i objdeff];
end

```

```

%%
%% Calculate weighted G-optimality criterion
%%
EV3;    % load fxt = the set of G-efficiency evaluation points
objopt=[];
for i=1:ndcho
    geffopt=[];
    xtmp = y((i-1)*ndp+1:i*ndp, 1:prm);    % xtmp = chromosome i
    for j = 1:nmodel
        gmax = 0;
        xtmpn=xtmp;
        loc=find(vec(j,)==0);
        xtmpn(:,loc)=[];
        xtx = xtmpn'*xtmpn;
        xtxinv = 1000*inv(xtx);
        fxtt=fxtb ;    % fxtt = canidate set of points
        fxtt(:,loc)=[];
        for a=1:Lfxtb
            gcrit=(ndp*fxtt(a,:)*xtxinv*fxtt(a,:))/1000;
            gmax = max(gmax,gcrit);
        end
        prms=sumvec(j);
        wgt=wgtvec(j);
        geff=(100*prms)/gmax ;
        wgeff = wgt*geff ;
        geffopt =[geffopt; wgeff]
    end
    objgeff = sum(geffopt(1:nmodel,1));
    objopt = [objopt; i objgeff];
end

```

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