# Some new designs for quantitative factors

*Citation for published version (APA):*
Berkum, van, E. E. M., & Upperman, P. M. (1995). *Some new designs for quantitative factors*. (Memorandum COSOR; Vol. 9503). Technische Universiteit Eindhoven.

*Document status and date:*
Published: 01/01/1995

*Document Version:*
Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Memorandum COSOR 95-03, 1995, Eindhoven University of Technology

# Some new designs for quantitative factors

E.E.M. van Berkum
Department of Mathematics and Computing Science
Eindhoven University of Technology
P.O. Box 513, 5600 MB Eindhoven, The Netherlands

P.M. Upperman
Quality Engineering Consultancy
Kapteynlaan 16, 5505 AZ Veldhoven, The Netherlands

$D$-optimal designs are given for some incomplete quadratic models in linear regression. The quadratic models are incomplete in the sense that not all quantitative factors have quadratic terms. The experimental region is a $q$-dimensional cube. Two methods are developed to construct small designs for quantitative factors. The first method uses the new concept of design generator. The second uses properties of $D$-optimal designs for the incomplete quadratic model. An application of a design with 8 experiments is included.

*Key words & Phrases*: $D$-optimal designs, approximate theory, linear regression, incomplete quadratic models, quantitative factors, design generator, orthogonality, exact designs.

# 1 Introduction

Many designs for quantitative factors have been developed during the past 40 years. They are very economical as regards the number of designs points needed, in spite of the fact that many of these designs, such as some response surface plans, use 5 levels for each factor.
Articles dealing with response surfaces where written by Box and Draper (1959, 1963), Box and Hunter (1957), Lucas (1974), Welch (1984) and Myers, Khuri and Carter (1988). Box and Behnken (1960), Hoke (1974), Mitchell and Bayne (1978) and Rechtschaffner (1967) deal with designs for quantitative factors with three levels. The designs for 3, 4, 5, 6, 7, 9, 10, 11, 12 or 16 factors, of Box and Behnken, are frequently used in practical work. Box and Draper (1974) discuss designs in which each factors has four unequally spaced levels, which may be a disadvantage in a practical situation.
There are several books dealing with response surface methodology such as Box, Hunter and Hunter (1978), Box and Draper (1987), Cochran and Cox (1957), Montgomery (1976) and Upperman (1974). It is mostly assumed that the response surface model can be presented by a second degree polynomial. Box and Draper (1987) is especially useful since it incorporates many results given in articles which were previously published.

# 2 The need for new designs with quantitative factors

Although an experimenter can choose from many designs for quantitative factors, our experience in statistical consultation has shown that available designs are not always satisfactory. There are three reasons:

(i) these designs have factors with the same number of levels, mostly 3 or 5;

(ii) designs with factors having four equally spaced levels are not available;

(iii) the number of experimental units is rather large.

Many experimenters only want to carry out small experiments because of time and costs involved. There is therefore a real need for a great variety of designs with quantitative factors having a small number of experimental units. The experimenter moreover wants some freedom as to the choice of the number of levels per factor. It may for instance be necessary to incorporate four available equally spaced levels, such as 4 wire diameters, in an experiment. It would then be unwise to use three levels, since it would force the experimenter to omit either the smallest or the largest diameter, although three levels would be sufficient to estimate linear and quadratic terms of a model. Especially in the preliminary states of experimental work, for instance research concerning integrated circuits, it is desirable to carry out small experiments in which a number of quantitative factors is varied simultaneously and knowledge as regards their main effects and two-factor interactions is required. This article describes some methods which enable us to construct small designs for quantitative factors, while maintaining as much orthogonality of the design as possible. To calculate the $D$-efficiency of these designs a class of $D$-optimal designs is developed in Section 3.
Two methods are discussed to construct small designs for quantitative factors:

(i) the first method constructs plans from the $2^n$ design using the new concept of "design generator". See Section 4;

(ii) the second method is described in Section 5.5 and uses properties of the $D$-optimal designs developed in Section 3.

The designs to be developed have been constructed using the following restrictions:

(i) factors have two, three or four levels;

(ii) the two-level factors may be qualitative or quantitative;

(iii) the three- and four-level factors are quantitative and the levels are equally spaced;

(iv) all interactions of more than two factors are ignored;

(v) the mathematical model of the observations is an incomplete quadratic model. See Section 3.1.

The two construction methods mentioned yield designs which have three advantages over many other designs with quantitative factors:

(i) the number of levels for each factor varies between 2 and 4 whereas many existing designs, such as the central composite designs of Cochran and Cox (1957) and the Box and Behnken (1960) designs, require each factor to have the same number of levels;

(ii) many designs contain a two-level factor which may of course be either qualitative or quantitative;

(iii) there is a great variety of small designs to choose from.

# 3 $D$-optimal designs for an incomplete quadratic model

## 3.1 Some basic definitions

It was announced in Section 2 that the designs to be developed have factors with two, three or four levels and that an incomplete quadratic model shall be used. The model we consider is incomplete in the sense that $k$ variables have linear and quadratic terms, but the other $(q-k)$ variables, corresponding with $(q-k)$ two-level factors, have only linear terms. All $\binom{q}{2}$ interactions of two factors are however included in the model. So we have the model

$$Y = \beta_0 + \beta_{11}x_1^2 + \ldots + \beta_{kk}x_k^2 + \beta_1 x_1 + \ldots + \beta_q x_q +$$
$$+\beta_{12}x_1x_2 + \ldots + \beta_{q-1,q}x_{q-1}x_q + \varepsilon \ , \qquad (1)$$

where each $x_i$ corresponds to a factor of the design, $Y$ is the response, and $\varepsilon$ is the error term of the response variable in the model. The experimental region $\mathcal{X}$ is defined by

$$\mathcal{X} = \{x \in I\!R^q | x = (x_1, ..., x_q)', -1 \le x_i \le 1 \text{ for all } i = 1, ..., q\} .$$

The experiment consists of $N$ runs. The number of parameters $p$ equals

$$p = q + \begin{pmatrix} q \\ 2 \end{pmatrix} + 1 + k = 1 + k + \tfrac{1}{2}q(q+1) .$$

The design matrix can be seen as a probability distribution giving weights $N^{-1}$ to $N$ not necessarily distinct elements of the experimental region $\mathcal{X}$. Such a design is called 'exact' because it can be realised in practice. The derivation of optimal designs is simplified by using the so-called approximate theory in which the $N$-trial design is replaced by a measure $\xi$ over $\mathcal{X}$. In the sequel we present $D$-optimal designs (approximate theory) for the model (1). These designs are new and have not previously been published. They will enable us to calculate the $D$-efficiency of the designs to be developed in Section 4 an 5.

### 3.2 $D$-optimal designs

First we give the $D$-optimal designs for model (1), where the experimental region $\mathcal{X}$ is a $q$-dimensional cube.

**Definition 1**. We define a design $\xi(\alpha, \beta, \gamma)$ consisting of three subsets as follows:

i) the $2^q$ vertices of the $q$-dimensional cube with weights $\alpha$.

ii) the $k2^{q-1}$ elements of $\mathcal{X}$, where one of the $k$ quadratic variables has the value zero, and all other variables have the value $-1$ or $+1$, these points are given weights $\beta$; the points are in the middle of some edges, but not all edges,

iii) the $\left( \begin{smallmatrix} k \\ 2 \end{smallmatrix} \right) 2^{q-2}$ elements, where two of the $k$ quadratic variables are equal to zero and all other variables have the value $-1$ or $+1$, these points are given weights $\gamma$ and are situated at the centers of some two-dimensional faces; if $k = 1$ this set is empty.

The spectrum of the designs $\xi(\alpha, \beta, \gamma)$ consists of $N = 2^{q-3}[8 + 4k + k(k-1)]$ points. Now define $\alpha_0, \beta_0$ and $\gamma_0$ as follows

$$\alpha_0 = [(k-2)(k-1) - 2k(k-2)u_0 + k(k-1)v_0]/2^{q+1} , \tag{2a}$$

$$\beta_0 = [-(k-2) + (2k-3)u_0 - (k-1)v_0]/2^{q-1} , \tag{2b}$$

$$\gamma_0 = [1 - 2u_0 + v_0]/2^{q-2} , \tag{2c}$$

where

$$u_0 = \frac{(2q-k+3)[2q(k+1) + k + 7 + (k-1)\sqrt{4q^2 + 12q + 17}]}{4(q+2)(2qk - k^2 + 3k + 2)} , \tag{3a}$$

and

$$v_0 = \frac{(2q-k+3)[(4q^2+8q+9)k+2q-5+(2qk+k+3)\sqrt{4q^2+12q+17}]}{8(q+2)^2(2qk-k^2+3k+2)} \ . \quad (3b)$$

**Theorem 1**. If $\alpha_0, \beta_0$ and $\gamma_0$ as defined in (2) are positive, then the design $\xi(\alpha_0, \beta_0, \gamma_0)$ of Definition 1 is $D$-optimal for model (1).

The weights $\alpha_0, \beta_0$ and $\gamma_0$ of (2) are positive when $q \leq 5, q = 6, 7$ and $k \leq q-1, 8 \leq q \leq 10$ and $k \leq q-2$. For $q > 10$ we did not compute the weights. However, it is clear that for $k = 1, \alpha_0$ and $\beta_0$ are positive for all $q$.
In Table 1 values are given for $q \leq 8$.

**Table 1**.
*Values determining the D-optimal designs*

| $q$ | $k$ | $u_0$ | $v_0$ | $2^q\alpha_0$ | $k2^{q-1}\beta_0$ | $k(k-1)2q^{q-3}\gamma_0$ |
|---|---|---|---|---|---|---|
| 1 | 1 | 0.6667 | – | 0.6667 | 0.3333 | – |
| 2 | 1 | 0.7500 | – | 0.7500 | 0.2500 | – |
| | 2 | 0.7435 | 0.5832 | 0.5832 | 0.3206 | 0.0962 |
| 3 | 1 | 0.8000 | – | 0.8000 | 0.2000 | – |
| | 2 | 0.7970 | 0.6549 | 0.6549 | 0.2842 | 0.0609 |
| | 3 | 0.7930 | 0.6516 | 0.5758 | 0.2274 | 0.1967 |
| 4 | 1 | 0.8333 | – | 0.8333 | 0.1667 | – |
| | 2 | 0.8317 | 0.7055 | 0.7055 | 0.2524 | 0.0421 |
| | 3 | 0.8297 | 0.7038 | 0.6223 | 0.2445 | 0.1332 |
| | 4 | 0.8271 | 0.7016 | 0.5927 | 0.1231 | 0.2843 |
| 5 | 1 | 0.8571 | – | 0.8571 | 0.1429 | – |
| | 2 | 0.8562 | 0.7432 | 0.7432 | 0.2260 | 0.0308 |
| | 3 | 0.8550 | 0.7421 | 0.6614 | 0.2421 | 0.0964 |
| | 4 | 0.8536 | 0.7409 | 0.6168 | 0.1807 | 0.2025 |
| | 5 | 0.8518 | 0.7394 | 0.6166 | 0.0259 | 0.3575 |
| 6 | 1 | 0.8750 | – | 0.8750 | 0.1250 | – |
| | 2 | 0.8744 | 0.7723 | 0.7723 | 0.2041 | 0.0236 |
| | 3 | 0.8736 | 0.7717 | 0.6940 | 0.2328 | 0.0731 |
| | 4 | 0.8728 | 0.7709 | 0.6431 | 0.2048 | 0.1520 |
| | 5 | 0.8717 | 0.7700 | 0.6236 | 0.1114 | 0.2649 |
| 7 | 1 | 0.8889 | – | 0.8889 | 0.1111 | – |
| | 2 | 0.8885 | 0.7955 | 0.7955 | 0.1859 | 0.0186 |
| | 3 | 0.8880 | 0.7951 | 0.7213 | 0.2213 | 0.0574 |
| | 4 | 0.8874 | 0.7946 | 0.6682 | 0.2133 | 0.1185 |
| | 5 | 0.8867 | 0.7940 | 0.6386 | 0.1566 | 0.2048 |
| | 6 | 0.8860 | 0.7933 | 0.6359 | 0.0440 | 0.3201 |
| 8 | 1 | 0.9000 | – | 0.9000 | 0.1000 | – |
| | 2 | 0.8997 | 0.8144 | 0.8144 | 0.1705 | 0.0105 |
| | 3 | 0.8994 | 0.8141 | 0.7443 | 0.2094 | 0.0463 |
| | 4 | 0.8990 | 0.8138 | 0.6909 | 0.2140 | 0.0951 |
| | 5 | 0.8985 | 0.8134 | 0.6559 | 0.1807 | 0.1634 |
| | 6 | 0.8980 | 0.8129 | 0.6415 | 0.1051 | 0.2535 |

**Remark**. The values for $q = k$ can also be found in Fedorov (1972). However there are some misprints in Table 1 of Fedorov (1972) on page 78. The table should read as follows.

**Table 2**.
*Correct values for $\alpha_0, \beta_0$ and $\gamma_0$ for $k = q \leq 5$*

| | $\alpha_0$ | $\beta_0$ | $\gamma_0$ |
|---|---|---|---|
| 1 | 0.333333 | 0.333333 | – |
| 2 | 0.145791 | 0.080161 | 0.096193 |
| 3 | 0.071977 | 0.018953 | 0.032792 |
| 4 | 0.037042 | 0.003845 | 0.011844 |
| 5 | 0.019268 | 0.000324 | 0.004469 |

### 3.3 Optimality of the designs

We shall prove the $D$-optimality of the design $\xi(\alpha_0, \beta_0, \gamma_0)$ given in Section 3.2 using the equivalence theorem of Kiefer and Wolfowitz (1960). For the information matrix of the design $\xi(\alpha_0, \beta_0, \gamma_0)$ we use the notation $M(\xi)$ and for the standardized variance of the estimated response in a point $x \in \mathcal{X}$

$$d(x, \xi) = (f(x))' M^{-1}(\xi) f(x) , \tag{4}$$

where

$$(f(x))' = (1, x_1^2, ..., x_k^2, x_1, ..., x_q, x_1 x_2, ..., x_{q-1} x_q) .$$

First we shall derive that the best design of the type $\xi(\alpha, \beta, \gamma)$ of Definition 1 has the weights $\alpha_0, \beta_0$ and $\gamma_0$, as given in (2). However, this does not prove that the design is $D$-optimal. It might be better (meaning a larger $\det(M(\xi))$ to use other points of the experimental region. But then we show that $\max_{x \in \mathcal{X}} d(x, \xi(\alpha_0, \beta_0, \gamma_0)) \leq p$ from which we conclude that the design is $G$-optimal and hence $D$-optimal.
Consider a design $\xi(\alpha, \beta, \gamma)$ as in Definition 1.
The information matrix $M(\xi)$ is equal to

$$M(\xi) = \left[ \begin{array}{c|cc|ccc} A & & & & & \\ \hline & uI_k & & & & \\ & & I_{q-k} & & & \\ \hline & & & vI_{\frac{1}{2}k(k-1)} & & \\ & & & & uI_{k(q-k)} & \\ & & & & & I_{\frac{1}{2}(q-k)(q-k-1)} \end{array} \right] , \tag{5}$$

where all the other entries are zero,

$$A = \left[ \begin{array}{c|c} 1 & u \dots u \\ \hline u & \\ \vdots & (u-v)I_k + vJ_k \\ u & \end{array} \right] ,$$

$I_m$ is the identity matrix of size $m \times m, J_m$ is a matrix of size $m \times m$ with $J_{ij} = 1$ for all $i$ and $j$, and $u$ and $v$ are defined by

$$u = 2^q\alpha + (k-1)2^{q-1}\beta + \tfrac{1}{2}(k-1)(k-2)2^{q-2}\gamma, (k \geq 1) \ , \tag{6}$$

$$v = 2^q\alpha + (k-2)2^{q-1}\beta + \tfrac{1}{2}(k-2)(k-3)2^{q-2}\gamma, (k \geq 2) \ . \tag{7}$$

The determinant of the matrix $M(\xi)$ is equal to

$$\det(M(\xi)) = u^{k(q-k+1)} v^{\frac{1}{2}k(k-1)} (u-v)^{k-1}(u + (k-1)v - ku^2) \text{ for } k \geq 2 \tag{8a}$$

and

$$\det(M(\xi)) = u^{q+1}(1-u) \text{ for } k = 1 \ . \tag{8b}$$

Maximizing $\det(M(\xi))$ with respect to $u$ and $v$ we obtain for $k = 1$ that $u = (q+1)/(q+2)$ and for $k \geq 2$ the two equations

$$\begin{aligned} &(q-k+2)\ u^2 + (k-2)(q-k+2)uv - (k(q-k) + 2k + 1)u^3 - \\ &\qquad (k-1)(q-k+1)v^2 + (k(q-k+1)+2)u^2v = 0 \end{aligned} \tag{9}$$

and

$$u^2 + (k-2)uv - ku^3 - (k+1)v^2 + (k+2)u^2v = 0 \ . \tag{10}$$

Solving the system of Equations (9) and (10) under the conditions $u > 0$ and $v > 0$ we obtain $u = u_0$ and $v = v_0$, where $u_0$ and $v_0$ are the values of (3).
The weights $\alpha, \beta$ and $\gamma$ can be found by solving the Equations (6), (7) and

$$1 = 2^q\alpha + k2^{q-1}\beta + \tfrac{1}{2}k(k-1)2^{q-2}\gamma \ . \tag{11}$$

This yields the values $\alpha_0, \beta_0$ and $\gamma_0$ of (2).
Now we shall prove

$$\max_{x \in \mathcal{X}} d(x, \xi(\alpha_0, \beta_0, \gamma_0)) \leq p \ . \tag{12}$$

We have to compute $M^{-1}(\xi)$.

$$M(\xi) = \left[\begin{array}{c|cc|ccc} A^{-1} & & & & & \\ \hline & \frac{1}{u}I_k & & & & \\ & & I_{q-k} & & & \\ \hline & & & \frac{1}{v}I_{\frac{1}{2}k(k-1)} & & \\ & & & & \frac{1}{u}I_{k(q-k)} & \\ & & & & & I_{\frac{1}{2}(q-k)(q-k-1)} \end{array}\right] , \tag{13}$$

with

$$A^{-1}=\frac{1}{u+(k-1)v-ku^2}\left[\begin{array}{c|c} u+k(k-1)v & -u\cdots -u \\ \hline -u & \\ \vdots & \dfrac{u+(k-1)v-ku^2}{u-v}I_k-\dfrac{v-u^2}{u-v}J_k \\ -u & \end{array}\right].$$

For $d(x,\xi_0)=d(x,\xi(\alpha_0,\beta_0,\gamma_0))$ we obtain

$$\begin{aligned} d(x,\xi_0)=&\frac{u_0+(k-1)v_0}{u_0+(k-1)v_0-ku_0^2}+\frac{u_0+(k-1)v_0-ku_0^2-v_0+u_0^2}{(u_0-v_0)(u_0+(k-1)v_0-ku_0^2)}\sum_{i=1}^k x_i^4- \\ &\frac{2u_0}{u_0+(k-1)v_0-ku_0^2}\sum_{i=1}^k x_i^2-2\frac{v_0-u_0^2}{(u_0-v_0)(u_0+(k-1)v_0-ku_0^2)}\sum\sum_{1\le i<j\le k} x_i^2x_j^2 \\ &+\frac{1}{u_0}\sum_{i=1}^k x_i^2+\sum_{j=k+1}^q x_j^2+\frac{1}{v_0}\sum\sum_{1\le i<j\le k} x_i^2x_j^2+\frac{1}{u_0}\sum_{i=1}^k\sum_{j=k+1}^q x_i^2x_j^2+\sum\sum_{k+1\le i<j\le q} x_i^2x_j^2\ . \end{aligned}\tag{14}$$

First we note that the $x_j^2$ (for $k+1\le j\le q$) only occur in positive terms. Therefore we can find an upper bound for $d(x,\xi_0)$ by substituting $x_j^2=1$ in (14) for $k+1\le j\le q$. Furthermore one can show using equation (10) that the coefficient of $\sum\sum_{1\le i<j\le k} x_i^2x_j^2$ is equal to zero, and using equation (9) that the coefficient of $\sum_{1\le i\le k} x_i^2$, say $c$, is equal to the coefficient of $-\sum_{1\le i\le k} x_i^2$.

From this we conclude

$$d(x,\xi_0)\le\frac{u_0+(k-1)v_0}{u_0+(k-1)v_0-ku_0^2}+(q-k)+\binom{q-k}{2}+c\sum_{i=1}^k(x_i^2-x_i^4)\ ,\tag{15}$$

with

$$c=\frac{(q-k+1)(u_0+(k-1)v_0-ku_0^2)-2u_0^2}{u_0(u_0+(k-1)v_0-ku_0^2)}\ .$$

Computation of the value of $c$ yields $c<0$ and therefore

$$d(x,\xi_0)\le\frac{u_0+(k-1)v_0}{u_0+(k-1)v_0-ku_0^2}+(q-k)+\binom{q-k}{2}\ .\tag{16}$$

Finally, substituting (3) in (16), we obtain (12).

### 3.4 Conclusion

In this section we derived $D$-optimal approximate designs for some models. In general these designs can not be realised in practice. It is possible to construct exact designs (i.e. designs that can be realised in practice) with efficiency $1 - \eta$ for any small positive value of $\eta$ (see Theorem 3.1.1. of Fedorov (1972)). For such a design, since the product of the weights and the number of observations must be an integer, in general a large number of observations has to be chosen. Such designs are not very useful for practical applications. Sometimes one is lucky. For $q = 3$ and $k = 1$ one can construct a 100% $D$-efficient design with only 20 observations as follows. At each of the 8 vertices two observations are taken and in each of 4 out of the 8 midpoints of the edges one observation (see Definition 1). Indeed we have $\alpha = \frac{2}{20} = 0.10$ and $\beta = \frac{1}{20} = 0.05$. In other cases one can use the $D$-optimal approximate designs to construct exact designs with a good efficiency. These will be presented in Section 5.5.

## 4 Construction of designs using design generators

### 4.1 Introduction

The designs to be constructed in this section will be derived from the $2^n$ design. To do so we shall use the techniques of replacement and collapsing, which will be explained in the following sections. The designs to be developed will have factors with two, three or four levels. These are given in column 2 of Table 3. The values of the corresponding variables are either given as $-1 \leq x_i \leq +1$ (column 3), or as orthogonal polynomial values (column 4). It will always be clear from the context which set of values is being used.

**Table 3.**
*Levels of factors and values of corresponding variables*

| 1 | 2 | 3 | 4 | |
|---|---|---|---|---|
| Number of levels | Levels used in experimental design | Values of corresponding variables | Values of orthogonal polynomials | |
| | | | linear | quadratic |
| two | 0 | $-1$ | $-1$ | |
| | 1 | $+1$ | $+1$ | |
| three (obtained from a four-level factor through collapsing) | 0 | $-1$ | $-\sqrt{2}$ | $+1$ |
| | 1 | 0 | 0 | $-1$ |
| | 1 | 0 | 0 | $-1$ |
| | 2 | $+1$ | $+\sqrt{2}$ | $+1$ |
| four | 0 | $-1$ | $-3/\sqrt{5}$ | $+1$ |
| | 1 | $-1/3$ | $-1/\sqrt{5}$ | $-1$ |
| | 2 | $+1/3$ | $+1/\sqrt{5}$ | $-1$ |
| | 3 | $+1$ | $+3/\sqrt{5}$ | $+1$ |

## 4.2 The technique of replacement

If we employ a $2^2$ design, we have four treatments as shown in Table 3. If we use a four-level factor we also have four treatments. We can therefore associate the treatments of the $2^2$ design with the treatments of the four-level factor and establish a one-to-one correspondence between them. This correspondence is given in Table 4, where the four equally spaced levels of the factor $P$ are indicated with $x_P = 0, 1, 2$ and 3.

**Table 4.**
*The $2^2$ design with four-level factor $P$*

<table>
<tr><td>$B$<br>$x_B$</td><td colspan="2">$-1$<br>0</td><td colspan="2">$+1$<br>1</td></tr>
<tr><td>$A$<br>$x_A$</td><td>$-1$<br>0</td><td>$+1$<br>1</td><td>$-1$<br>0</td><td>$+1$<br>1</td></tr>
<tr><td>obs.</td><td>$y_1$</td><td>$y_2$</td><td>$y_3$</td><td>$y_4$</td></tr>
<tr><td>value<br>of $x_P$</td><td>0</td><td>1</td><td>2</td><td>3</td></tr>
</table>

The relation given in Table 4 has a great practical value, because it is now possible to take two factors out of a $2^n$ design or a fraction thereof and replace these two factors by an equally spaced four-level factor $P$. This technique is called replacement. See Addelman (1962a, 1963). We are now able to use a $2^n$ design as a building block for designs with a number of quantitative factors having four levels. In Section 2 we stipulated that the mathematical model of the observations can be described by an incomplete quadratic model. Since the factor $P$ has four levels we can represent its effect with a second degree polynomial in $x_P$. However, to ensure orthogonality as much as possible, which means many zeros in the $X'X$ matrix, we shall employ orthogonal polynomials to represent the $P$-effect. The first and second degree orthogonal polynomials of an equally spaced four-level factor are

$$\begin{aligned} P(\text{linear}) &= Pl = (-3 + 2x_P)/\sqrt{5}\ , \\ P(\text{quadratic}) &= Pq = 1 - 3x_P + x_P^2\ . \end{aligned} \tag{17}$$

The method to calculate these orthogonal polynomials is described in Addelman (1962a). Substituting the values $x_{Pi} = 0, 1, 2,$ and 3 in (17) we obtain orthogonal polynomial values for a four-level factor as given in Table 5. See also Table 3.

**Table 5.**
*Orthogonal polynomial values for a four-level factor*

| $x_{Pi}$ | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| $Pl_i$ | $-3/\sqrt{5}$ | $-1/\sqrt{5}$ | $1/\sqrt{5}$ | $3/\sqrt{5}$ |
| $Pq_i$ | 1 | $-1$ | $-1$ | 1 |

Replacing the two-level factors $A$ and $B$ by one four-level factor is equivalent to replacing the column vectors $A, B$ and $AB$ in the $X$ matrix of a design by the column vectors $Pl$ and $Pq$ of Table 5. See also Table 6.

**Table 6.**
*Values of $x_{Pi}$ and column vector elements $A_i, B_i, A_iB_i, Pl_i$ and $Pq_i$*

| $x_{Pi}$ | $A_i$ | $B_i$ | $A_iB_i$ | $Pl_i = (A_i + 2B_i)/\sqrt{5}$ | $Pq_i = A_iB_i$ |
|---|---|---|---|---|---|
| 0 | –1 | –1 | 1 | $-3/\sqrt{5}$ | 1 |
| 1 | 1 | –1 | –1 | $-1/\sqrt{5}$ | –1 |
| 2 | –1 | 1 | –1 | $1/\sqrt{5}$ | –1 |
| 3 | 1 | 1 | 1 | $3/\sqrt{5}$ | 1 |

The orthogonal polynomials (17) have been scaled in such a way that $\sum_{i=1}^{4} Pl_i^2 = \sum_{i=1}^{4} Pq_i^2 = 4 = N$, where $N$ equals the number of observations. The diagonal elements of $X'X$ will then be equal to $N$. The first advantage of it is that the variance of the $\widehat{\beta}$'s, the estimated parameters of the model are equal for an orthogonal design and nearly equal if the design is nearly orthogonal. A second advantage is that it will be easy to compare the quality of designs which have an equal number of experimental units. We now return to the $2^n$ design of Table 4. To facilitate the construction of new designs later on it is necessary to find the relation between the elements of the set of column vectors $(A, B, AB)$ and $(Pl, Pq)$. These sets are, together with $x_{Pi}$, given in Table 6.
The following relations now hold

$$\begin{aligned} Pl_i &= (A_i + 2B_i)/\sqrt{5} = (-3 + 2x_{Pi})/\sqrt{5} \text{ or } x_{Pi} = (3 + Pl_i\sqrt{5})/2 \ , \\ Pq_i &= A_iB_i = 1 - 3x_{Pi} + x_{Pi}^2 \ . \end{aligned} \tag{18}$$

We shall use (18) to construct new designs.

## 4.3 The technique of collapsing

In the preceding section it was shown that the $2^n$ design can be used to construct designs of which some quantitative factors have four equally spaced levels. The factors in the $2^n$ design which have not been used for replacement will still have two levels. This replacement technique therefore generates designs with some or all quantitative factors having four equally spaced levels and the remaining factors having two levels. It was however pointed out in Section 2 that experimenters want some freedom as to the choice of the number of levels. It is therefore logical that they may wish to have designs, in which some quantitative factors have three levels. This can be achieved by making use of the technique of collapsing. See *Addelman* (1962a, 1962b), *Margolin* (1969). This technique establishes for our purpose a correspondence between the levels of the four-level factor and the levels of a three-level factor. The scheme of Table 7 gives a method to achieve collapsing.

**Table 7.**
*Collapsing a four-level factor to a three-level factor with relevant column vectors*

| Four-level factor $x'_{Pi}$ | Three-level factor $x_{Pi}$ | $A_i$ | $B_i$ | $A_iB_i$ | $Pl_i$ | $Pq_i$ |
|---|---|---|---|---|---|---|
| 0 | 0 | $-1$ | $-1$ | $+1$ | $-\sqrt{2}$ | $+1$ |
| 1 | 1 | $+1$ | $-1$ | $-1$ | 0 | $-1$ |
| 2 | 1 | $-1$ | $+1$ | $-1$ | 0 | $-1$ |
| 3 | 2 | $+1$ | $+1$ | $+1$ | $+\sqrt{2}$ | $+1$ |

The quantities in Table 7 are related as follows

$$\begin{aligned} Pl_i &= (A_1 + B_i)/\sqrt{2} = (-1 + x_{Pi})\sqrt{2} \rightarrow x_{Pi} = 1 + Pl_i/\sqrt{2} \ , \\ Pq_i &= A_iB_i \qquad\qquad = 1 - 4x_{Pi} + 2x_{Pi}^2 \ . \end{aligned} \tag{19}$$

When we compare formulae (18) with (19), we see that $Pl$ remains a linear function of $A$ and $B$, whereas the expression for $Pq$ has not changed at all. This property is very convenient because it means that we can change a satisfactory design with a four-level factor into a design with that particular factor collapsed into a three-level factor, which zero elements in the $X'X$ matrix remain zero. An orthogonal design with a four-level factor can therefore easily be changed into an orthogonal design with a three-level factor. In the next sections we shall use the techniques of replacement and collapsing to construct some new designs.

## 4.4 The $2^3$ design as a building block for other designs

### 4.4.1 Main-effect designs

The $2^3$ design has a well-known structure as given in Table 8.

**Table 8.**
$2^3$ *design*

| | | | | | | |
|---|---|---|---|---|---|---|
| | | $A$ | $-1$ | | $+1$ | |
| | | $x_A$ | 0 | | 1 | |
| | | $B$ | $-1$ | $+1$ | $-1$ | $+1$ |
| | | $x_B$ | 0 | 1 | 0 | 1 |
| $C$ | $x_C$ | | | | | |
| $-1$ | 0 | | $y_1$ | $y_3$ | $y_2$ | $y_4$ |
| $+1$ | 1 | | $y_5$ | $y_7$ | $y_6$ | $y_8$ |

The $X$ matrix of column vectors corresponding to the $2^3$ design is given in Table 9.

**Table 9.**
*The $X$ matrix of column vectors for the $2^3$ design*

| Experimental unit | $x_{0i}$ | $A_i$ | $B_i$ | $C_i$ | $A_iB_i$ | $A_iC_i$ | $B_iC_i$ | $A_iB_iC_i$ |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | −1 | −1 | −1 | +1 | +1 | +1 | −1 |
| 2 | 1 | +1 | −1 | −1 | −1 | −1 | +1 | +1 |
| 3 | 1 | −1 | +1 | −1 | −1 | +1 | −1 | +1 |
| 4 | 1 | +1 | +1 | −1 | +1 | −1 | −1 | −1 |
| 5 | 1 | −1 | −1 | +1 | +1 | −1 | −1 | +1 |
| 6 | 1 | +1 | −1 | +1 | −1 | +1 | −1 | −1 |
| 7 | 1 | −1 | +1 | +1 | −1 | −1 | +1 | −1 |
| 8 | 1 | +1 | +1 | +1 | +1 | +1 | +1 | +1 |

The $X$ matrix of Table 9 has excellent properties because $X'X$ is orthogonal which means that the inner product of two different column vectors always equals zero. Each column vector with the exception of column $x_0$ has four values −1 and four values +1. This means that this $X$ matrix can be used as a design matrix for experimental design with $3, 4, ..., 7$ two-level factors. In this way a number of small (8 experimental units) main-effect designs for two-level factors can and have been constructed. See *Addelman* (1962a, 1963). In the next section we shall investigate whether it is possible to construct a $4 \times 2 \times 2$ design with eight experimental units from the $X$ matrix of Table 9 using the restrictions mentioned in Section 2.
Such a design shall be indicated as a $4 \times 2 \times 2/8$ design.

### 4.4.2 The $4 \times 2 \times 2$ design in eight experimental units

The factors to be used are the following.

P: A quantitative factor with four equally spaced levels 0, 1, 2 and 3.

Q: A two-level factor with levels $Q_1 = -1$ and $Q_2 = +1$ or $x_{Q1} = 0$ and $x_{Q2} = 1$.
If follows that $x_Q = (Q + 1)/2$.

R: A two-level factor with levels $R_1 = -1$ and $R_2 = +1$ or $x_{R1} = 0$ and $x_{R2} = 1$ and $x_R = (R + 1)/2$.

Using the orthogonal polynomials $Pl$ and $Pq$ as defined in Section 4.2, see (18), we have the following mathematical model

$$y_i = \beta_0 x_{0i} + \beta_1 Pl_i + \beta_{23} Q_i R_i + \beta_{11} Pq_i + \beta_2 Q_i + \beta_{13} Pl_i R_i + \beta_3 R_i + \beta_{12} Pl_i Q_i + \varepsilon_i \ , \quad (20)$$

$(i = 1, 2, ..., 8)$ . See also model (1)

Since (20) contains 8 parameters it must be possible to employ an experiment with 8 experimental units to estimate these parameters. To find the levels of the four-level factor $P$ we use the technique of replacement as in Section 4.2 and replace the column vector elements $A_i, B_i$ and $A_iB_i$ of Table 9 by $Pl_i$ and $Pq_i$ using formula (18). As to the choice of $Q_i$ and $R_i$ from Table 9 we can choose two elements from the set $C_i, A_iC_i, B_iC_i, A_iB_iC_i$. A good choice appears to be $Q_i = C_i$ and $R_i = A_iC_i$. Using (18) we obtain the following design generators.

**Table 10.**
*Design generators for a $4 \times 2 \times 2/8$ design*

$$\boxed{\begin{array}{l} Pl_i = (A_i + 2B_i)/\sqrt{5} \\ Pq_i = A_iB_i \\ Q_i = C_i \\ R_i = A_iC_i \end{array}}$$

With the aid of the design generators of Table 10 we can write each independent variable of model (20) as a function of the column vector elements of Table 9.
We find

$$\begin{aligned} & x_{0i} = 1 \\ & Pl_i = (A_i + 2B_i)/\sqrt{5} \\ & Pq_i = A_iB_i \\ & Q_i = C_i \\ & R_i = A_iC_i \\ & Q_iR_i = C_i(A_iC_i) = A_i \\ & Pl_iR_i = (A_i + 2B_i)(A_iC_i)/\sqrt{5} = (C_i + 2A_iB_iC_i)/\sqrt{5} \\ & Pl_iQ_i = (A_i + 2B_i)(C_i)/\sqrt{5} = (A_iC_i + 2B_iC_i)/\sqrt{5}\ . \end{aligned} \tag{21}$$

**Table 11.**
*Design matrix and $X$ matrix*

| Exp.unit | $x_P$ | $x_Q$ | $x_R$ | $x_{0i}$ | $Pl_i$ | $Q_iR_i$ | $Pq_i$ | $Q_i$ | $Pl_iR_i$ | $R_i$ | $Pl_iQ_i$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | 1 | $-3/\sqrt{5}$ | $-1$ | 1 | $-1$ | $-3/\sqrt{5}$ | 1 | $3/\sqrt{5}$ |
| 2 | 1 | 0 | 0 | 1 | $-1/\sqrt{5}$ | 1 | $-1$ | $-1$ | $1/\sqrt{5}$ | $-1$ | $1/\sqrt{5}$ |
| 3 | 2 | 0 | 1 | 1 | $1/\sqrt{5}$ | $-1$ | $-1$ | $-1$ | $1/\sqrt{5}$ | 1 | $-1/\sqrt{5}$ |
| 4 | 3 | 0 | 0 | 1 | $3/\sqrt{5}$ | 1 | 1 | $-1$ | $-3/\sqrt{5}$ | $-1$ | $-3/\sqrt{5}$ |
| 5 | 0 | 1 | 0 | 1 | $-3/\sqrt{5}$ | $-1$ | 1 | 1 | $3/\sqrt{5}$ | $-1$ | $-3/\sqrt{5}$ |
| 6 | 1 | 1 | 1 | 1 | $-1/\sqrt{5}$ | 1 | $-1$ | 1 | $-1/\sqrt{5}$ | 1 | $-1/\sqrt{5}$ |
| 7 | 2 | 1 | 0 | 1 | $1/\sqrt{5}$ | $-1$ | $-1$ | 1 | $-1/\sqrt{5}$ | $-1$ | $1/\sqrt{5}$ |
| 8 | 3 | 1 | 1 | 1 | $3/\sqrt{5}$ | 1 | 1 | 1 | $3/\sqrt{5}$ | 1 | $3/\sqrt{5}$ |

The design matrix and the $X$ matrix of column vectors can now be derived from Table 9 and are presented in Table 11 using the relations (18), (21) and the formulae $x_Q = (Q+1)/2, x_R = (R+1)/2$.
We can of course calculate $X'X$ easily from the $X$ matrix of Table 11. It is, however, more elegant and we obtain more insight into the structure of $X'X$ when the expressions (21) are used.
We find for example

$$(Pl, QR) = ((A+2B)/\sqrt{5}, A) = \tfrac{1}{5}\sqrt{5}((A,A)+2(A,B)) = \tfrac{8}{5}\sqrt{5} \ , \tag{22}$$

where $Pl, QR, A$ and $B$ are vectors.
This yields

$$X'X = 8 \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & F & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & F & 0 \\ 0 & 0 & 0 & 0 & F \end{pmatrix} , \tag{23}$$

with

$$F = \begin{pmatrix} 1 & \tfrac{1}{5}\sqrt{5} \\ \tfrac{1}{5}\sqrt{5} & 1 \end{pmatrix} .$$

According to linear regression theory we have

$$\mathrm{Cov}(\widehat{\beta}) = \sigma^2 (X'X)^{-1} = \sigma^2 \tfrac{1}{8} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & F^{-1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & F^{-1} & 0 \\ 0 & 0 & 0 & 0 & F^{-1} \end{pmatrix} . \tag{24}$$

The matrix $(X'X)^{-1}$ is an important one since the diagonal elements are proportional to the variances of the estimated regression coefficients $\widehat{\beta}$ and a zero off-diagonal element means that the corresponding coefficient of correlation between two $\widehat{\beta}$'s equals zero. The number of zero off-diagonal elements is therefore a measure for the orthogonality of the design. When we examine (24) in more detail it appears that the estimated values $\widehat{\beta}$ can be divided into 5 groups, namely

$$\widehat{\beta}_0, (\widehat{\beta}_1, \widehat{\beta}_{23}), \widehat{\beta}_{11}, (\widehat{\beta}_2, \widehat{\beta}_{13}), (\widehat{\beta}_3, \widehat{\beta}_{12}) \ .$$

It is striking that all linear effect belong to different groups and that each linear effect of a factor is correlated with the linear interaction component of the two other factors; $\widehat{\beta}$'s belonging to different groups are orthogonal estimates and therefore uncorrelated. Some authors call this clumpwise orthogonality (see Margolin, 1969). A large measure of orthogonality is therefore maintained.

Now we discuss the choice of the design generators in Table 10. We could have chosen for example $Q_i = C_i$ and $R_i = B_iC_i$. This choice results in a matrix $X'X$ with structure given in (23) where now

$$F = \begin{pmatrix} 1 & \frac{2}{5}\sqrt{5} \\ \\ \frac{2}{5}\sqrt{5} & 1 \end{pmatrix} .$$

The values $8 \cdot \frac{2}{5}\sqrt{5} = \frac{16}{5}\sqrt{5}$ in the matrix $X'X$ are the result of the inner products $(Pl, QR)$, $(PlR, Q)$ and $(PlQ, R)$. We have for example

$$(Pl, QR) = ((A + 2B)/\sqrt{5}, B) = 2(B, B)/\sqrt{5} = \tfrac{16}{5}\sqrt{5} . \tag{25}$$

We prefer the first choice for two reasons

- the diagonal elements corresponding to the variances of $\widehat{\beta}_1, \widehat{\beta}_{23}, \widehat{\beta}_2, \widehat{\beta}_{13}$ and $\widehat{\beta}_{12}$ are four times smaller
- the correlation coefficient between two $\widehat{\beta}$'s within the pairs $(\widehat{\beta}_1, \widehat{\beta}_{23}), (\widehat{\beta}_2, \widehat{\beta}_{13})$ and $(\widehat{\beta}_3, \widehat{\beta}_{12})$ equals $-1/\sqrt{5}$ for the first and $-2/\sqrt{5}$ for the second choice.

Comparing (25) and (22), we see that the value $\frac{16}{5}\sqrt{5}$ originated from the term $2B$ in $Pl$. We can now formulate an important rule.
Having once chosen $Pl = (A + 2B)/\sqrt{5}$ and $Pq = AB$ it is necessary not to equate the $B$ and $AB$ columns of the $2^3$ design to any of the $2^3$ design to any of the columns for $Q, R$ and $QR$. Applying this rule indicates that apart from the choice $Q_i = C_i$ and $R_i = A_iC_i$ only the choice $Q_i = B_iC_i$ and $R_i = A_iB_iC_i$ generates a suitable design. The latter choice turns out to have the same information matrix as (23). It therefore appears that there is only one suitable $4 \times 2 \times 2$ design in 8 runs.

### 4.4.3 The $D$-efficiency of the $4 \times 2 \times 2/8$ design

The $D$-efficiency of a design $\xi$ is defined as

$$D\text{-efficiency} = 100(\det(M(\xi))/\det(M(\xi^*)))^{(1/P)} , \tag{26}$$

where $\xi^*$ is a $D$-optimal design.
The value $\det(M(\xi^*))$ is obtained by substituting the relevant $u_0$ and $v_0$ values from Table 1 in (8). Therefore we obtain

$$\det(M(\xi^*)) = 2^8/5^5 . \tag{27}$$

The value det $(M(\xi))$ can be computed from

$$\det(M(\xi)) = \det((X'X)/N) \tag{28}$$

where $N$ equals the number of observations. However, we should remember that (27) was obtained using model (1) and $-1 \leq x_i \leq 1$ for $i = 1, 2, 3$. We therefore have to calculate $\det(M(\xi))$ using the scaling $-1 \leq x_i \leq 1$ for the independent variables $x_i$ and the model (1). We obtain a new matrix $X_2 = XL$, where $X$ equals the matrix in Table 11, and

$$L = \begin{pmatrix} 1 & 0 & 0 & 5/9 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{5}/3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4/9 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{5}/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{5}/3 \end{pmatrix} . \tag{29}$$

Therefore

$$\det(X_2'X_2) = (\det(L))^2 \det(X'X) = 2^{10} \cdot 8^8/3^{10} \tag{30}$$

and

$$\det(M(\xi)) = 2^{10}/3^{10} .$$

This yields a $D$-efficiency of 82.4%.

### 4.4.4 An application of the $4 \times 2 \times 2/8$ design

To study the ligth output of a particular type of lamp, it was decided to examine the effect of three factors $P, Q$ and $R$. These factors and their levels are presented in Table 12. The model used is given in (20).

**Table 12.**
*Factors and levels of lamp experiment*

| Factor | | Levels |
|---|---|---|
| $P$ | The amount of amalgam | 3, 5, 7, 9, |
| $Q$ | Type of gas in the lamp | G1, G2 |
| $R$ | Type of glas used | I, II |

Only a small experiment could be carried out because the lamps were expensive and the available time in which to carry out the experiment was limited. It was therefore decided to carry out a half replicate of a $4 \times 2 \times 2$ design. The results, the ligth output of one lamp in each "cell", are given in Table 13. This design has a structure as given in Table 11.

**Table 13.**
*Data of the lamp experiment*

| | $Q$: Type of gas | G1 | | G2 | |
|---|---|---|---|---|---|
| | $x_Q$ | 0 | | 1 | |
| $P$ : | $R$: Type of glas | I | II | I | II |
| Amount of amalgam | $x_R$ | 0 | 1 | 0 | 1 |
| | $x_P$ | | | | |
| 3 | 0 | | 32.9 | 13.9 | |
| 5 | 1 | 21.7 | | | 5.0 |
| 7 | 2 | | 24.2 | 14.6 | |
| 9 | 3 | 24.5 | | | 15.9 |

The vector of least squares estimates for the unknown parameters in (20) equals

$$\widehat{\beta} = (19.09,\ 0.80,\ -2.67,\ 2.71,\ -6.66,\ 0.18,\ -0.68,\ 2.45)' \ .$$

From the results of previous experiments we have an estimate of $\sigma^2$, namely $\widehat{\sigma}^2 = 16.28$ with 20 degrees of freedom. Using linear regression theory, we obtain that $\beta_0, \beta_{11}$ and $\beta_2$ are significant ($\alpha = 0.10$). A significant value of $\beta_{11}$ implies an effect of factor $P$. We therefore decide to use the estimate $\widehat{\beta}_1$ as well in order to obtain a correct measure of the $P$-effect. Our estimated model therefore is

$$\widehat{E(y_i)} = \widehat{\beta}_0 x_{0i} + \widehat{\delta}_1 Pl_i + \widehat{\beta}_{11} Pq_i + \widehat{\delta}_2 Q_i \ ,$$

where $\widehat{\delta}_1$ and $\widehat{\delta}_2$ are new estimates of the parameters $\beta_1$ and $\beta_2$, namely

$$\widehat{\delta}_1 = 0.40 \text{ and } \widehat{\delta}_2 = -6.74 \ .$$

The relation between the amount of amalgam and light output for two types of gas has been plotted in Figure 1.

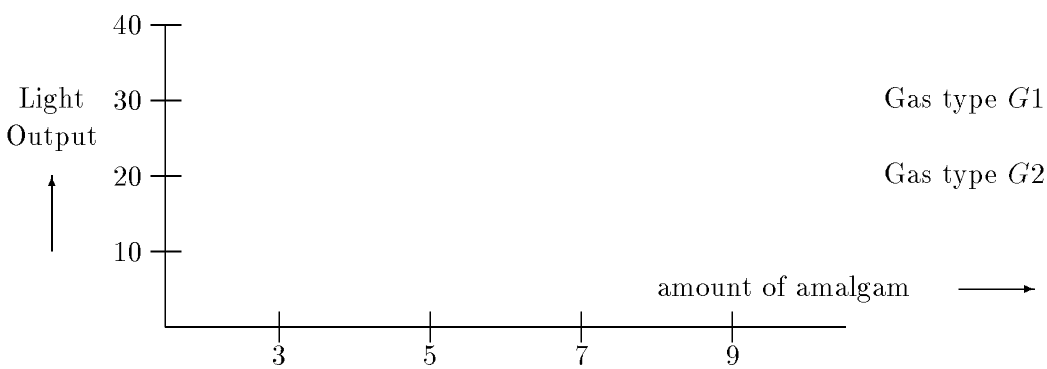


Fig. 1. Relation between the amount of amalgam and light output for two types of gas.

Figure 1 is very interesting because it shows the large and constant difference between the two types of gas and a minimum value of light output for an amount of amalgam of 6.14. The highest light output is obtained for an amount of amalgam of 3 and gas type G1. The expected corresponding light output equals 29.08.

#### 4.4.5 The $3 \times 2 \times 2$ design in 8 experimental units

In order to construct a $3 \times 2 \times 2$ design in 8 experimental units, we again employ the $X$ matrix of column vectors for a $2^3$ design a presented in Table 9.

The factors to be used are as follows:

P: A quantitative three-level factor with equally spaced levels 0, 1 and 2.

Q: A two-level factor with levels $Q_1 = -1$ and $Q_2 = +1$, or $x_{Q1} = 0$ and $x_{Q2} = 1$.

R: A two-level factor with levels $R_1 = -1$ and $R_2 = +1$, or $x_{R1} = 0$ and $x_{R2} = 1$.

We use the model (20), so a design of 8 experimental units should again be sufficient. We shall employ the technique of replacement and collapsing as summarized in Table 7 of Section 4.3 to find the column vector elements $Pl_i, R_i, ..., Pl_iQ_i$. The relations according to (19) can be used to replace the two factors $A$ and $B$ with two levels each by a three-level factor. The column vectors $Q$ and $R$ can be obtained by choosing two vectors from the set $C, AC, BC, ABC$. A good choice is $Q = C, R = AC$.
This yields the design given in Table 14.

**Table 14.**
*A $3 \times 2 \times 2/8$ design*

<table>
<tr><td>$x_Q$</td><td colspan="2">0</td><td colspan="2">1</td></tr>
<tr><td>$x_P$ \ $x_R$</td><td>0</td><td>1</td><td>0</td><td>1</td></tr>
<tr><td>0</td><td></td><td>×</td><td>×</td><td></td></tr>
<tr><td>1</td><td>×</td><td>×</td><td>×</td><td>×</td></tr>
<tr><td>2</td><td>×</td><td></td><td></td><td>×</td></tr>
</table>

Using the same method as in Section 4.4.2, we may write the elements of the column vectors of the $X$ matrix of this design as given in Table 15.

**Table 15.**
*Column vector elements for a $3 \times 2 \times 2/8$ design*

| | |
|---|---|
| $x_{0i} = 1$ | $Pl_i = (A_i + B_i)/\sqrt{2}$ |
| $Q_iR_i = A_i$ | $Pq_i = A_iB_i$ |
| $Q_i = C_i$ | $Pl_iR_i = (C_i + A_iB_iC_i)/\sqrt{2}$ |
| $R_i = A_iC_i$ | $Pl_iQ_i = (A_iC_i + B_iC_i)/\sqrt{2}$ |

The $X'X$ matrix has the structure given in (23) where now

$$F = \begin{pmatrix} 1 & \frac{1}{2}\sqrt{2} \\ \\ \frac{1}{2}\sqrt{2} & 1 \end{pmatrix} .$$

The $(X'X)^{-1}$ matrix shows that correlation within the same pairs of $\widehat{\beta}$'s, namely ($\widehat{\beta}_1$, $\widehat{\beta}_{23}$), ($\widehat{\beta}_2$, $\widehat{\beta}_{13}$) and ($\widehat{\beta}_3$, $\widehat{\beta}_{12}$), occurs as with the $4 \times 2 \times 2/8$ design.
The relevant correlation coefficient equals

$$\rho_{pq} = \frac{\mathrm{cov}(\widehat{\beta}_p, \widehat{\beta}_q)}{\sqrt{(\mathrm{var}(\widehat{\beta}_p)\mathrm{var}(\widehat{\beta}_q)}} = -\tfrac{1}{2}\sqrt{2} = -0.71 \ .$$

This correlation coefficient is fairly high and we can ask ourselves whether a better design than the one given in Table 14 can be found. The $D$-efficiency of this design equals 68.4%. A $3 \times 2 \times 2/8$ design using a different collapsing procedure was found by Upperman (1993). It had a $D$-efficiency of 81.3%. A disadvantage of the latter design is the fairly large value of $\sigma^2_{\widehat{\beta}_{11}}$ .

# 5 Designs using 16 experimental units

## 5.1 The $2^4$ design

The $2^4$ design shall now be used to construct designs with three or four factors, each of which has two, three or four levels. As before we stipulate that the three- and four-level factors are quantitative and have equally spaced levels. We shall, as already announced in Section 2, use two construction methods. The first one uses design generators and will be dealt with in the Sections 5.2, 5.3 and 5.4. The second method uses the properties of the $D$-optimal designs as discussed in Section 3. Designs derived from $D$-optimal designs will be treated in Section 5.5. In Section 4 we found that only a few suitable designs with factors having more than two levels could be derived from the $2^3$ design. We shall see that the number of designs which can be derived from the $2^4$ designs is far greater. Because we shall frequently make use of the $X$ matrix of column vectors of the $2^4$ design we give this matrix in Table 16.

**Table 16.**
*The $X$ matrix of column vectors for the $2^4$ design*

| Nr.exp. | $x_0$ | $A$ | $B$ | $C$ | $D$ | $AB$ | $AC$ | $AD$ | $BC$ | $BD$ | $CD$ | $ABC$ | $ABD$ | $ACD$ | $BCD$ | $ABCD$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | 1 |
| 2 | 1 | 1 | −1 | −1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | 1 | 1 | 1 | −1 | −1 |
| 3 | 1 | −1 | 1 | −1 | −1 | −1 | 1 | 1 | −1 | −1 | 1 | 1 | 1 | −1 | 1 | −1 |
| 4 | 1 | 1 | 1 | −1 | −1 | 1 | −1 | −1 | −1 | −1 | 1 | −1 | −1 | 1 | 1 | 1 |
| 5 | 1 | −1 | −1 | 1 | −1 | 1 | −1 | 1 | −1 | 1 | −1 | 1 | −1 | 1 | 1 | −1 |
| 6 | 1 | 1 | 1 | −1 | 1 | −1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | −1 | 1 | 1 |
| 7 | 1 | −1 | 1 | 1 | −1 | −1 | −1 | 1 | 1 | −1 | −1 | −1 | 1 | 1 | −1 | 1 |
| 8 | 1 | 1 | 1 | 1 | −1 | 1 | 1 | −1 | 1 | −1 | −1 | 1 | −1 | −1 | −1 | −1 |
| 9 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 |
| 10 | 1 | 1 | −1 | −1 | 1 | −1 | −1 | 1 | 1 | −1 | −1 | 1 | −1 | −1 | 1 | 1 |
| 11 | 1 | −1 | 1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | −1 | 1 | −1 | 1 | −1 | 1 |
| 12 | 1 | 1 | 1 | −1 | 1 | 1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | −1 | −1 | −1 |
| 13 | 1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | 1 |
| 14 | 1 | 1 | −1 | 1 | 1 | −1 | 1 | 1 | −1 | −1 | 1 | −1 | −1 | 1 | −1 | −1 |
| 15 | 1 | −1 | 1 | 1 | 1 | −1 | −1 | −1 | 1 | 1 | 1 | −1 | −1 | 1 | −1 | −1 |
| 16 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

The $X$ matrix of Table 16 has similar properties as the $X$ matrix of the $2^3$ design as discussed in Section 4.4.1. It is well known from the literature that the $2^4$ design can be used to estimate effects of $4, 5, ..., 15$ two-level factors. For 4 and 5 factors it is possible to estimate all main effects and two-factor interactions. If more than 5 factors are used, only the main effects and under certain conditions some two-factor interactions can be estimated. In the next sections we shall construct designs, using the $2^4$ design, with factors having more than two levels. We shall however ignore the $4 \times 2 \times 2/16$ design since it contains 16 experimental units. Its construction and analysis is therefore straightforward. We shall instead try to construct a half replicate of the $4 \times 4 \times 2$ design from the $X$ matrix of Table 16.

## 5.2 The $4 \times 4 \times 2$ orthogonal design with 16 experimental units

The factors to be used are the following:

P,Q: Two quantitative factors with 4 equally spaced levels $x_P = 0, 1, 2, 3$ and $x_Q = 0, 1, 2, 3$

R: A two-level factor with levels $R_1 = -1$ and $R_2 = +1$ or $x_{R1} = 0$ or $x_{R2} = 1$.

Using the restrictions as given in Section 2 we have the mathematical model of the observations $y_i$ as given in (31).

$$\begin{aligned} y_i = {} & \beta_0 x_{0i} + \beta_1 Pl_i + \beta_{11} Pq_i + \beta_2 Ql_i + \beta_{22} Qq_i + \beta_3 R_i + \beta_{12} Pl_i Ql_i + \\ & \beta_{13} Pl_i R_i + \beta_{23} Ql_i R_i + \varepsilon_i, \quad i = 1, 2, ..., 16 \,, \end{aligned} \tag{31}$$

where $E(\varepsilon) = 0$ and $E(\varepsilon'\varepsilon) = \sigma^2 I$; $I$ is the identity matrix.

**Table 17.**
*Column vector elements for the $4 \times 4 \times 2/16$ design*

$x_{0i} = 1$

$Pl_i = (A_i + 2B_i)/\sqrt{5}$

$Pq_i = A_i B_i$

$Ql_i = (C_i + 2D_i)/\sqrt{5}$

$Qq_i = C_i D_i$

$R_i = A_i B_i C_i D_i$

$Pl_i Ql_i = (A_i C_i + 2A_i D_i + 2B_i D_i + 2B_i C_i + 4B_i D_i)/5$

$Pl_i R_i = (B_i C_i D_i + 2A_i C_i D_i)/\sqrt{5}$

$Ql_i R_i = (A_i B_i D_i + 2A_i B_i C_i)/\sqrt{5}$ .

Since (31) contains 9 parameters $\beta$, the number of 16 experimental units is sufficient and allows an estimate of $\sigma^2$ with $16 - 9 = 7$ degrees of freedom. To construct the matrix of column vectors for (31) we employ a procedure similar to the one used in Section 4.4.2. We find, using the column vectors $A, B, ..., ABCD$ of Table 16 the expressions given in Table 17.

The manner in which the expressions of Table 17 were found will now be explained. The expressions for $Pl_i$, $Pq_i$, $Ql_i$ and $Qq_i$ imply that we have used the technique of replacement twice, since we assigned the column vectors $A, B$ and $AB$ to $Pl$ and $Pq$ while those for $C, D$ and $CD$ were assigned to $Ql$ and $Qq$. We therefore replaced the factors $A$ and $B$ by the four-level factor $P$ and the factors $C$ and $D$ by the four-level factor $Q$. See also Section 4.2. We therefore used 6 columns of Table 16 to calculate the 4 column vectors for the factors $P$ and $Q$. We have to select one more column vector in Table 16 for the remaining two-level factor $R$. We have in principle the choice from nine vectors, but it will appear that only one of these is suitable. First of all it is evident that from the choice

$$Pl_i = (A_i + 2B_i)/\sqrt{5} \text{ and } Ql_i = (C_i + 2D_i)/\sqrt{5} \,,$$

it follows that

$$Pl_iQl_i = (A_iC_i + 2A_iD_i + 2B_iC_i + 4B_iD_i)/\sqrt{5} \,. \tag{32}$$

Formula (32) shows that the column vector for $PlQl$ is calculated from 4 "interaction columns" of Table 16. If we use one of these columns for the factor $R$, we immediately introduce a non zero off-diagonal element in $X'X$ and hence correlation between $\widehat{\beta}$'s. To avoid this we have to choose from the remaining column vectors $ABC, ABD, ACD, BCD$ and $ABCD$. Suppose we choose $R_i = A_iB_iC_i$. We then have $Pl_iR_i = (B_iC_i + 2A_iC_i)/\sqrt{5}$ which are terms already in (32) and we again introduce non zero off-diagonal elements in $X'X$. It appears that the only way to avoid this phenomenon is to choose $R_i = A_iB_iC_iD_i$ as was done in Table 17. When we examine the expressions in Table 17 more closely we see that all column vectors of Table 16 appear only once. It follows that all inner products of the vectors in Table 17 such as $(x_0, Pl)$, $(Pl, Pq)$, $(Pl, Ql), ..., (PlR, QlR)$ are equal to zero and that means that $X'X$ corresponding to model (32) is diagonal and we therefore have an orthogonal design. The vector elements $Pl_iQl_i$, $Pl_iR_i$ and $Ql_iR_i$ in Table 17 are calculated from the *design generators*, as given in Table 18.

**Table 18.**
*Design generators for the* $4 \times 4 \times 2/16$ *design*

| | | |
|---|---|---|
| $Pl_i = (A_i + 2B_i)/\sqrt{5}$ | $Pq_i = A_iB_i$ | |
| $Ql_i = (C_i + 2D_i)/\sqrt{5}$ | $Qq_i = C_iD_i$ | $R_i = A_iB_iC_iD_i$ |

It is extremely important to choose these generators very carefully since they determine the structure of the $X'X$ and therefore of the $(X'X)^{-1}$ matrix. It is also stressed that the design generator not only yield some of the expressions in Table 18 but also enable us to calculate $X'X$ analytically.
We find

$$X'X = 16I \ . \tag{33}$$

It appears that $X'X$ is not only diagonal, but also has as diagonal elements the numbers 16. This was achieved by choosing the orthogonal polynomial values as given in Table 6. The matrices $X'X$ and $(X'X)^{-1}$ are therefore equal to the $X'X$ and $(X'X)^{-1}$ of the $2^4$ design. Having the number 16 as diagonal elements in $X'X$ is especially important since it facilitates the comparison with other designs. To find the design matrix we use the equations (18) and we obtain the relations

$$x_{Pi} = (3 + Pl_i\sqrt{5})/2 = (3 + A_i + 2B_i)/2 \tag{34a}$$

$$x_{Qi} = (3 + Ql_i\sqrt{5})/2 = (3 + C_i + 2D_i)/2 \tag{34b}$$

$$x_{Ri} = (1 + R_i)/2 = (1 + A_iB_iC_iD_i)/2 \ . \tag{34c}$$

Substituting the values $Pl_i, Ql_i$ and $R_i$ of Table 17 or $A_i, B_i, C_i, D_i$ and $A_iB_iC_iD_i$ of Table 16 into the equations (34) results in the design matrix for the $4 \times 4 \times 2/16$ design, which is given in Table 19.

**Table 19.**
*Design matrix for the orthogonal* $4 \times 4 \times 2/16$ *design*

| $x_P$ | $x_Q$ | $x_R$ |
|---|---|---|
| 0 | 0 | 1 |
| 1 | 0 | 0 |
| 2 | 0 | 0 |
| 3 | 0 | 1 |
| 0 | 1 | 0 |
| 1 | 1 | 1 |
| 2 | 1 | 1 |
| 3 | 1 | 0 |
| 0 | 2 | 0 |
| 1 | 2 | 1 |
| 2 | 2 | 1 |
| 3 | 2 | 0 |
| 0 | 3 | 1 |
| 1 | 3 | 0 |
| 2 | 3 | 0 |
| 3 | 3 | 1 |

## 5.3 The $4 \times 3 \times 2$ design with 16 experimental units

In order to construct the $4 \times 3 \times 2$ design, we shall collapse the four-level factor $Q$ used in the previous section to a three-level factor $Q$. We use the collapsing procedure as given in Section 4.3 and can therefore use the design generators of Table 18 if we only change the expression for $Ql_i$ into

$$Ql_i = (C_i + D_i)/\sqrt{2} \ .$$

Again we have

$$X'X = 16I \ .$$

The design matrix is given in Table 20.

**Table 20.**
*Design matrix for the orthogonal* $4 \times 3 \times 2/16$ *design*

| $x_P$ | $x_Q$ | $x_R$ |
|---|---|---|
| 0 | 0 | 1 |
| 1 | 0 | 0 |
| 2 | 0 | 0 |
| 3 | 0 | 1 |
| 0 | 1 | 0 |
| 1 | 1 | 1 |
| 2 | 1 | 1 |
| 3 | 1 | 0 |
| 0 | 1 | 0 |
| 1 | 1 | 1 |
| 2 | 1 | 1 |
| 3 | 1 | 0 |
| 0 | 2 | 1 |
| 1 | 2 | 0 |
| 2 | 2 | 0 |
| 3 | 2 | 1 |

### 5.4 Other designs with 16 experimental units

Upperman (1993) derived a total of 7 designs wit 16 experimental units using methods described in Section 5.2 and 5.3 these are listed in Table 21.

**Table 21.**
*Designs with 16 experimental units constructed by using design generators and collapsing*

| | | | |
|---|---|---|---|
| $4 \times 4 \times 2/16$ | 1/2 | 82.0 | Orthogonal design (Section 5.2) |
| $4 \times 3 \times 2/16$ | 2/3 | 81.3 | Orthogonal design (Section 5.3) |
| $4 \times 2 \times 2 \times 2/16$ | 1/2 | 90.1 | Orthogonal design |
| $3 \times 2 \times 2 \times 2/16$ | 2/3 | 88.6 | Orthogonal design |
| $4 \times 4 \times 2 \times 2/16$ | 1/4 | 75.2 | Clumpwise othogonality |
| $4 \times 3 \times 2 \times 2/16$ | 1/3 | 69.0 | Clumpwise othogonality |
| $3 \times 3 \times 2 \times 2/16$ | 4/9 | 68.1 | Clumpwise othogonality |

Further details of these designs can be found in Upperman (1993), where design characteristics, other than $D$-efficiency are discussed. It is possible to construct an additional 13 fractional designs with 16 experimental units using the techniques of replacement, design generators and collapsing, but these designs have a low $D$-efficiency. In Section 5.5 we shall therefore use a different method to construct fractional designs with 16 experimental units.

## 5.5 The construction of designs with 16 experimental units using $D$-optimal designs

The appropriate model to be used for the $4 \times 4 \times 4/16$ design is the model described in (1) for $k = q = 3$. Using Table 1 we find that for $k = q = 3$ the $D$-optimal design consists of design points as given in Table 22.

**Table 22.**
*Design points of the $D$-optimal $3 \times 3 \times 3$ design*

| |
|---|
| 57.6% of the points are the type $\pm 1, \pm 1, \pm 1$ |
| 22.7% of the points are the type $0, \pm 1, \pm 1$ |
| 19.7% of the points are the type $0, 0, \pm 1$ |

Since we only use 16 design points we can never realize the percentages of Table 22 in practice and we therefore have to use approximate values. Moreover, since we employ 4 levels, we do not have the level 0, but have to use $\pm$ (1/3) instead, remembering that levels $\pm$ (1/3) will become a level 0 after collapsing.
We then set up the design of Table 23.

**Table 23.**
*A $4 \times 4 \times 4/16$ design*

| Exp.unit | $x_{1i}$ | $x_{2i}$ | $x_{3i}$ |
|---|---|---|---|
| 1 | −1 | −1 | −1 |
| 2 | 1 | −1 | −1 |
| 3 | −1 | −1 | −1 |
| 4 | 1 | −1 | −1 |
| 5 | −1 | −1 | −1 |
| 6 | 1 | −1 | −1 |
| 7 | −1 | −1 | −1 |
| 8 | 1 | −1 | −1 |
| 9 | −1/3 | −1/3 | −1/3 |
| 10 | 1 | −1 | −1/3 |
| 11 | −1/3 | 1 | −1 |
| 12 | 1 | 1/3 | −1 |
| 13 | −1 | −1/3 | 1 |
| 14 | 1/3 | −1 | 1 |
| 15 | −1 | 1 | 1/3 |
| 16 | 1/3 | 1/3 | 1/3 |

Examining Table 23 we see that

$$8 \text{ points} = 50\% \text{ are of the type } \pm 1 \ \pm 1 \ \pm 1 \ ,$$

these points form a $2^3$ design,

$$6 \text{ points} = 37.5\% \text{ are of the type } \pm 1/3 \ \pm 1 \ \pm 1$$

$$2 \text{ points} = 12.5\% \text{ are of the type } \pm 1/3 \ \pm 1/3 \ \pm 1/3 \ .$$

When we compare these percentages with those in Table 22 we see some discrepancies as regards the groups ($\pm$ 1, $\pm$ 1, $\pm$ 1) and (0, $\pm$ 1, $\pm$ 1). Moreover, we used two points of the type $\pm$ 1/3 $\pm$ 1/3 $\pm$ 1/3 which do not occur at all in Table 22, but we used these, to have two "center points" when the three four-level factors are collapsed to three-level factors. These center points are however not desirable from the $D$-efficiency point of view because they do not occur at all in the $D$-optimal design of Table 22. It is, on the other hand, very often desirable to include these points in an experiment, because they represent "normal" or "standard" operating conditions. We nevertheless calculated the $D$-efficiency of the design in Table 23.
For the design of Table 23 we obtain

$$\det((X'X)/16) = 1.566 \times 10^{-4} \ .$$

From Table 1 and (8a) we obtain

$$\max \det \ (M(\xi)) = 0.000578313 \ .$$

So, the $D$-efficiency of the design of Table 23 equals 87.8%. Three other designs were derived from the $4 \times 4 \times 4/16$ design by collapsing 1, 2 and 3 four-level factors into three-level factors. The collapsing is achieved as indicated in Table 24.

**Table 24.**
*Collapsing a four-level factor into a three-level factor*

| Four-level factor | | Three-level factor | |
|---|---|---|---|
| $x'_P$ or $x'_Q$ or $x'_R$ | $x'_1$ or $x'_2$ or $x'_3$ | $x_P$ or $x_Q$ or $x_R$ | $x_1$ or $x_2$ or $x_3$ |
| 0 | –1 | 0 | –1 |
| 1 | –1/3 | 1 | 0 |
| 2 | 1/3 | 1 | 0 |
| 3 | 1 | 2 | 1 |

The collapsing procedure of Table 24 is identical to the method used in Table 7. Three other groups of design were similarly constructed namely

– A $4 \times 4 \times 2 \times 2/16$ design and two additional designs derived through collapsing one and two four-level factors.

– A $4 \times 4 \times 4 \times 2/16$ design and three other designs obtained by collapsing.

– A $4 \times 4 \times 4 \times 4/16$ design and four other designs also constructed by collapsing one, two, three and four factors.

These designs are listed in Table 25. For further details we refer to Upperman (1993).

**Table 25.**
*Designs with 16 experimental units constructed by using D-optimal designs and collapsing*

| Design | Fraction | $D$-efficiency | Remarks |
|---|---|---|---|
| $4 \times 4 \times 4/16$ | 1/4 | 87.8 | Linear effects orthogonal |
| $4 \times 4 \times 3/16$ | 1/3 | 89.2 | Linear effects orthogonal |
| $4 \times 3 \times 3/16$ | 4/9 | 90.9 | Linear effects orthogonal |
| $3 \times 3 \times 3/16$ | 16/27 | 92.6 | Linear effects orthogonal |
| | | | |
| $4 \times 4 \times 4 \times 2/16$ | 1/4 | 84.6 | Clumpwise orthogonality |
| $4 \times 3 \times 2 \times 2/16$ | 1/3 | 81.1 | Clumpwise orthogonality |
| $3 \times 3 \times 2 \times 2/16$ | 4/9 | 76.4 | Clumpwise orthogonality |
| | | | |
| $4 \times 4 \times 4 \times 2/16$ | 1/8 | 87.5 | |
| $4 \times 4 \times 3 \times 2/16$ | 1/6 | 87.2 | |
| $4 \times 3 \times 3 \times 2/16$ | 2/9 | 86.8 | |
| $3 \times 3 \times 3 \times 2/16$ | 8/27 | 87.2 | |
| | | | |
| $4 \times 4 \times 4 \times 4/16$ | 1/16 | 84.9 | |
| $4 \times 4 \times 4 \times 3/16$ | 1/12 | 86.2 | |
| $4 \times 4 \times 3 \times 3/16$ | 1/9 | 86.0 | |
| $4 \times 3 \times 3 \times 3/16$ | 4/27 | 85.8 | |
| $3 \times 3 \times 3 \times 3/16$ | 16/81 | 85.8 | |

## References


Addelman, S. (1962a), Orthogonal Main-effect Plans for Asymmetrical Factorial Experiments. *Technometrics 4*, 21–46.

Addelman, S. (1962b), Symmetrical and Asymmetrical Fractional Factorial Plans, *Technometrics 4*, 47–58.

Addelman, S. (1963), Techniques for constructing fractional replicate plans, *Journal of the American Statistical Association 58*, 45–71.

Atkinson, A.C. (1988), Recent developments in the methods of optimum and related experimental designs. *International Statistical Review 56*, 99–115.

Box, G.E.P. and Behnken, D.W. (1960), Some New Three-Level Designs for the Study of Quantitative Variables, *Technometrics 2*, 455–475.

Box, G.E.P. and Draper, N.R. (1959), A basis for the selection of a response surface design, *Journal of the American Statistical Association 54*, 622–654.

Box, G.E.P. and Draper, N.R. (1963), The choice of a second order rotatable design, *Biometrika 50*, 335–352.

Box, M.J. and Draper, N.R. (1974), On Minimum Point Second-Order Design, *Technometrics 16*, 613–616.

Box, G.E.P. and Draper, N.R. (1987), *Empirical Model-Building and Response Surfaces*, John Wiley & Sons, New York.

Box, G.E.P. and Hunter, J.S. (1957), Multifactor Experimental Designs for Exploring Response Surfaces, *Annals of Mathematical Statistics 28*, 195–241.

Box, G.E.P., Hunter, W.G. and Hunter, J.S. (1978), *Statistics for Experimenters*, John Wiley & Sons, New York.

Cochran, W. and Cox, G.M. (1957), *Experimental Designs*, John Wiley & Sons, New York.

Fedorov, V.V. (1972), *Theory of Optimal Experiments*, Academic Press Inc., London, New York.

Hoke, A.T. (1974), Economical Second-Order Designs Based on Irregular Fractions of the $3^n$ Factorial, *Technometrics 16*, 375–384.

Kiefer, J. and Wolfowitz, (1960), The equivalence of two extremum problems, *Canadian Journal of Mathematics 12*, 363–366.

Lucas, J.M. (1974), Optimum Composite Designs, *Technometrics 16*, 561–567.

Margolin, B.H. (1969), Orthogonal Main-Effect Plans Permitting Estimation of All Two-Factor Interactions for the $2^n3^m$ Fractional Series of Designs, *Technometrics 11*, 747–762.

Mitchell, T.J. and Bayne, C.K. (1978), $D$-Optimal Fractions of Three-Level Factorial Designs, *Technometrics 20*, 369–380.

Montgomery, D.C. (1976), *Design and Analysis of Experiments*, John Wiley & Sons, New York.

Myers, R.H., Khuri, A.I. and Carter, H.W. (1988), Response Surface Methodology 1966–1988, *Technometrics 31*, 137–157.

Rechtschaffner, R.L. (1967), Saturated Fractions of $2^n$ and $3^n$ Factorial Designs, *Technometrics 9*, 569–575.

Upperman, P.M. (1974), *Statistische Methoden en Proefopzetten*, Universitaire Pers, Rotterdam.

Upperman, P.M. (1993), *Designs with a small number of runs for factorial experiments.* Dissertation, Technische Universiteit Eindhoven, Eindhoven.

Welch, W.J. (1984), Computer-Aided Design of Experiments for Response Estimation, *Technometrics 26*, 217–224.