Blocking Schemes for Definitive Screening Designs

Bradley JONES
SAS Institute
Cary, NC 27513 (Bradley.Jones@jmp.com)

Christopher J. NACHTSHEIM
Carlson School of Management
University of Minnesota
Minneapolis, MN 55455 (nacht001@umn.edu)

In earlier work, Jones and Nachtsheim proposed a new class of screening designs called definitive screening designs. As originally presented, these designs are three-level designs for quantitative factors that provide estimates of main effects that are unbiased by any second-order effect and require only one more than twice as many runs as there are factors. Definitive screening designs avoid direct confounding of any pair of second-order effects, and, for designs that have more than five factors, project to efficient response surface designs for any two or three factors. Recently, Jones and Nachtsheim expanded the applicability of these designs by showing how to include any number of two-level categorical factors. However, methods for blocking definitive screening designs have not been addressed. In this article we develop orthogonal blocking schemes for definitive screening designs. We separately consider the cases where all of the factors are quantitative and where there is a mix of quantitative and two-level qualitative factors. The schemes are quite flexible in that the numbers of blocks may vary from two to the number of factors, and block sizes need not be equal. We provide blocking schemes for both fixed and random blocks. Supplementary materials for this article are available online.

KEY WORDS: Alias; Conference matrix; Confounding; D-efficiency; Foldover; Orthogonal blocks; Small response surface designs.

1. INTRODUCTION

Definitive screening designs (DSDs) were recently introduced by Jones and Nachtsheim (2011). The structure of these designs is shown in Table 1, where \( x_{i,j} \) denotes the setting of the \( j \)th factor for the \( i \)th run. From the table, one can observe that an \( m \)-factor DSD requires \( 2m + 1 \) runs and that the \( 2m + 1 \) runs are comprised of \( m \) fold-over pairs and a run consisting of the center values of all the factors called a center run. The center run was added to allow the design to estimate the saturated model consisting of the intercept and linear plus quadratic main effects. With the exception of the center run, each run has exactly one factor level at its center value and all others at the extremes. We refer to these as edge runs because in any three-factor projection involving this factor such points are on the edges of the cube. Jones and Nachtsheim (2011) chose the specific values of the \( \pm 1 \) entries using the coordinate-exchange algorithm (Meyer and Nachtsheim 1995) to maximize the determinant of the information matrix for the model consisting of all linear and quadratic main effects. Thus, as originally introduced, DSDs were defined to be designs that are D-optimal subject to the structural constraints implied by Table 1. However, as developed below, subsequent work has broadened the definition and applicability of DSDs.

Jones and Nachtsheim (2011) identified various advantages of these designs, relative to the standard \( 2^{k-p} \) system (Box and Hunter 1961). Among them are (1) the number of required runs is only one more than twice the number of factors; (2) main effects are completely independent of two-factor interactions; (3) two-factor interactions are not completely confounded (though correlated) with any other two-factor interactions; (4) all quadratic effects are estimable; (5) quadratic effects are orthogonal to linear main effects and not completely confounded (though correlated) with two-factor interaction effects; and (6) with six through 16 factors, the designs are capable of estimating all possible full second-order models involving three or fewer factors with very high levels of statistical efficiency. Similarly, with 17 through 20 factors, these designs are capable of estimating efficiently all possible full second-order models involving four or fewer factors, and with 21 through at least 32 factors, they can estimate efficiently all full second-order models for five or fewer factors. The capability to project these designs to efficient response surface designs makes possible the screening and optimization of a system in a single step.

As stated previously, a number of extensions to the class of definitive screening designs have been proposed since the designs were introduced by Jones and Nachtsheim (2011). Xiao, Lin, and Fengshan (2012) showed that for many values of even \( m \), an \( m \times m \) conference matrix and its foldover could be used to guarantee the orthogonality of the linear main effects. This makes it possible to construct an orthogonal DSD for an odd number of factors by generating an orthogonal DSD for \( m' = m + 1 \) factors and then dropping the extraneous column. This results in an \( m \)-factor DSD with \( 2(m + 1) + 1 \) runs. Similarly, to increase the power of the design for detecting smaller linear effects and two-factor interactions, an investigator may create a design for a larger number of factors (say \( m' = m + k \) factors).
Then, the \( k \) spurious columns can be dropped yielding a design with \( m \) columns and \( 2(m + k) + 1 \) runs. If \( k \geq 1 \), then there are also runs without center values for any factor. We refer to these as vertex runs. This design if created using conference matrices also has orthogonal main effects that are unaliased by any second-order effects. Using this construction scheme, Jones and Nachtsheim (2013) showed how to incorporate two-level categorical factors while retaining key properties of DSDs. We treat all such modified designs as members of the class of DSDs.

DSDs with two-level categorical factors are mixed-level screening designs. Related approaches include Hedayat, Sloane, and Stufken (1999), Nguyen (1996), Wang and Wu (1992), and Xu (2002).

To date, the development of blocking schemes for DSDs has not been addressed in the literature. In what follows, we develop orthogonal blocking plans applicable for definitive screening designs. Related approaches include Hedayat, Sloane, and Stufken (1999), Nguyen (1996), Wang and Wu (1992), and Xu (2002).

The outline of the rest of this article is as follows. In Section 2 we provide schemes for orthogonal blocking treating the blocks as fixed effects. Section 3 deals with the relative D-efficiency of the proposed designs versus D-optimally blocked designs with the same number of runs and blocks. Section 4 provides results showing the effect of adding blocks on the power to detect main effects, quadratic effects and additional two-factor interactions. We also show the effect of adding blocks on the D-efficiency for estimating the full quadratic model across three-factor projections. Section 5 provides guidance for blocking when the blocks are treated as random instead of fixed. We provide a real example of a blocked DSD in Section 6. We conclude in Section 7 with a short discussion.

## 2. FIXED-EFFECTS BLOCKING SCHEMES

In this section, we take up the construction of blocking plans when we treat block effects as fixed. Throughout, we assume that there are \( B \) blocks, \( 2 \leq B \leq m' \), and that the number of runs in the \( b \)th block is \( n_b \geq 2 \). Let \( y_i \) denote the \( i \)th observation, which is contained in block \( b(i) \), where \( 1 \leq b(i) \leq B \). The \( j \)th quantitative factor setting of the \( i \)th run is denoted by \( x_{ij} \), for \( j = 1, \ldots, m \). If a full, second-order linear model with additive block effect is applicable, we write:

\[
y_i = \sum_{j=1}^{m} \beta_{ij} x_{ij} + \gamma_{b(i)} + \epsilon_i, \quad b(i) \in \{1, \ldots, B\}, \quad i = 1, \ldots, n.
\]

where the parameters \( \beta_0, \ldots, \beta_{mm} \) are unknown constants (of which many are zero by the sparsity of effects assumption), \( \gamma_1, \ldots, \gamma_B \) are the block effects, \( \gamma_{b(i)} \) is the block effect of the block containing the \( i \)th run, and the \( \{\epsilon_i\} \) are iid N(0, \( \sigma^2 \)). As model (1) implies, we employ indicator coding for the blocks, and we assume that all third- and higher-order effects, as well as all block-by-treatment interactions, are negligible. Since the goal is screening, and the number of runs is too small to permit estimation of the full second-order model, we assume that the experimenter might initially fit a first-order model to the response. This model is

\[
y_i = \sum_{j=1}^{m} \beta_{ij} x_{ij} + \epsilon_i, \quad b(i) \in \{1, \ldots, B\}, \quad i = 1, \ldots, n.
\]

In matrix terms, we write

\[
Y = L\beta_1 + Z\gamma + \epsilon,
\]

where \( Y \) is the response vector, \( L \) is the design matrix corresponding to the linear effects of the \( m \) factors, \( \beta_1 \) is the vector of linear main effects regression coefficients, and \( Z = (z_1, z_2, \ldots, z_B) \) is the matrix of block indicator columns, \( \gamma \) is the vector of block effects, and \( \epsilon \) is the random error vector. We refer to (2) as the linear main effects model. We will also refer, at times, to the model consisting of linear and quadratic main effects terms:

\[
y_i = \sum_{j=1}^{m} \beta_{ij} x_{ij} + \sum_{j=1}^{m} \gamma_{ij} x_{ij}^2 + \gamma_{b(i)} + \epsilon_i, \quad b \in \{1, \ldots, B\}, \quad i = 1, \ldots, n.
\]

In matrix terms, this model is

\[
Y = L\beta_1 + Q\beta_2 + Z\gamma + \epsilon,
\]

where \( Q \) denotes the quadratic main effects columns and \( \beta_2 \) is the vector of quadratic effect regression coefficients. We refer to (4) as the linear-plus-quadratic main effects model.

As we will demonstrate, we may need to add runs to guarantee the estimability of quadratic main effects. For an even number of factors (with no dropped columns) estimating the quadratic main effects requires one additional run per block. When all factors are continuous and \( m' > m \), only \( \max(B - (m' - m), 0) \) additional runs are needed. In other words, if the number of dropped columns is greater than or equal to the number of blocks, no additional center runs are needed. For simplicity, we first discuss blocking in the all-continuous-factors case. We then show how a simple modification of the all-continuous-factors scheme can be used to handle two-level categorical factors. Finally, we show some special results for the two-block case.
2.1 Blocking With Continuous Factors

In this subsection, our objective is to develop blocking plans such that the block effects are orthogonal to the linear main effects model terms and such that the linear-plus-quadratic main effects model is estimable. Assume that all $m$ factors are quantitative and that an $m'$-factor DSD has been constructed, where $m' = m + k$, having $n = 2(m + k) + 1$ runs. Delete the center run from the DSD, giving a $(2(m + k))$-run design. Assigning these runs to blocks is a two-step procedure. We first construct a blocked design that is nonsingular for the linear-plus-quadratic main effects model and for which the block effects are orthogonal to the linear main effects. Orthogonality results by assigning both members of any foldover pair to the same block. We then use an interchange procedure, described below, to obtain the D-optimal assignment of foldover pairs to blocks. In what follows, the model we employ for the D-optimality criterion includes both the treatment effects and the block effects. Moreover, we refer to designs constructed algorithmically based on the $D$ criterion as D-optimal designs. There is, of course, no guarantee that the designs constructed in this fashion are globally D-optimal, although we use multiple random starts in an effort to find the globally optimal solution.

Step 1: Obtain a nonsingular starting design. The procedure is as follows:

1.a Construct the base design. The base design is the DSD for $m$ factors based on $m'$ foldover pairs, omitting the center run. $m$ of these foldover pairs are edge runs, and $k$ pairs of runs are vertex runs. For illustration, the base design for $m = 5$ and $m' = 6$ is displayed in the first 12 runs for factors $X_1$ through $X_5$ in Table 2.

1.b Sequentially assign foldover pairs to blocks. In Table 2, where we construct a design in three blocks, we assign foldover pair 1 to block 1, foldover pair 2 to block 2, foldover pair 3 to block 3, foldover pair 4 to block 1, and so on, until all foldover pairs are assigned to blocks. The results of this step for the $m = 5$ and $m' = 6$ example are shown in runs 1 through 12 of columns $z_1$ through $z_3$ of Table 2. If the desired block sizes are unequal, the procedure for initial assignment of foldover pairs to blocks is exactly the same as the equal-block-size case, except that a check is made before assigning the next foldover pair to a block. If the block does not have space available for another foldover pair, we continue checking sequentially until we come to a block that still has available space. The pair is then assigned to that block.

1.c If $k = 0$, add $B$ center runs, one per block. If $k > 0$, $k$ of the vertex foldover pairs have been assigned to blocks at this point. Add max$(B - k, 0)$ center runs, one per block, to the blocks that do not already contain a vertex run. In the example of Table 2, $k = 1$, and note that the one vertex run foldover pair has been assigned to block 3. Thus $B - k = 3 - 1 = 2$ center runs are added, with one center run placed in block 1 and one center run placed in block 2.

Theorem 1. The starting design constructed using Steps 1a to 1c above is nonsingular for the linear-plus-quadratic main effects model. Moreover, the block effects are orthogonal to the linear main effects.

We provide the proof of Theorem 1 in the supplementary materials. Theorem 1 indicates that block effects are orthogonal to linear main effects and that the starting design is nonsingular for the linear-plus-quadratic main effects model. It is worth restating that the block effects are fully orthogonal to the linear main effects in model (2); however, if model (4) is operative, block effects will be correlated with the quadratic main effects. Finally, Theorem 1 does not guarantee optimality of the blocking scheme. We take up the issue of optimality next.

Step 2: Find the optimal assignment of foldover pairs to blocks. Since block effects are correlated with the quadratic main effects, interchanging foldover pairs from different blocks can affect the value of the $D$ criterion for the linear-plus-quadratic main effects model. For small designs, one can determine an optimal assignment of foldover pairs to blocks by exhaustive search. For larger designs, an interchange procedure avoids the exponential time required by exhaustive search. Our interchange procedure is a greedy optimization approach that sequentially considers the exchange of each foldover pair with all foldover pairs residing in other blocks. If an improvement can be made by an interchange, or swap, of foldover pairs between blocks, the interchange is made, the determinant is updated, and the procedure restarts. The procedure continues until no further improvements via block interchanges can be found. In our implementation, we use a random ordering of the $m'$ foldover pairs in Table 2 to construct a “random” starting design. We then apply the interchange procedure and find a best assignment of foldover pairs to blocks. We then repeat this procedure for $s$ random starting designs and retain the best of the $s$ solutions. We constructed optimal designs in this fashion and compared the results to the globally optimal design found by exhaustive search. Our experience suggests that using $s = 20$ random starts consistently
identifies the optimal design. For the example of Table 2, the interchange procedure was not able to make any improvements to the starting design.

It is common in many fields to employ uniform block sizes. For this reason, we have provided, in Figure 1, all blocking schemes for six through 12 factors that provide the most uniform distribution of block sizes for given numbers of factors and blocks. Note that Figure 1 does not reflect the full flexibility of the blocking scheme. For example, the uniform blocking scheme for six factors is comprised of three blocks of size five. Two other orthogonally blocked arrangements in three blocks exist: namely, three blocks comprised of seven, five, and three runs or three blocks comprised of nine, three, and three runs.

2.2 Adding Two-Level Categorical Treatment Factors

In this section we describe blocking schemes for DSDs with added two-level categorical factors. In particular we will focus on the blocking of DSDs constructed using the DSD-augment method of Jones and Nachtsheim (2013). The form of the linear-main-effects model and the quadratic-main-effects models change, due to the presence of two-level categorical factors. The linear-main-effects model becomes

\[ y_i = \sum_{j=1}^{m+c} \beta_{ij} x_{ij} + \gamma_{b(i)} + \varepsilon_i, \quad b \in 1, \ldots, B, \]

\[ i = 1, \ldots, n, \quad (6) \]

while the linear-plus-quadratic-main-effects model becomes

\[ y_i = \sum_{j=1}^{m+c} \beta_{ij} x_{ij} + \sum_{j=1}^{m} \beta_{ij} x_{ij}^2 + \gamma_{b(i)} + \varepsilon_i, \quad b \in 1, \ldots, B, \]

\[ i = 1, \ldots, n, \quad (7) \]

Consider, for illustration, the case in which the number of continuous factors is \( m = 4 \), the number of categorical factors is \( c = 2 \), and the number of blocks is \( b = 4 \). The DSD design matrix obtained using the DSD-augment procedure is shown in rows 1 through 12 of Table 3(a). The DSD-augment procedure first obtains a conference matrix and its foldover for \( m' = m + c + k \) factors, where \( k \) is chosen so that \( m' \) is even. The center values for the categorical columns in each foldover pair are then changed from zeros to best settings \( \pm 1 \) using an optimization procedure. The starred settings in rows 9–12 of Table 3(a) reflect these changes. The starting design algorithm for the fixed-effects blocking scheme for continuous factors can now be applied with two modifications:

1. Whenever a center run is required, we add two center runs. In the first run, the values of the categorical factors are arbitrarily set to \(-1\); in the second, these values are set to \(+1\). The resulting starting design has rank \( 2m + c + B \). (This fact is easily shown with a minor modification to the proof of Theorem 1.)
2. The starting settings for the categorical factors will likely not be optimal. These settings must be optimized, along with the assignment of foldover pairs to blocks in the interchange procedure. Pseudo code and a JMP script for the combined interchange procedure are provided in the supplementary materials.

The design produced by the combined interchange procedure is shown in Table 3(b). The improvement resulting from the interchange procedure is generally not large. In this case the efficiency of the final design, relative to the starting design, is 108%.

2.3 Blocking via Added Categorical Factor

The ORTH-augment procedure of Jones and Nachtsheim (2013) provides a method for augmenting a DSD with a small number of two-level categorical factors, such that the added factors are orthogonal to each other, and to the continuous factors. This suggests an alternative approach to blocking when the number of desired blocks is \( B = 2 \). One can simply use
the ORTH-augment procedure with an odd number of continuous factors to add one two-level categorical factor, and then use the levels of the added factor to define the block levels. We investigate this alternative briefly in this subsection.

Table 4(b) shows the blocked DSD using the scheme of Section 2.1, while Table 4(b) shows the orthogonal DSD for 5 continuous factors and one two-level categorical factor of Jones and Nachtsheim (2013). To use Table 4(b) as a design with continuous factors and one two-level categorical factor of Jones and Nachtsheim (2013) does not extend to designs created using the fixed-effects blocking scheme. Therefore, we prefer the blocked design in Table 4(b) over the fixed-effects blocking approach of Section 2.1. However, for designs having an even number of continuous factors, the designs of Jones and Nachtsheim (2013) require two more runs than the designs created using the fixed-effects blocking scheme. Finally, the method of Jones and Nachtsheim (2013) does not extend to designs having more than two blocks, making it a special case rather than a general purpose tool.

3. EFFICIENCY OF BLOCKING SCHEMES

One concern about adding sufficient center runs to allow for the estimation of all the quadratic effects is that the resulting efficiency of the blocked DSD might drop unacceptably. To
investigate this, we generated blocked D-optimal designs using JMP for six and 12 factors in two through six blocks. The a priori model used for the D-optimal design was linear-plus-quadratic main effects model (4).

We then evaluated the relative D-efficiency of the blocked DSDs for the same cases with the same number of runs. The results appear in Table 5. We compared the relative D-efficiency of the two designs for both the linear main effects model and the a priori model used to generate the D-optimal design. As expected, the DSD does not perform well compared to the D-optimal design for the linear-plus-quadratic effects model (4). Also as the number of blocks increases the relative efficiency of the blocked DSD decreases. For six factors this decrease is from 88% for two blocks to 62% for six blocks. For 12 factors this decrease is from 74% for two blocks to 60% for six blocks. However, for estimating the linear main effects model the DSD generally outperforms the D-optimal design though the relative efficiency still drops as the number of blocks increases. For six factors this decrease is from 88% for two blocks to 62% for six blocks. For 12 factors blocks is 128% which falls to 113% for six blocks.

For 12 factors the relative efficiency for a DSD having two blocks is greater. Thus, our orthogonally blocked DSDs are capable of detecting strong curvature in the effect of one continuous factor if such curvature exists.

DSDs, whether blocked or not, have the capability of fitting two-factor interactions instead of quadratic effects. We investigated the effect of the number of factors and the number of blocks on the average, minimum and maximum power for signal-to-noise (SN) ratios of 1, 2, and 3. The results appear in Table 8. Two main patterns that emerge from an examination of Table 8. First, as the number of blocks increases, the power for detecting a quadratic effect decreases. Second, as the number of factors increases, the power for detecting a two-factor interaction increases. In general, the power for detecting a two-factor interaction varies across the set of interactions. Interestingly, we found that if the number of blocks equals the number of factors blocks SN $\frac{\beta_0}{\sigma}$.

Table 6. Power of DSD in any number of blocks to detect any main effect

| $m$ | $\text{SN} = 1$ | $\text{SN} = 2$ | $\text{SN} = 3$ |
|-----|----------------|----------------|----------------|
| 6   | 0.750          | 0.999          | 1.000          |
| 8   | 0.900          | 0.999          | 1.000          |
| 10  | 0.967          | 1.000          | 1.000          |
| 12  | 0.990          | 1.000          | 1.000          |

4. IMPACT ON POWER AND PROJECTION PROPERTIES

In this section we consider the power and projection properties of the orthogonally blocked DSD using the fixed-effects blocking scheme. We begin by calculating the power to detect active main effects as a function of the number of factors and the magnitude of the effect. Table 6 shows the power to detect any main effect for model (2) for signal-to-noise (SN) ratios of 1, 2, and 3 and for designs with 6, 8, 10, and 12 factors. We define the SN ratio as the ratio of the absolute value of the regression coefficient to the error standard deviation (i.e., $|\beta_0|/\sigma$). We also assume, in all of our power calculations, that hypothesis tests will employ an $\alpha = 0.05$ level of significance. Each of the four designs employed in the power study summarized in Table 6 include a center run in each block. None of the reported power values in Table 6 are a function of the number of blocks. As expected, the power increases as the number of factors or SN ratio increases. We see that it is virtually certain that a DSD with six or more factors will detect any main effect with a SN ratio of 2 or greater.

Table 7 shows the effect of changing the number of factors, number of blocks and SN ratio on the power to detect a single added quadratic effect. The power for detecting a quadratic effect added to the main effects model is not a function of the specific quadratic effect chosen. Power increases with increases in the SN ratio, the number of factors or the number of blocks. However, the power to detect a quadratic effect is substantially lower than the power to detect a main effect of the same magnitude. We observe that to be assured of detecting an active quadratic effect that effect needs to have an SN ratio of 3 or greater. Thus, our orthogonally blocked DSDs are capable of detecting strong curvature in the effect of one continuous factor if such curvature exists.

Table 7. Power of DSD in two through $m$ blocks to detect one quadratic effect

| Number of factors | Number of blocks | $\text{SN} = 1$ | $\text{SN} = 2$ | $\text{SN} = 3$ |
|-------------------|-----------------|----------------|----------------|----------------|
| 6                 | 2               | 0.257          | 0.728          | 0.966          |
| 6                 | 6               | 0.317          | 0.828          | 0.990          |
| 8                 | 2               | 0.313          | 0.829          | 0.991          |
| 8                 | 8               | 0.462          | 0.957          | 1.000          |
| 10                | 2               | 0.349          | 0.878          | 0.997          |
| 10                | 10              | 0.589          | 0.991          | 1.000          |
| 12                | 2               | 0.375          | 0.904          | 0.998          |
| 12                | 12              | 0.694          | 0.998          | 1.000          |
number of factors, then the power for detecting any two-factor interaction is the same for all two-factor interactions.

We now consider the projection properties of the orthogonally blocked DSDs. Jones and Nachtsheim (2011) stated that for DSDs with 6 to 12 factors, any three factor projection results in a design capable of fitting the full quadratic model with high D-efficiency. Table 9 reproduces that analysis for orthogonally blocked DSDs with either two blocks or $m$ blocks each containing one center run.

Using JMP, we created D-optimal designs having the same number of observations and blocks as each blocked DSD we considered. The D-efficiencies we report are relative to the D-efficiencies of these D-optimal blocked designs each with three continuous factors and a model consisting of all the main effects, two-factor interactions, quadratic effects, and block effects.

We again observe two main patterns in Table 9. The average relative D-efficiency over all the three-factor projections of the blocked DSDs increases as the number of factors increases. However, for a given number of factors the average relative D-efficiency decreases as the number of blocks increases.

Again interestingly, when the number of blocks equals the number of factors, the relative D-efficiency for the quadratic model of all the three-factor projections of the blocked DSDs is the same.

5. RANDOM BLOCKS

The models for analyzing data from blocked experiments using random blocks has the same form as (3) and (5) except that the effects $\gamma$ are random rather than fixed. We therefore assume that the block effects as well as the residual errors are random effects that are all independent and normally distributed with zero mean. We also assume that the block effects have variance $\sigma^2_\gamma$, and that the residual errors have variance $\sigma^2_\varepsilon$.

Given these assumptions, the variance–covariance matrix of the response vector is $\mathbf{V} = \sigma^2_\gamma \mathbf{Z} \mathbf{Z}' + \sigma^2_\varepsilon \mathbf{I}_n$. A design that is D-optimal for a linear model with random blocks maximizes the determinant of the information matrix $\mathbf{X}' \mathbf{V}^{-1} \mathbf{X}$. In general, the information of a design with random blocks is a function of the ratio $\sigma^2_\gamma / \sigma^2_\varepsilon$, which we designate $\eta$. We set $\eta$ to 1 for our efficiency comparisons below.

One advantage to using random instead of fixed blocks is that, for designs requiring many blocks, it is unnecessary to add as many center runs as blocks to the DSD to estimate both the linear and quadratic fixed effects. The DSD with one center run is saturated for model (4). Adding two more center runs is sufficient for estimating the error variance and the block variance. Mylona, Goos, and Jones (2014) provided a method to ensure the estimability of $\sigma^2_\gamma$ when a design is saturated or nearly saturated for estimating the fixed effects and variance components. They accomplish this by replicating a run within one block. Replicating a center run in one block provides a pure error degree of freedom for the estimation of $\sigma^2_\gamma$. Adding a third center run to a different block ensures the estimability of $\sigma^2_\gamma$. So, this way of apportioning three center runs neatly divides the degrees of freedom for estimating the two variance components while maintaining the many good features of the DSD.

Table 10 displays the six factor design in three blocks constructed in this manner. The first column shows the assignment of runs to blocks. Note that there are six runs in the first block, five in the second block, and four in the third block. The replicated center run in block 2 provides one degree of freedom for

| Number of Factors | Number of blocks | Number of projections | Average D-efficiency | Minimum D-efficiency | Maximum D-efficiency |
|-------------------|-----------------|-----------------------|----------------------|----------------------|----------------------|
| 6                 | 2               | 20                    | 0.856                | 0.856                | 0.856                |
| 6                 | 6               | 20                    | 0.695                | 0.695                | 0.695                |
| 8                 | 2               | 56                    | 0.942                | 0.855                | 0.959                |
| 8                 | 8               | 56                    | 0.786                | 0.786                | 0.786                |
| 10                | 2               | 120                   | 0.893                | 0.777                | 0.944                |
| 10                | 10              | 120                   | 0.719                | 0.719                | 0.719                |
| 12                | 2               | 220                   | 0.894                | 0.750                | 0.928                |
| 12                | 12              | 220                   | 0.737                | 0.737                | 0.737                |

TECHNOMETRICS, FEBRUARY 2016, VOL. 58, NO. 1
error variance estimation. The third center run provides one degree of freedom for estimating the block variance. As shown by Mylona, Goos, and Jones (2014), taking these precautions helps to avoid convergence problems in restricted maximum likelihood (REML) estimation and allows for inference on all of the fixed effects.

Column 2 of Table 10 shows the random block assignments to the DSD runs for the case having five blocks and 15 runs. Note that since the first block already has four runs, the first pair of center runs is assigned to the second block and the final center run to the third block. This leads to block sizes of 4, 4, 3, 2, and 2, respectively. This arrangement for the five blocks provides the most uniform block sizes possible, given the restrictions required for avoiding inference problems.

To investigate the utility of this approach we created D-optimal random block designs for model (4) for four cases. For six factors we considered three blocks of five runs and five blocks of three runs. For 12 factors we considered three blocks of nine runs and nine blocks of three runs. We constructed blocked DSDs using the method described above.

Results of this investigation appear in Table 11. The relative D-efficiencies of the DSD compared to the D-optimal random block design generated using JMP now increase as the number of blocks increases for both the linear-main-effects model and the linear-plus-quadratic main effects model. The random block DSDs are uniformly better than the corresponding D-optimal designs for estimating the linear main effects model.

### 6. An Example: Laser Etch Experiment

In'Tech Industries is a global supplier of miniature plastic hearing aid component parts. Labeling of these miniature parts is accomplished using a laser etching process. The depth, width, and overall readability of the etch is affected by machine settings that include the speed of the etch (Mark Speed), the number of times that the etch is repeated (Repetitions), the percentage power level (Percent Power), and the laser frequency (Frequency). Other potential uncontrollable factors include the ambient temperature, ambient humidity, and operator. Etching is normally carried out by one of three operators in the company.

In an effort to identify key factors and (if possible) optimal operating conditions, In'Tech constructed a DSD based on the four control factors. The experiment was run in three blocks, with each block assigned to a different operator. With four factors, an 11-run DSD could be constructed with block sizes of 4, 4, and 3. The engineers felt that these block sizes were too small and that equal block sizes of five or more would be preferable. For this reason, we added two pseudo-factors and constructed a six-factor DSD in 13 runs. This design could be fielded in three blocks of size five—with one center run per block plus four vertex runs all assigned to the first block. The design is reproduced in Table 12. Each run involved etching a blank plastic chip with the letters “DOE Run XX” and the date of the run etched below. Once the etching was complete, width, depth, and readability of the etches were recorded. Readability is a subjective measurement that was obtained as follows. Each of seven technicians ranked the 15 chips from best (rank 1) to worst (rank 15) in terms of clarity and readability. Average ranks (across the seven technicians) were then obtained for each chip. The rankings were fairly consistent across raters.

To model the data, a forward stepwise analysis based on the AICc criterion was conducted, where potential terms included all first and second order terms among the control factors and the two block terms. The model found by the AICc stepwise procedure is

\[
\hat{Y} = 4.081 + 1.171X_2 - 1.743X_3 + 6.193X_2^2 + 1.743X_1X_2
\]

using scaled units from −1 to 1 for \(X_1\) through \(X_3\). (The same model resulted when using a p-value threshold criterion, with the threshold equal to 0.05.) Neither the block effect nor the Repetition effect entered our final model. Assuming the fitted model is correct, the best setting for Mark Speed is 15,000 (the high level). For frequency and percent power, the best settings are 1 and 38%, respectively. Five confirmatory tests made at these settings led to etchings that were extremely readable and consistent. (A JMP 11 regression summary and associated profile plots of factor effects are provided in the supplementary materials.)

As sometimes happens, the block effect was small in this experiment. Investigators block experiments when they fear that an uncontrollable source of variation will swamp the effects if the design is completely randomized instead of being run in blocks. We reran the analysis of the experiment after adding
two units to the response for each run in the first block and subtracting one unit from each run in the other two blocks. This simulated a block effect with a sum of squares nearly 10 times greater than the error sum of squares. Our analysis procedures found exactly the same treatment effects while accommodating for the strong block effect.

7. DISCUSSION

In this article we have shown how to create orthogonally blocked DSDs, investigated their statistical properties and provided a real application. It is surprisingly simple to create orthogonal blocks from a DSD. All that is required is that runs in foldover pairs appear together in a block. Thus, for an even number of factors, \( m \), we can have \( m \) blocks each having one foldover pair. Alternatively, we can have two blocks with half of the foldover pairs in each block. These two cases represent the extremes but there are other possibilities. Blocks need not have the same number of runs. For example some blocks could have only one foldover pair while others have two or more.

For studies employing quantitative factors only, we advocate adding a center run to each of \( \max(B-k,0) \) blocks to guarantee estimability of the linear-plus-quadratic main effects model. However, adding a center run to each of these blocks is not strictly necessary if the cost of each run is high and the practitioner is willing to accept the risk of model ambiguity should either block effects or quadratic effects be active. The supplementary materials provide a greedy blocking scheme for fixed blocks and shows the resulting aliasing of block effects with quadratic effects.

If there is a mix of quantitative and two-level categorical factors, we suggest adding a pair of center runs to each of \( \max(B-k,0) \) blocks to guarantee estimability of the linear-plus-quadratic main effects model. The levels of the categorical factors in each of these added pairs is determined algorithmically.

The fixed-effects blocking scheme indicates that center runs must be added to each of \( \max(B-k,0) \) blocks to guarantee estimability of the linear-plus-quadratic main effects model. This has an interesting implication for unblocked DSDs—in which case \( B = 1 \). If any vertex runs are present, \( k > 0, \max(B-k,0) = 0 \), and Theorem 1 indicates that no center runs are needed for estimation of the linear-plus-quadratic main effects model. Stated simply, a center run is not required in an unblocked DSD whenever vertex runs are present.

Finally, we note a more general result concerning the orthogonal blocking of designs that are self-fold-over designs. For such designs any blocking scheme where the two runs in each fold-over pair appear together in a block is orthogonally blocked.

SUPPLEMENTARY MATERIALS

Supplementary files available on the Technometrics website are as follows:

Proof: Theorem1Proof.pdf. Restatement and proof of Theorem 1.
Greedy blocking scheme: GreedyBlockingScheme.pdf. Description of Greedy blocking scheme that confounds block and quadratic effects.
Computer code: DSDBlockInterchange.jsl. JMP scripting language (JSL) code for creating Blocked DSDs.
Algorithm: DSD Pseudocode.pdf. Pseudo-code for implementing blocked DSDs.
Analysis Output: EtchStudyAnalysis.pdf. JMP computer output for the Laser Etch Study.
Text: ReadMe.txt. Explanations of the supplementary material contents.

[Received July 2013. Revised January 2015.]

REFERENCES

Box, G. E. P., and Hunter, J. S. (1961), “The \( 2^{k-p} \) Fractional Factorial Designs,” Technometrics, 3, 449–458. [74]
Hedayat, A. S., Sloane, N. J. A., and Stufken, J. (1999), Orthogonal Arrays: Theory and Applications, New York, NY: Springer. [75]
Jones, B., and Nachtsheim, C. J. (2011), “A Class of Three-Level Designs for Definitive Screening in the Presence of Second-Order Effects,” *Journal of Quality Technology*, 43, 1–14. [74,80]
——— (2013), “Definitive Screening Designs With Added Two-Level Categorical Factors,” *Journal of Quality Technology*, 45, 121–129. [75,77,78]
Meyer, R. K., and Nachtsheim, C. J. (1995), “The Coordinate-Exchange Algorithm for Constructing Exact Optimal Experimental Designs,” *Technometrics*, 37, 60–69. [74]
Mylona, K., Goos, P., and Jones, B. (2014), “Optimal Design of Blocked and Split-Plot Experiments for Fixed Effects and Variance Component Estimation,” *Technometrics*, 56, 132–144. [80]
Nguyen, N.-K. (1996), “A Note on the Construction of Near-Orthogonal Arrays With Mixed Levels and Economic Run Size,” *Technometrics*, 38, 279–283. [75]
Wang, J. C., and Wu, C. F. J. (1992), “Nearly Orthogonal Arrays With Mixed Levels and Small Runs,” *Technometrics*, 34, 409–422. [75]
Xiao, L., Lin, D. K. J., and Fengshan, B. (2012), “Constructing Definitive Screening Designs Using Conference Matrices,” *Journal of Quality Technology*, 44, 1–7. [74]
Xu, H. (2002), “An Algorithm for Constructing Orthogonal and Nearly-Orthogonal Arrays With Mixed Levels and Small Runs,” *Technometrics*, 44, 356–368. [75]