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ORTHOGONAL MINIMALLY ALIASED RESPONSE SURFACE DESIGNS FOR THREE-LEVEL QUANTITATIVE FACTORS AND TWO-LEVEL CATEGORICAL FACTORS

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Abstract: Orthogonal minimally aliased response surface (OMARS) designs constitute a new family of three-level experimental designs for studying quantitative factors. Many experiments, however, also involve one or more two-level categorical factors. In this work, we derive necessary conditions for the existence of mixed-level OMARS designs, and present three construction methods based on integer programming. Like the original three-level OMARS designs, the new mixed-level designs are orthogonal main-effect plans in which the main effects are also orthogonal to the second-order effects. These properties distinguish the new designs from definitive screening designs with additional two-level categorical factors and other mixed-level designs recently presented in the literature. To demonstrate the flexibility of our construction methods, we provide 587 mixed-level OMARS designs in the online Supplementary Material.

Key words and phrases: Definitive screening design, foldover design, OMARS design, mixed integer programming, orthogonal array.

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1. Introduction

The dominant experimental designs in process optimization and response surface modeling, where all experimental factors are quantitative, have long been central composite designs (Box and Wilson (1951)), small central composite designs (Hartley (1959)), and Box–Behnken designs (Box and Behnken (1960)). With the introduction of exchange algorithms in the last few decades of the previous century, response surface experiments using optimal experimental designs (Goos and Jones (2011)) gained substantial popularity as well. More recently, many experimenters have switched to definitive screening designs (DSDs, see Jones and Nachtsheim (2011); Xiao et al. (2012)), because these designs allow the study of many quantitative factors using a limited number of experimental runs. However, these response surface designs all possess certain weaknesses. First, central composite designs, small central composite designs, and Box–Behnken designs are often too large to be of practical use. Second, DSDs have a low power to detect any quadratic effect, and may exhibit substantial aliasing among the second-order effects (Vazquez et al. (2020)). Finally, in optimal designs, the main effects are, in general, partially aliased with each other and with the second-order effects. Recently, Núñez-Ares and Goos (2020) introduced the family of orthogonal minimally aliased response surface (OMARS) designs. These designs exist for many different run sizes. Some involve fewer runs than DSDs, while others have the same or a larger run size. Compared with DSDs, many OMARS designs involve less aliasing among the second-order effects, allow more interactions to be estimated simultaneously, have a higher power to detect any quadratic effect, and have better projection properties. Just like definitive screening designs, OMARS designs have three levels for each factor, are orthogonal for the main effects, and involve no aliasing between the main effects and the second-order effects (i.e., the two-factor interaction

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effects and the quadratic effects). For all of these reasons, many OMARS designs appear to be attractive alternatives to traditional response surface designs, optimal designs, and definitive screening designs.

It should be clear that the literature on response surface designs for quantitative experimental factors is extensive. At the same time, many studies have examined designs for experiments involving only categorical factors. For these experiments, it is common to base the designs on orthogonal arrays (OAs; e.g., see Hedayat et al. (1999)). In recent years, much work has been done on the enumeration and evaluation of various kinds of OAs. Schoen et al. (2010) presented an enumeration algorithm and a large catalog of OAs. Schoen et al. (2017), Schoen and Mee (2012), and Vazquez et al. (2019), among others, performed detailed studies on two-level OAs. Sartono et al. (2012) investigated a large collection of three-level OAs, assuming all factors are categorical.

The literature on designs for both quantitative and categorical factors is scarce. Atkinson and Donev (1989) were the first to propose a method for constructing designs for experiments involving both quantitative and categorical factors. In Chapter 14 of Atkinson et al. (2007), the authors present mixed-level designs and provide some additional examples. In Chapter 4 of Goos and Jones (2011), the authors present a case study involving a response surface design with an extra categorical factor.

In recent years, several research teams have proposed methods for creating mixed-level designs for three-level quantitative and two-level categorical factors. First, Jones and Nachtsheim (2013) presented two heuristic methods to extend definitive screening designs, which originally only included three-level quantitative factors, to also include two-level categorical factors. Their first method is called DSD-based column augmentation, and

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the resulting designs are called DSD-A designs. Their second method is called orthogonal column augmentation and the resulting designs are referred to as ORTH-A designs. DSD-A designs are foldover designs in which there is no aliasing between the main effects and the second-order effects. However, unlike the original definitive screening designs, they are not orthogonal main-effect plans. ORTH-A designs are orthogonal for the main effects, but the main effects are aliased to some extent with interaction effects involving one or two categorical factors. As a result, none of the definitive screening designs with two-level categorical factors in Jones and Nachtsheim (2013) simultaneously possess the properties that they are orthogonal for the main effects and that the main effects and the second-order effects are not aliased. In a follow-up article, Nachtsheim et al. (2017) presented *compromise designs* that balance the pros and cons of the DSD-A and ORTH-A designs in Jones and Nachtsheim (2013). However, these compromise designs also do not possess the attractive orthogonality and minimal aliasing properties of definitive screening and OMARS designs for quantitative factors. A commonality of the work of Jones and Nachtsheim (2013) and that of Nachtsheim et al. (2017) is that the majority of the factors in their mixed-level designs are quantitative and have three levels.

Nguyen et al. (2020) also proposed a method to generate mixed-level designs for experiments involving three-level quantitative and two-level categorical factors simultaneously. More specifically, they presented a heuristic foldover algorithm based on two-level orthogonal matrices that converts some of the two-level columns into three-level ones. The goal of Nguyen et al. (2020) was to obtain designs with the same kind of correlation structure as DSD-A designs, while minimizing the aliasing between the quadratic effects. They named their newly constructed designs mixed-level foldover designs (MLFO designs). In

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these designs, most of the factors are two-level categorical ones. Like the DSD-A, ORTH-A, and compromise designs discussed above, MLFO designs do not possess the attractive orthogonality and minimal aliasing properties of the DSDs or the OMARS designs for quantitative factors.

The rest of this article is structured as follows. In Section 2, we formally define the properties of mixed-level OMARS designs and study the necessary conditions for their existence. In Section 3, we present the system of linear integer equations we used to generate mixed-level OMARS designs, and discuss three complementary solution approaches. In Section 4, we present three examples of mixed-level OMARS designs, obtained using the different solution approaches. Next, to demonstrate the versatility of our construction methods, in Section 5, we report on a computational search for mixed-level OMARS designs with up to 48 runs and 14 factors, resulting in 587 mixed-level OMARS designs. To the best of our knowledge, these designs are new to the literature. Finally, Section 6 contains our conclusions and directions for future research.

2. Existence of mixed-level OMARS designs

2.1 Properties

A mixed-level OMARS design possesses the following three properties:

Property 1. *There are three equidistant levels for the quantitative factors.*

Without loss of generality, we code the levels of the quantitative factors as -1, 0, and 1, and those of the two-level categorical factors as -1 and 1.

Property 2. *All odd design moments up to order three are equal to zero.*

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The concept of an odd design moment is defined in Section 7.4.2 of Myers et al. (2016). Property 2 is equivalent to the following:

(2.1) The average level of all quantitative factors is zero, and the two levels of each categorical factor are balanced.

(2.2) Any two main-effect columns of the model matrix are orthogonal.

(2.3) Any main-effect column in the model matrix is orthogonal to any two-factor interaction column and to any quadratic-effect column of the model matrix.

Property 3. *The number of zero entries in the main-effect columns of the model matrix is the same for all quantitative factors.*

Property 4. *The number of zero entries in the interaction-effect columns corresponding to two quantitative factors is equal.*

We denote the number of zero entries in each main-effect column for a quantitative factor by n_0^{ME}, and the number of zero entries in each interaction-effect column corresponding to two quantitative factors by n_0^{IE}. As pointed out by Núñez-Ares and Goos (2020), the n_0^{ME} and n_0^{IE} values give rise to different sets of OMARS designs. For definitive screening designs, for instance, $(n_0^{ME}, n_0^{IE}) = (2, 4)$ if we ignore the center run(s).

2.2 Necessary conditions for the existence of mixed-level OMARS designs

In this section, we derive necessary conditions for mixed-level OMARS designs involving one, two, and three or more two-level categorical factors to exist. First, Property 2 implies that the levels are balanced for each two-level factor. Therefore, the number of runs in any mixed-level OMARS design must be even.

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For designs with two or more two-level categorical factors, we can be even more specific. In the event that there are two two-level factors, the two-level part of a mixed-level OMARS design necessarily has to be a replicated 2^2 factorial design, because this is the only two-factor two-level orthogonal design that is balanced and involves no aliasing between the main effects and the two-factor interaction. As a result, mixed-level OMARS designs with two two-level categorical factors only exist for run sizes that are multiples of four.

In the event that there are three or more two-level categorical factors, the two-level part of a mixed-level OMARS surface design necessarily has to be a strength-3 OA, because this is the only family of two-level orthogonal designs that are balanced and involve no aliasing between the main effects and the two-factor interactions. Because strength-3 OAs only exist when the number of runs is a multiple of eight, mixed-level OMARS designs with three or more two-level categorical factors only exist for run sizes that are multiples of eight.

This line of reasoning is summarized by the following three conditions for the existence of mixed-level OMARS designs:

Lemma 1. *A necessary condition for the existence of a mixed-level OMARS design with one two-level factor is that the number of runs n is even.*

Lemma 2. *A necessary condition for the existence of a mixed-level OMARS design with two two-level factors is that the number of runs n is a multiple of four.*

Lemma 3. *A necessary condition for the existence of a mixed-level OMARS design with three or more two-level factors is that the number of runs n is a multiple of eight.*

To connect the existence of mixed-level OMARS designs to the number of zeros in the main-effect columns of the quantitative factors, n_0^{ME}, and in the interaction-effect columns

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involving these factors, n_0^{IE}, we need the following proposition of Núñez-Ares and Goos (2020):

Proposition 1. *A necessary condition for the existence of a three-level OMARS design with n runs and n_0^{IE} zero entries in the interaction-effect columns of the model matrix is that $n - n_0^{IE} \equiv 0 \pmod 4$.*

According to Lemma 1, the number of runs n has to be even for one two-level factor. Thus, Proposition 1 implies that n_0^{IE} must also be even for the case of one two-level factor. More specifically, either n and n_0^{IE} should both be multiples of four or they should both be odd multiples of two:

Corollary 1. *Necessary conditions for the existence of a mixed-level OMARS design with one two-level factor, n runs, and n_0^{IE} zero entries in the quantitative factors' interaction-effect columns of the model matrix are that n and n_0^{IE} should be even and that $n - n_0^{IE} \equiv 0 \pmod 4$.*

According to Lemmas 2 and 3, the number of runs n has to be a multiple of four or eight for two or more two-level factors. Thus, Proposition 1 implies that n_0^{IE} should be a multiple of four if there are two or more two-level factors:

Corollary 2. *A necessary condition for the existence of a mixed-level OMARS design with two or more two-level factors, n runs, and n_0^{IE} zero entries in the quantitative factors' interaction-effect columns of the model matrix is that n_0^{IE} should be a multiple of four.*

The following proposition connects the run size n with the number of zeros in the main-effect columns of the quantitative factors:

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Proposition 2. *A necessary condition for the existence of a mixed-level OMARS design with one or more two-level factors is that* $n - n_0^{ME} \equiv 0 \pmod 4$.

Proof. Let $\mathbf{a}$ be a three-level column and $\mathbf{x}$ be a two-level column of the model matrix of a mixed-level OMARS design. Both $\mathbf{a}$ and $\mathbf{x}$ have size n, which is the number of runs. Denote by a_i and x_i the ith entries of $\mathbf{a}$ and $\mathbf{x}$, respectively. Finally, consider the partition A_{-1}, A_0, and A_1 of $\mathscr{N} = \{1, \ldots, n\}$, where A_{-1}, A_0, and A_1 represent the sets of indices i for which a_i is equal to -1, 0, or 1, respectively.

Then, from Property (2.1) of any mixed-level OMARS design, we know that

$$\sum_{i=1}^{n} a_i x_i = \sum_{i \in A_1} x_i - \sum_{i \in A_{-1}} x_i = 0,$$

so that

$$\sum_{i \in A_1} x_i = \sum_{i \in A_{-1}} x_i.$$

From Property (2.3), we also know that

$$\sum_{i=1}^{n} a_i^2 x_i = \sum_{i \in A_1} x_i + \sum_{i \in A_{-1}} x_i = 0,$$

so that

$$\sum_{i \in A_1} x_i = -\sum_{i \in A_{-1}} x_i.$$

As a result,

$$\sum_{i \in A_1} x_i = \sum_{i \in A_{-1}} x_i = 0. \tag{2.1}$$

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Now, from Property (2.1),

$$\sum_{i=1}^{n} x_i = \sum_{i \in A_{-1}} x_i + \sum_{i \in A_0} x_i + \sum_{i \in A_1} x_i = 0,$$

so that

$$\sum_{i \in A_0} x_i = 0. \tag{2.2}$$

Equations (2.1) and (2.2) imply that the entries of $\mathbf{x}$ are balanced within each of the sets A_{-1}, A_1, and A_0. Consequently, the cardinalities $|A_{-1}|, |A_1|$, and $|A_0|$ and $n = |A_{-1}| + |A_1| + |A_0|$ are even numbers. In addition, from Property (2.1), the entries of vector $\mathbf{a}$ sum to zero, which implies that $|A_{-1}| = |A_1|$, and that $|A_{-1}| + |A_1| = n - |A_0| = n - n_0^{ME}$ is a multiple of four.

□

Combining Corollary 2 and Proposition 2, we obtain our final corollary:

Corollary 3. *A necessary condition for the existence of a mixed-level OMARS design with one or more two-level factors is that* $n_0^{IE} - n_0^{ME} \equiv 0 \pmod 4$.

An immediate consequence of Corollary 3 is that some sets of three-level OMARS designs, as characterized by the pair (n_0^{ME}, n_0^{IE}), cannot be extended to mixed-level OMARS designs by adding one or more two-level factors. For instance, it is impossible to convert definitive screening designs into mixed-level OMARS designs by adding several two-level factors. This is because, for definitive screening designs involving k center runs, $(n_0^{ME}, n_0^{IE}) = (2+k, 4+k)$, and therefore $n_0^{IE} - n_0^{ME}$ is not a multiple of four. Corollary 3 thus explains why Jones and Nachtsheim (2013) were unable to add multiple two-level factors to definitive screening

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designs to obtain a design that is orthogonal for the main effects and involves no aliasing between the main effects and the second-order effects.

3. Construction methods

After discussing a few preliminaries, we describe three alternative construction methods for mixed-level OMARS designs. The first constructs designs from scratch, ignoring any available knowledge on three-level OMARS designs or two-level OAs. Our second construction starts from a known strength-3 two-level OA, and our third construction starts from a known three-level OMARS design.

3.1 Preliminaries

We are interested in constructing n-run mixed-level OMARS designs, with m_1 quantitative factors with levels -1, 0, and 1, m_2 two-level categorical factors, n_0^{ME} occurrences of the zero level for each quantitative factor, and n_0^{IE} zeros in the columns of the model matrix that correspond to interactions of two quantitative factors. Therefore, every mixed-level OMARS design we construct is characterized by a tuple of five integers, $(m_1, m_2, n, n_0^{ME}, n_0^{IE})$.

Núñez-Ares and Goos (2020) created their catalog of OMARS designs for three-level quantitative factors in two steps. First, they created basic OMARS designs that did not contain any center runs (i.e., runs at which all factor levels are zero). Next, they added up to six center points to each basic OMARS design. As a result, each basic design they generated gave rise to seven different OMARS designs. When creating the basic OMARS designs, Núñez-Ares and Goos (2020) could ignore the center runs initially, because these neither affect the orthogonality of the main-effect columns of the model matrix nor do they

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impact the aliasing between the main effects and the second-order effects. In the presence of two-level categorical factors, the concept of a center run no longer exists, because there is no such thing as a middle value for a two-level categorical factor. Moreover, adding runs with all quantitative factors set at their middle level now potentially does affect the orthogonality of the main-effect columns in the model matrix, the aliasing between the main effects of the categorical factors and their interactions, and the aliasing between the main effects of the categorical factors and the second-order effects of the quantitative factors. Therefore, unlike Núñez-Ares and Goos (2020), we do allow all quantitative factors to act at their middle level simultaneously.

3.2 Construction from scratch

Let Ω_{m_1} be the set of all 3^{m_1} possible row vectors of size m_1 with entries equal to -1, 0, or 1, and let Ω_{m_2} be the set of all 2^{m_2} possible vectors of size m_2 with entries equal to -1 or 1. The set $\Omega = \Omega_{m_1} \times \Omega_{m_2} = \{(x_1 \parallel x_2) \mid x_1 \in \Omega_{m_1}, x_2 \in \Omega_{m_2}\}$, where $\times$ indicates the Cartesian product, and $x_1 \parallel x_2$ denotes the vector of size $m_1 + m_2$ produced by concatenating x_1 and x_2. Clearly, Ω has $3^{m_1}2^{m_2}$ elements and contains all possible factor-level combinations that can be used in a mixed-level OMARS design with m_1 three-level quantitative factors and m_2 two-level categorical factors.

Let $p \in \Omega$ be one of these possible factor-level combinations, and denote by α_i^p the ith entry of p. By construction, $\alpha_i^p \in \{-1, 0, 1\}$, for $i = 1, \ldots, m_1$, and $\alpha_i^p \in \{-1, 1\}$, for $i = m_1 + 1, \ldots, m_1 + m_2$. Based on the elements α_i^p, we can define two kinds of subsets of Ω that are needed in our construction. The first is defined as $\Omega_{0i} := \{p \in \Omega : \alpha_i^p = 0\}$, for $i = 1, \ldots, m_1$. The second is defined as $\Omega_{0ij} := \{p \in \Omega : \alpha_i^p \alpha_j^p = 0\}$, for $1 \leq i < j \leq m_1$.

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Finally, we use a binary variable y^p for each $p \in \Omega$. That variable takes the value one if vector p is selected in the mixed-level OMARS design, and zero otherwise.

A solution to the following system of binary linear equations is a mixed-level OMARS design of the type $(m_1,\, m_2, n, n_0^{ME}, n_0^{IE})$:

$$\sum_{p \in \Omega} y^p = n \tag{3.1}$$

$$\sum_{p \in \Omega_{0i}} y^p = n_0^{ME} \qquad 1 \leq i \leq m_1 \tag{3.2}$$

$$\sum_{p \in \Omega_{0ij}} y^p = n_0^{IE} \qquad 1 \leq i < j \leq m_1 \tag{3.3}$$

$$\sum_{p \in \Omega} \alpha_i^p \alpha_j^p y^p = 0 \qquad 1 \leq i < j \leq m_1 + m_2 \tag{3.4}$$

$$\sum_{p \in \Omega} \alpha_i^p \alpha_j^p \alpha_k^p y^p = 0 \qquad 1 \leq i < j < k \leq m_1 + m_2 \tag{3.5}$$

$$\sum_{p \in \Omega} \alpha_i^p \alpha_i^p \alpha_j^p y^p = 0 \qquad 1 \leq i \leq m_1, 1 \leq j \leq m_1 + m_2 \tag{3.6}$$

$$\sum_{p \in \Omega} \alpha_i^p y^p = 0 \qquad m_1 + 1 \leq i \leq m_1 + m_2 \tag{3.7}$$

$$y^p \in \{0, 1\} \qquad p \in \Omega. \tag{3.8}$$

Equation (3.1) ensures that exactly n of the binary decision variables y^p take the value one, so that an n-run design is obtained. Equations (3.2) ensure that every main-effect column of the model matrix corresponding to a quantitative factor has n_0^{ME} zeros, and Equations (3.3) ensure that every interaction-effect column corresponding to two quantitative

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factors involves n_0^{IE} zeros. Thus, together, Equations (3.2) and (3.3) make sure that the created design created possesses Property 3 and Property 4. Equations (3.4)–(3.7) translate Property 2 into mathematical notation. More specifically, Equations (3.4) force the main effects of all factors to be orthogonal to each other, irrespective of whether the factors are quantitative or categorical. Equations (3.5) guarantee that there is no aliasing between a main effect of any factor and the interaction of two other factors. Equations (3.6) have two functions. First, they ensure that, for each quantitative factor, the sum of all entries in a main-effect column of the model matrix is zero, so that the main effects can be estimated independently from the intercept. Second, it ensures that all main-effect columns of the model matrix are orthogonal to the columns corresponding to the quadratic effects. Equations (3.7) force the two-level factors of the design to be level balanced. Finally, Equations (3.8) define the binary nature of the decision variables y^p. The binary nature of the decision variables y^p and the construction of Ω imply that, just like the definitive screening designs with categorical factors from Jones and Nachtsheim (2013), the mixed-level OMARS designs produced by our first construction do not involve replicated runs.

3.3 Construction starting from a given OA

In the event that many two-level experimental factors are included in an experiment, the experimenter may desire to include a known high-quality n-run strength-3 OA. In that case, the two-level part of the design is fixed, and only the three-level part has to be determined.

This approach, which exploits existing knowledge about two-level designs, requires a few modifications to the approach described in Section 3.2. The first modification is that Ω_{m_2} should no longer be the set of all 2^{m_2} possible vectors of size m_2 with entries equal to -1 or 1.

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Instead, Ω_{m_2} should be the set of n rows of -1s or 1s of the selected strength-3 OA. In that event, Ω involves $3^{m_1} \times n$ instead of $3^{m_1}2^{m_2}$ elements. When starting from a given strength-3 OA, the constraints in Equation (3.7) are redundant, and the indices in the constraints in Equations (3.4) and (3.5) need to be adjusted.

When starting the construction from a strength-3 OA without replicates, the mixed-level OMARS designs produced by our second construction do not involve replicates either. If, however, our second construction starts from an OA that does involve replicates, then it is possible that it produces a design with replicates.

3.4 Construction starting from a given OMARS design

It is also possible to construct a mixed-level OMARS design starting from a known high-quality n-run OMARS design involving m_1 quantitative factors by adding m_2 two-level factors. This approach also necessitates a few modifications to the approach described in Section 3.2. The first is that Ω_{m_1} should no longer be the set of all 3^{m_1} possible vectors of size m_1 with entries equal to -1, 0, or 1. Instead, Ω_{m_1} should be the set of n rows of -1s, 0s, or 1s of the selected three-level OMARS design. In that event, Ω involves $n \times 2^{m_2}$ instead of $3^{m_1}2^{m_2}$ elements. Obviously, all constraints involving solely three-level factors can then be removed from the above system of linear equations.

As is the case with the previous construction method, we can obtain a design with replicates if the initial OMARS design involves replicates.

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4. Design examples

In this section, we present three examples obtained using each of the solution approaches presented in Section 3. Table 1 contains the set of values $(n, m_1, m_2, n_0^{ME}, n_0^{IE})$ characterizing each design example. All designs have four or more two-level categorical factors. From Lemma 3, the number of runs n is therefore a multiple of eight in each case. We can also verify that Propositions 1 and 2 and Corollary 3 are satisfied for all designs.

Feature	Design 1	Design 2	Design 3
n	24	48	40
m_1	4	5	6
m_2	4	14	4
n_0^{ME}	4	24	16
n_0^{IE}	8	36	24

Table 1: Key features of the three example designs.

4.1 Example 1: a 24-run eight-factor design

Design 1 is a 24-run design involving four three-level quantitative factors and four two-level categorical factors, constructed from scratch (see Section 3.2). Because it is a mixed-level OMARS design, Design 1 is orthogonal for the main effects of all factors, and all main-effect columns of its model matrix are orthogonal to the columns for the second-order effects. None of the designs available in the literature share both of these properties.

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run		*run*	
1	0 − + + + + + −	13	0 − + − − − − +
2	0 + − − − − − +	14	0 + − + + + + −
3	− 0 + + + − − −	15	− 0 − + − + + +
4	+ 0 − − − + + +	16	+ 0 + − + − − −
5	− − 0 − + − + +	17	− + 0 − − + − −
6	+ + 0 + − + − −	18	+ − 0 + + − + +
7	− − − 0 − − + −	19	− + + 0 − − + −
8	+ + + 0 + + − +	20	+ − − 0 + + − +
9	− + − + + − − +	21	− − − − + + − −
10	+ − + − − + + −	22	+ + + + − − + +
11	− + + − + + + +	23	− − + + − + − +
12	+ − − + − − − −	24	+ + − − + − + −

Design 1: 24-run mixed-level OMARS design involving four three-level quantitative factors and four two-level categorical factors.

A close inspection of Design 1 reveals that its three-level part is composed of two 12-run four-factor definitive screening designs (without center runs). Runs 1–12 form one definitive screening design, and runs 13–24 form the other. A three-quarter fraction of the 2^4 factorial design is appended to each of the two definitive screening designs to accommodate the four two-level categorical factors. The full design is a foldover design. This result suggests that one method for constructing large designs, with or without two-level categorical factors, might be to concatenate two definitive screening designs or, more generally, two OMARS designs. Such constructions have been proven to be successful for large two-level OAs (Li and Lin (2016); Vazquez et al. (2019)). Design 1 allows the estimation of any full second-order model in any three quantitative factors and one categorical factor. In addition, the maximum absolute correlation between the model matrix columns corresponding to the quadratic effects is 0.2,

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and the average absolute correlation between the columns corresponding to all second-order effects is 0.15.

The construction from scratch presented in Section 3.2 is suitable for problems where the researcher does not have an OA or OMARS design to start from. However, when the total number of factors is greater than 10, this approach is computationally expensive, owing to the large number of variables in the system of linear equalities.

4.2 Example 2: a 48-run 19-factor design

The solution approach of Section 3.3, which starts from a given OA, is convenient for designs requiring many two-level factors. As an example, Design 2 is a 48-run mixed-level OMARS design obtained from the OA-based construction. We started from a 14-factor 48-run strength-3 OA recommended by Schoen and Mee (2012), and added five three-level factors. Thus, unlike in Design 1, most of the factors in Design 2 are two-level categorical ones. The large number of two-level factors implies that the design can be considered a traditional two-level screening design, augmented with five three-level quantitative factors, for which quadratic effects are anticipated. As a matter of fact, the design offers large power for detecting any existing quadratic effect of the quantitative factors. This is because $n_0^{ME} = 24$ in the design, indicating that, for each quantitative factor, the zero level is used 24 times. This is very different in a DSD of this run size, for which $n_0^{ME} = 2$, if we ignore the center run. Like Design 1, Design 2 is a foldover design. The average correlation between the second-order effects' columns in the model matrix is 0.138, and the maximum correlation is 0.5. Finally, Design 2 allows the estimation of a full second-order model in any subset of four quantitative factors and two categorical factors, in any subset of five quantitative

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factors and any one categorical factor, and in any subset of three categorical factors and two quantitative factors. For subsets of higher cardinality, the proportion of estimable models is very high. For example, Design 2 allows the estimation of a full second-order model for 99% of all subsets containing two quantitative factors and four categorical factors, and for 97% of all subsets containing one quantitative factor and five categorical ones.

run		*run*	
1	0 − + 0 0 − − − − − − − − − − − − − −	25	0 0 0 0 − + − − − + + + − + + + − + +
2	0 + 0 0 0 − − − − − − − − − + + + + +	26	+ 0 0 − 0 + − − − + + + + − − + − − −
3	0 0 0 + 0 − − − − − − + + + − − − + +	27	+ − − + 0 + − − + − − + + − + + + + −
4	0 0 − + + − − − − + + − − + − + + − −	28	− − 0 − + + − − + − + + − + − − + + +
5	0 0 − − − − − − + − + − + − + − − − +	29	0 0 + 0 0 + − − + + − − − + + + − − +
6	0 + 0 − + − − − + + − + + + + − + − −	30	− + + + − + − − + + + − + − − − + + −
7	− − + 0 − − − + − − + + + + + + + − −	31	− + − − 0 + − + − − − − + + − + − + −
8	+ 0 0 0 0 − − + − + + − + + + − + + +	32	+ + 0 0 0 + − + − − + + − − − − + − +
9	0 + + 0 + − − + + − + + − − + + − + −	33	0 − 0 − 0 + − + − + − − − − + − + + −
10	− 0 − 0 − − − + + + − + − − − + + − +	34	− 0 0 + + + − + − + − + + − + − − − +
11	+ 0 0 0 − − − + + + − + − + − − − + −	35	+ 0 + 0 0 + − + + − − − + + − + + − +
12	0 − 0 0 + − − + + + + − + − − + − + +	36	0 0 − + 0 + − + + − + − − + + − − − −
13	0 0 + − 0 − + − − + − + + − − + + + +	37	0 + 0 0 − + + − − − − + − + + − + − −
14	− 0 − 0 0 − + − − + + + − − + − − + −	38	− 0 0 0 + + + − − − + − + − + + + − +
15	+ 0 0 − − − + − + − + − − + − + + + −	39	+ 0 + 0 + + + − − − + − + + + − − + −
16	0 + 0 + 0 − + − + − + + + + − + − − +	40	0 − − 0 − + + − − + − − + + − − + − +
17	− − 0 0 0 − + − + + − − + + + + − + −	41	− 0 0 0 0 + + − + − − + − − − + − − −
18	+ − + + 0 − + − + + + + − − + − + − +	42	+ + − 0 + + + − + + − − − − − − − + +
19	+ − − − + − + + − − − + − + + + − − +	43	0 − 0 + − + + + − − + − − − − + − + +
20	0 0 − 0 0 − + + − − + + + − − − + + −	44	0 0 + + + + + + − + − + − + − + + + −
21	+ + 0 + − − + + − + − − + − + + − − −	45	0 0 + − − + + + + − − + + − + − − + +
22	− + + − 0 − + + − + + − − + − − − − +	46	0 0 0 − 0 + + + + + + − − − + + + − −
23	− 0 0 + 0 − + + + − − − − + + − + + +	47	0 − 0 0 0 + + + + + + + + + − − − − −
24	0 0 0 0 + − + + + − − − + − − − + − −	48	0 + − 0 0 + + + + + + + + + + + + + +

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Design 2: 48-run mixed-level OMARS design involving five three-level quantitative factors and 14 two-level categorical factors.

4.3 Example 3: a 40-run 10-factor design

Design 3 was constructed from a 34-run three-level OMARS design in the catalog of Núñez-Ares and Goos (2020), involving six three-level quantitative factors and augmented with six center runs. Therefore, we used the construction from Section 3.4 to obtain the design. The design, which in total involves six quantitative and four categorical factors and turns out to be a foldover design, possesses attractive projection properties. It can fit a full second-order model for any five quantitative factors, any subset of four quantitative factors and one categorical factor, and any subset of three quantitative and two categorical factors. It is also able to fit an interaction-effect model for any six quantitative factors and any subset of five quantitative factors and one categorical factor.

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run		*run*		*run*	
1	− − − − − − − − − −	15	0 − 0 − − + + + − +	29	+ 0 − + 0 + − − − −
2	− − − + − − − + + +	16	0 − + + 0 + − + − −	30	+ 0 0 − + − − + − +
3	− − 0 − + 0 + − + −	17	0 0 − − + + − − + +	31	+ + − 0 0 − + + + −
4	− − + 0 0 + − − − +	18	0 0 + + − − + + − −	32	+ + 0 + − 0 − + − +
5	− 0 0 + − + + − + −	19	0 + − − 0 − + − + +	33	+ + + − + + + − − −
6	− 0 + − 0 − + + + +	20	0 + 0 + + − − − + −	34	+ + + + + + + + + +
7	− 0 + 0 + − + + − −	21	0 + + − − 0 − − + −	35	0 0 0 0 0 0 − + + −
8	− 0 + + + 0 − − + +	22	0 + + 0 − − − − − +	36	0 0 0 0 0 0 − + + −
9	− + − 0 + 0 − + − +	23	+ − 0 0 + − − − − −	37	0 0 0 0 0 0 − + + −
10	− + − + 0 0 + − − −	24	+ − 0 + 0 − + − + +	38	0 0 0 0 0 0 + − − +
11	− + 0 − 0 + − + − −	25	+ − + − 0 0 − + + +	39	0 0 0 0 0 0 + − − +
12	− + 0 0 − + + + + +	26	+ − + 0 − 0 + − + −	40	0 0 0 0 0 0 + − − +
13	0 − − 0 + + + + + −	27	+ 0 − − − 0 + + − −		
14	0 − − + + 0 + + − +	28	+ 0 − 0 − + − − + +		

Design 3: 40-run mixed-level OMARS design involving six three-level quantitative factors and four two-level categorical factors.

A remarkable characteristic of Design 3 is that it involves two triplicated factor level combinations. This allows a model-independent estimation of the error variance. The triplicates are possible because of the six center runs in the OMARS design used to start the construction.

We recommend using the solution approach from Section 3.4 when the requirements concerning the quantitative factors are demanding, such as high projection capabilities, low fourth-order correlations, high powers to detect quadratic effects, or the presence of replicates. In these situations, it pays to start from an OMARS design that fulfills these requirements.

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5. A computational search for mixed-level OMARS designs

Using the three construction methods outlined in Section 3, we explored the existence of mixed-level OMARS designs with up to 32 runs (the 48-run Design 2 and the 40-run Design 3 were obtained by a dedicated search for a few large designs). We focused on run sizes up to 32 because these are the ones typically used for screening experiments and for response surface experiments. Our exploration resulted in 587 different designs, which demonstrates the usefulness of the construction methods.

For our exploration, we first determined tuples $(n, m_1, m_2, n_0^{ME}, n_0^{IE})$ that satisfy the necessary conditions for mixed-level designs to exist from Section 2. For each tuple, we investigated which of the three construction methods were applicable, and then built the appropriate system of binary linear equations. Finally, we solved the system of equations using CPLEX 12.71. We performed the required computations on the Tier-1 and Tier-2 infrastructure at the Flemish Supercomputer Centrum, and set a computing time limit of one hour. For each system of linear equations, there were three possible outcomes: (i) a solution was found by CPLEX within the computing time limit; (ii) CPLEX indicates that the system of equations has no solution; or (iii) CPLEX neither finds a solution within the computing time limit, nor does it indicate that no solutions exist.

Table 2 provides an overview of the results we obtained for the three construction methods outlined in Section 3. The first column of Table 2 shows the number of instances considered for each of the three construction methods, which indicate the number of attempts we made to find a mixed-level OMARS design. For the construction from scratch, an instance is simply defined by a tuple of the form $(n, m_1, m_2, n_0^{ME}, n_0^{IE})$. For the construction from a given OA, an instance is defined by the input OA, the number of three-level quantitative

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Construction	Instances	Solutions	Infeasible	Unresolved	Time
From Scratch	1314	245	488	581	30.4
From OA	1173	123	894	156	18.4
From OMARS	973	219	572	182	13.5

Table 2: Summary of the computation results and total computing time (expressed in days) for the three construction methods for designs with up to 32 runs.

factors added (m_1), and the number of zeros in the model matrix's main-effect and interaction-effect columns for the quantitative factors (n_0^{ME} and n_0^{IE}). Finally, for the construction from a given three-level OMARS design (with given m_1, n_0^{ME}, and n_0^{IE} values), an instance is defined by the input OMARS design and the number of two-level categorical factors added (m_2). The second column of Table 2 shows the number of instances for which CPLEX reported a solution, and thus produced a mixed-level OMARS design, within the computing time limit. The third column shows the number of instances for which CPLEX reported that no solution exists. The fourth column reports the number of instances for which one hour of computing did not suffice to produce a solution or to prove the infeasibility of the system of linear equations. The final column reports the total computing time for each construction method, expressed in days.

As shown in the second column of Table 2, we set up 3460 systems of linear equations, and solved them using CPLEX. These systems were partitioned as follows: 1314 systems corresponded to a construction from scratch, 1173 corresponded to a construction starting from a given OA, and 973 corresponded to a construction starting from a given three-level OMARS design. For the construction method from scratch, the instances are determined by the tuple $(n, m_1, m_2, n_0^{ME}, n_0^{IE})$. We selected all tuples with an even number of runs ranging from 14 to 32, all combinations of two- and three-level factors such that there were two to seven three-level factors and the total number of factors did not exceed half of the

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number of runs and, finally, all feasible values for (n_0^{ME}, n_0^{IE}) given the run size. As input to the construction from a given OA, we used 57 strength-3 OAs, all of which are optimal in terms of the generalized word length pattern. More specifically, we used two OAs with 16 runs, six with 24 runs, and 49 with 32 runs. As input to the construction from a given three-level OMARS design, we used 223 six- and seven-factor OMARS designs, selected from Núñez-Ares and Goos (2020).

CPLEX was able to construct 245 mixed-level OMARS designs from scratch within one hour of computing, 123 designs starting from an OA, and 219 designs starting from a three-level OMARS design. CPLEX also found 488, 894, and 572 systems of linear equations to be infeasible for the constructions from scratch, from a given OA, and from a given three-level OMARS design, respectively. For a given run size n, the probability that a system of equations is infeasible and no mixed-level OMARS design exists increases with the number of factors involved. The probability that CPLEX does not finish its computation within one hour increases with the run size n.

Figure 1 provides a graphical summary of our results for run sizes up to 32. Figure 1a uses three symbols to show the combinations of the total number of factors $(m_1 + m_2)$ and the run size n for which we obtained a mixed-level OMARS design using at least one of the three construction methods. Figure 1b shows the combinations of the number of three-level factors m_1 and the number of two-level factors m_2 for which we found a mixed-level OMARS design using at least one construction method. The figures clearly show that we obtained multiple designs with 10 or more factors, and that each of the three methods allows us to construct designs with that many factors. Our computational results thus provide evidence that small mixed-level OMARS designs exist for large numbers of factors.

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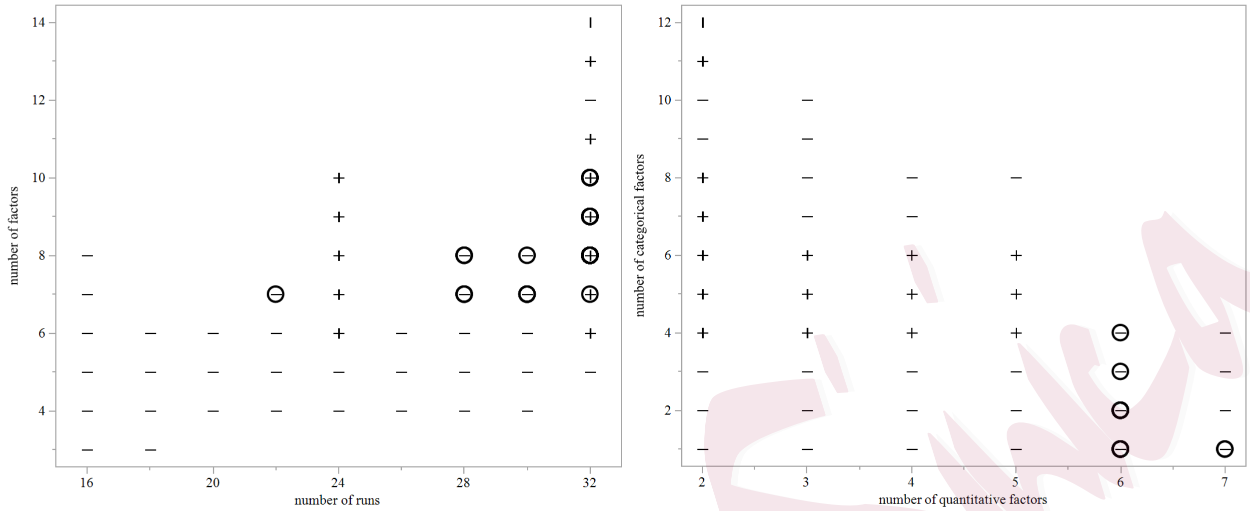

(a) Number of factors and design size

(b) Number of two- and three-level factors

Figure 1: OMARS designs found using the three construction methods, where the symbols −, I, and O indicate designs obtained using the construction methods from scratch, an existing OA, and an existing OMARS, respectively.

Figure 1 shows that we obtained mixed-level OMARS designs for all even run sizes from 14 to 32. For even run sizes that are not multiples of four, the mixed-level designs found involve one two-level categorical factor only. We also obtained mixed-level OMARS designs with 20 and 28 runs. Because these run sizes are odd multiples of four, these mixed-level designs involve at most two two-level categorical factors. All mixed-level OMARS designs with three or more two-level categorical factors have run sizes that are multiples of eight. Most of the designs obtained are foldover designs. However, 15 of the mixed-level OMARS designs are not foldover designs.

The mixed-level OMARS designs we obtained are available at `https://github.com/jnares/mixed-omars-designs-article.git`.

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6. Discussion

The original OMARS designs were intended for experiments with quantitative factors only, and they involve three levels per factor. The family of OMARS designs generalizes the family of definitive screening designs for quantitative factors, as well as the families of Box–Behnken and central composite designs. Here, we have studied mixed-level OMARS designs involving three-level quantitative factors and two-level categorical factors. We have derived several necessary conditions for the existence of these designs, and presented three alternative construction methods. One of our construction methods for mixed-level OMARS designs exploits existing catalogs of three-level OMARS designs, while another exploits existing catalogs of strength-3 two-level OAs. Using the three construction methods, we were able to generate designs with various numbers of quantitative and categorical factors and numbers of runs used in practice.

Our construction methods constitute a breakthrough in the experimental design literature, because several studies have attempted and failed to find orthogonal designs for three-level quantitative and two-level categorical factors possessing the minimal aliasing property. In general, of course, the categorical part of the designs presented here can also be used for quantitative factors when the quadratic effects are of no interest.

We view our work as a proof of concept. In future research, we will investigate algorithms for a complete enumeration of non-isomorphic mixed-level OMARS designs. If successful, such a complete enumeration would allow us to either confirm that the designs identified here are the best ones, or identify even more attractive ones. Similar enumerations have been performed for OAs (Schoen et al. (2010)) and for OMARS designs (Núñez-Ares and Goos (2020)).

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