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A Mixed-Effect Model for Analyzing Experiments with Multistage Processes

Kaibo Wang* and Chenxu Dai

Department of Industrial Engineering, Tsinghua University, Beijing, China
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Abstract: In industrial practice, most products are produced by processes that involve multiple stages. In studying multistage processes via designed experiments, some practitioners treat them as single-stage processes and follow the usual factorial designs or split-plot designs. In this paper, through an analysis of the error transmission mechanism, we propose a mixed-effect model for analyzing experiments with multistage processes. Based on an analysis of simulated and real experimental data, we find that different conclusions about factor significance may be drawn if the data are analyzed differently. In addition, the mixed-effect model can help separate errors at different stages and hence provide more information on process improvement.

Keywords: Design of experiments, mixed-effect model, multistage process.

1. Introduction

Design of experiments (DOE) is an efficient and widely used technique for process investigation, data collection and model building. In a controlled experiment, the process to be studied is treated as a black box; controllable factors, such as x_1 and x_2, that may affect the process output y are identified first and then are changed manually according to a design matrix. Figure 1(a) shows a diagram that represents the general scenario of experimental design: all of the factors are treated equally, and the impacts of the factors are applied to the process simultaneously.

However, in some processes, the factors are physically positioned at different stages, as Figure 1(b) shows. Compared to the process in Figure 1(a), the process in Figure 1(b) has two distinct features: first, there is a distinct difference in terms of the time or location of the factors. In Figure 1(b), factor x_1 functions first at stage 1, while the second factor, x_2, functions at a later stage, after the effect of x_1 on y', which is unobservable in practice. Second, a new interaction structure is presented in the process. With the variation propagating from upstream stages to downstream stages, the error term from stage 1, ε', enters stage 2 and may interact with x_2, while it is physically impossible for the disturbance at stage 2, ε, to move backward to interact with x_1.

The process in Figure 1(b) is a typical multistage manufacturing system (MMS). An MMS is a process that consists of more than one stage (or work station). In an MMS, each product moves through multiple manufacturing stages, there are controllable factors at each stage, and the accumulated effect of the factors is embedded in the final quality of the product. Because it is difficult to finish a product in a single operation, nearly all products

* Corresponding author. E-mail: kbwang@tsinghua.edu.cn

are produced by an MMS. For example, a semiconductor manufacturing process for producing integrated circuits (ICs) usually involves hundreds of stages (Mee and Bates [10]). A process for making a car also has dozens of stages (Shi [15]). Wu and Hamada [18] introduced a soap bar example consisting of two sub-processes: mixing and forming. The output of a multistage process is not a simple summation of all the individual stages; rather, control actions taken at later stages may interfere with the results of actions performed at earlier stages (Zhong *et al.* [21]).

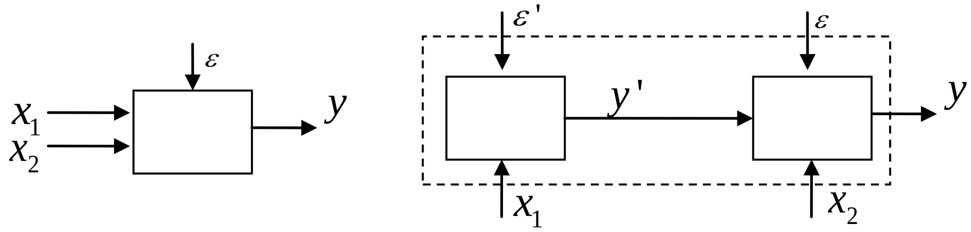

Figure 1. General model for a single-stage and two-stage process.

A considerable amount of research has been carried out on the modeling, monitoring and control of MMSs. Jin and Shi [6] developed a state-space model to characterize the variation propagation of a sheet metal assembly process in automobile production. Yao and Gao [19] suggested that a multistage process may be divided into blocks for model building. Li and Zhou [8] presented a robust variation source identification method for quality improvement in manufacturing processes, assuming a linear relationship between the variation sources. Gaver *et al.* [5] studied the reliability growth of a multistage system. Shi and Zhou [16] presented a survey of recent research into the modeling, monitoring, diagnosis, and control of multistage processes. Zi *et al.* [22] presented examples on monitoring a multistage process. However, research on the design and analysis of experiments for multistage processes is still limited.

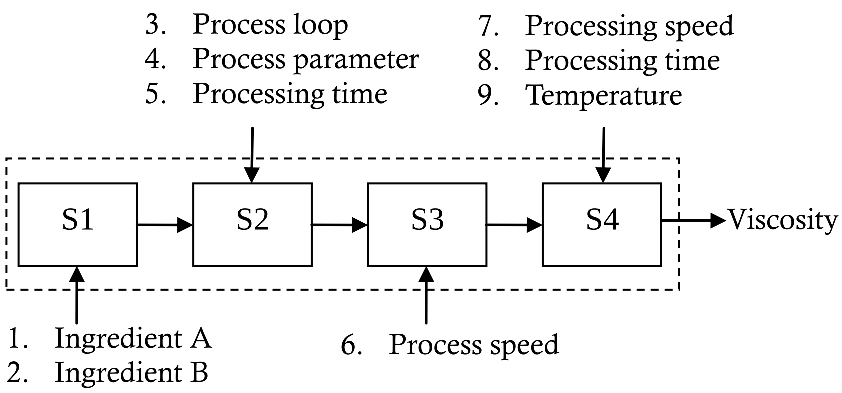

Figure 2. The multistage nature of the coffee cream-making process introduced by Schoen *et al.* [13].

To study a multistage process, it is preferable that each stage is studied individually if the intermediate response variables are observable, so that the physical mechanism of the engineering process is easier to understand. If such intermediate observations are difficult or impossible, the typical current practice is to treat the multiple stages as a single process. For example, Schoen *et al.* [13] studied a process for making coffee cream. The whole process consists of four consecutive stages. Nine controllable factors are identified in total, with two factors at the first stage, three at the second stage, one at the third stage and two at the last stage, as shown in Figure 2. The authors classified these factors as being easy to change or hard to change and then used a split-plot design to study the process.

As another example, Schoen [14] introduced a wood construction experiment involving 6 factors. The construction process has six stages: sawing, immersing, pretreatment, gluing, press, and storage. Again, the author treated the six-step process as a single stage and ignored the successive effects of the factors.

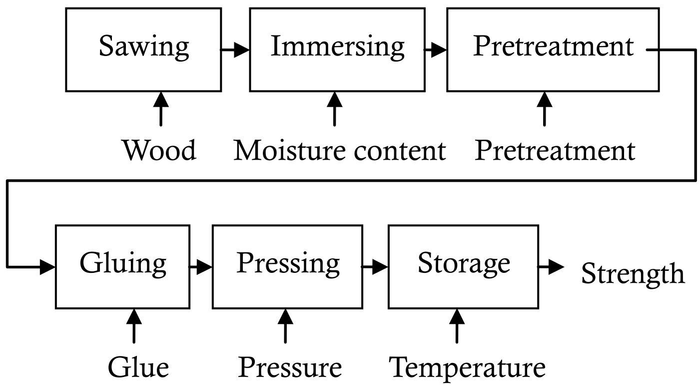

Figure 3. The multistage nature of the wood construction experiment introduced by Schoen [14].

In a later section of this paper, we examine a wafer-rinsing process. The process is designed to improve the smoothness of lapped wafers in semiconductor manufacturing. In this process, each wafer moves through several tanks sequentially. Each tank has its own factors, such as solution density and time. The wafers cannot be measured until they are treated in all tanks. A designed experiment is needed to study this process and optimize the settings of each tank. Conventionally, the tanks could be treated as one "big tank" with the factors of all the tanks being treated as equal. However, this approach obviously ignores the multistage nature of the process and may reduce the efficiency of the data analysis. The experiment is introduced in greater detail later. We also show the differences if the same experiment is analyzed in different ways.

Because the multistage nature of processes is widely observed, the design and analysis of experiments for multistage processes become important in practice. To optimize a multistage process, it is critical to collect data from the process efficiently and analyze the data appropriately. DOE is an important way to help identify significant factors in a process and construct statistical models to express the relationships between process output and input variables.

In the literature, some researchers have noticed the unique nature of multistage processes and have proposed ways to design and run experiments more efficiently at lower costs. For example, Miller [11] presented a laundry example with two stages: clothes need to go through washing and drying machines. The washing and drying steps obviously happen in sequence. Miller proposed the use of a strip-lot design (Mee and Bates [10] called this a two-way split-unit design) to reduce the resources needed for the experiment. Mee and Bates [10] presented an example of IC fabrication: wafers move through many manufacturing steps in their production. The authors suggested the use of multi-way split-lot designs. The name comes from the fact that in semiconductor manufacturing, wafers are processed in lots (batches). A split-lot design can be considered a typical design with incomplete blocks in which some main effects are confounded with blocking effects (see Section 3.5 of Mee [9]). Instead of using a fixed lot, Mee and Bates [10] suggested removal of the restriction of separate replicates so that a higher degree of randomization is achieved. Yuangyai *et al.* [20] proposed a robust parameter design method for a multistage process. However, they did not provide details regarding how the experiment should be analyzed; rather, they suggested methods for analyzing linear models for full-factorial split-plot designs.

Butler [2] suggested that split-lot designs are potentially useful for multistage processes. In such a design, each stage has a split-plot structure. This has the same implication as the multi-way split-unit design proposed by Taguchi [17]. Butler [2] also mentioned that a split-lot design with two stages is equivalent to a strip-plot design as described by Miller [11] and provided guidelines for constructing two-level split-lot fractional factorial designs for multistage processes. However, these studies only focused on the design of experiments for multistage processes; they did not emphasize the analysis of the experiments.

Alternatively, Schoen *et al.* [13] treated the experiment for a multistage process as a split-plot design. A split-plot experiment (which is referred to as a split-unit experiment in chapter 9 of Ryan [12]) is a blocked experiment in which blocks are formed with hard-to-change factors. Complete randomization is only implemented within subplots. If an experiment involves factors that are hard to change, it is a natural choice to adjust the hard-to-change factors less frequently (Mee and Bates [10]). In a split-plot design, hard-to-change factors are treated as whole-plot factors. The levels of a whole-plot factor are first randomized, and then the levels of the split-plot factors (easy-to-change factors) are randomized under each level of the whole-plot factor (Jones and Nachtsheim [7]). As Anbari and Lucas [1] noted, split-plot designs are widely used because of their accuracy, efficiency and low cost.

The purposes of this paper are to investigate the variation propagation mechanism in experiments for multistage processes and to propose a mixed-effect model for analyzing data collected from multistage processes. The remainder of this paper is organized as follows. Section 2 establishes a mixed-effect model for experiments with multistage processes. In Section 3, different model strategies for the experiments are studied. In Section 4, a comparison of the different modeling strategies are carried out based on simulated and real data. Lastly, Section 5 concludes with suggestions for future research.

2. A Mixed-Effect Model for Characterizing the Output of a Multistage Process

To better understand the data collected from DOE for a multistage process, we first try to capture the behavior of the process using a statistical model. For simplicity, we focus on a two-stage process that is similar to the one shown in Figure 1(b). There are S_1 factors at the first stage and S_2 factors at the second stage. The intermediate invisible output of the first stage, y', is given as follows:

$$y' = a_1 + \sum_{i=1}^{S_1} b_{1i} x_{1i} + \sum_{i,i'=1:S_1;i\neq i'} b'_{1ii'} x_{1i} x_{1i'} + \varepsilon', \tag{1}$$

where a_1, b_{1i}, and $b'_{1ii'}$ are the intercept and coefficients of the factors and their interactions. The first stage is assumed to have a normally distributed disturbance, $\varepsilon' \sim N(0,\sigma_1^2)$.

In Equation (1), each interaction effect can be observed as a new factor (for example, we can define $x_3 = x_1 x_2$). Because the focus of this paper is the study of the multistage nature of a process, to simplify the equations and their explanation, in the following, we hide all interaction effects of *the factors at the same stage* from the model. However, these effects could easily be added to the model, and all derivations still hold.

In a multistage process, the output of the upstream stages becomes the input of the downstream stages. In the two-stage process, the output of the second stage is therefore given by the following expression:

$$y = a_2 + \sum_{j=1}^{S_2} b_{2j} x_{2j} + ky' + \sum_{j=1}^{S_2} c_j x_{2j} y' + \varepsilon, \tag{2}$$

where k is the magnificent coefficient of y' on y and c_i is the coefficient of the interaction between the factors at the second stage, x_{2i}, and the output of the first stage, y'. Again, the second stage itself is also affected by a normally distributed disturbance, ε, and $\varepsilon \sim N(0,\sigma_2^2)$. Substituting Equation (1) for y' in Equation (2), we obtain the following expression:

$$\begin{aligned} y &= (ka_1 + a_2) + k\sum_{i=1}^{S_1} b_{1i} x_{1i} + \sum_{j=1}^{S_2} \left(b_{2j} + a_1 c_j\right) x_{2i} + \left(\sum_{j=1}^{S_2} c_j x_{2j} \left(\sum_{i=1}^{S_1} b_{1i} x_{1i}\right)\right) + k\varepsilon' + \sum_{j=1}^{S_2} c_j x_{2j} \varepsilon' + \varepsilon \\ &= \beta_0 + \sum_{i=1}^{S_1} \beta_{1i} x_{1i} + \sum_{j=1}^{S_2} \beta_{2j} x_{2j} + \sum_{j=1}^{S_2} \sum_{i=1}^{S_1} \beta_{ij} x_{1i} x_{2j} + \tau_0 + \sum_{j=1}^{S_2} x_{2j} \tau_{1j} + \varepsilon, \end{aligned} \tag{3}$$

where $\beta_{\bullet}$ reflect the effects of the factors and interactions; τ_0 is the stage-specific random effect, which is rooted in the transmission of the error at stage 1 to stage 2 and only appears in a multistage model; τ_{1j} is the random effect due to the interaction between the factors at the second stage and the propagated errors from the first stage, and

$$\tau_0 \sim N(0,\sigma_{\tau_0}^2),\ \tau_{1i} \sim N(0,\sigma_{\tau_{1i}}^2),\ \varepsilon \sim N(0,\sigma^2).$$

Equation (3) shows the components of the output of a multistage process. First, the output has several fixed effects, including the intercept and the main effects. Second, the output is also affected by the random effects in the system. Specifically, τ_0 is the effect of the error passing through from the first stage, and τ_1 is the interaction between the same error passing through from the first stage and the factors at the second stage. Third, the disturbance of the second stage is the global error shown directly in y.

Equation (3) can be observed as a special form of a mixed-effect model. The general form of the mixed-effect model is as follows (Fox [4]):

$$\mathbf{y}_i = \mathbf{X}_i \boldsymbol{\beta}_i + \mathbf{Z}_i \boldsymbol{\tau}_i + \boldsymbol{\varepsilon}_i,\quad \boldsymbol{\tau}_i \sim \mathbf{N}_q(\mathbf{0},\boldsymbol{\psi}^2),\ \ \boldsymbol{\varepsilon}_i \sim \mathbf{N}_{n_i}(\mathbf{0},\sigma^2\boldsymbol{\Lambda}_i).$$

In a multistage experiment, the special structure of the $\mathbf{Z}$ matrix is determined by the design matrix and the run order. In the following section, we examine several specific design scenarios and analyze the data based on the mixed-effect model.

If the multistage process is wrongly treated as a single-stage process, the model for the output would be expressed as follows:

$$y = \beta_0 + \sum_{i=1}^{S_1} \beta_{1i} x_{1i} + \sum_{j=1}^{S_2} \beta_{2j} x_{2j} + \sum_{j=1}^{S_2} \sum_{i=1}^{S_1} \beta_{ij} x_{1i} x_{2j} + \varepsilon", \quad (4)$$

where $\varepsilon"$ represented the effect of the two disturbance sources in the process. Compared with Equation (3), the random effects are missing, which may lead to an inaccurate estimation of the effects and erroneous conclusions about the factor significance. Simulated and real examples are presented later to show the difference between these models.

If the design is treated as a split-plot design, the model would be expressed as follows (see Jones and Nachtsheim [7]):

$$y = \beta_0 + \sum_{i=1}^{S_1} \beta_{1i} x_{1i} + \sum_{j=1}^{S_2} \beta_{2j} x_{2j} + \sum_{j=1}^{S_2} \sum_{i=1}^{S_1} \beta_{ij} x_{1i} x_{2j} + \tau_0 + \varepsilon", \quad (5)$$

where τ_0 is a random effect corresponding to the whole plot error in the split-plot design, rooted in the transmitted error of stage 1 to stage 2 in Equation (3). Obviously, this formulation does not consider the interaction effect between the transmitted error and the factors at stage 2.

The formulation in Equation (3) is also different from the model presented by Miller [11], in which the transmission and propagation of errors were also missing. In the following section, we apply the above formulation to different DOE scenarios and study how the experiments should be analyzed if the multistage nature is to be appropriately considered.

3. Modeling Strategies of Experiments for Multistage Processes

When dealing with experiments for multistage processes, the unique error transmission mechanism makes the modeling of the experiment different. In practice, some practitioners may ignore the multistage nature of the process and treat it as a typical factorial design. Some may analyze the experiment as a split-plot experiment. In the following section, for illustration purposes, we study a simple process with two stages. Different experimental design schemes are applied to the process. For each design, we then apply different modeling strategies and compare their differences.

3.1. Unreplicated Experiments with Two Factors

In the first scenario, we assume that in the two-stage process, each stage has a single controllable factor. Therefore, the process has two factors in total. Four experimental runs are used to study this process. The experiment could be treated in four different ways: (a) with a simple randomized factorial design, (b) with a randomized factorial design with consideration of the multistage nature, (c) with a split-plot design or (d) with a split-plot design with consideration of the multistage nature. We will show the model for each way of treating the experiment and compare the differences.

3.1.1. Modeling as a Single-Stage Randomized Factorial Design

In practice, some practitioners may simply treat an experiment for a multistage process as they would a factorial experiment for a single-stage process. In such a case, an unreplicated 2^2 full factorial design would be modeled as follows:

$$\mathbf{y}=\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}=\begin{bmatrix} 1 & x_{1+} & x_{2+} & x_{1+}x_{2+} \\ 1 & x_{1+} & x_{2-} & x_{1+}x_{2-} \\ 1 & x_{1-} & x_{2+} & x_{1-}x_{2+} \\ 1 & x_{1-} & x_{2-} & x_{1-}x_{2-} \end{bmatrix}\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}+\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{bmatrix}. \tag{6}$$

The covariance matrix of $\mathbf{y}$ is expressed as follows:

$$V=\begin{bmatrix} \sigma^2 & 0 & 0 & 0 \\ 0 & \sigma^2 & 0 & 0 \\ 0 & 0 & \sigma^2 & 0 \\ 0 & 0 & 0 & \sigma^2 \end{bmatrix}. \tag{7}$$

In this modeling framework, the two-stage process is treated as a black box on the whole. The errors of the two stages are not separable.

3.1.2. Modeling as a Multistage Randomized Design

Following the multistage model in Equation (3), if the multistage nature is considered for the completely randomized experiment, the observations of the four runs are modeled in the following way:

$$\begin{aligned}\mathbf{y}=\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}&=\begin{bmatrix} 1 & x_{1+} & x_{2+} & x_{1+}x_{2+} \\ 1 & x_{1+} & x_{2-} & x_{1+}x_{2-} \\ 1 & x_{1-} & x_{2+} & x_{1-}x_{2+} \\ 1 & x_{1-} & x_{2-} & x_{1-}x_{2-} \end{bmatrix}\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} \\ &+\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} \tau_{01} \\ \tau_{02} \\ \tau_{03} \\ \tau_{04} \end{bmatrix}+\begin{bmatrix} x_{2+} & 0 & 0 & 0 \\ 0 & x_{2-} & 0 & 0 \\ 0 & 0 & x_{2+} & 0 \\ 0 & 0 & 0 & x_{2-} \end{bmatrix}\begin{bmatrix} \tau_{11} \\ \tau_{12} \\ \tau_{13} \\ \tau_{14} \end{bmatrix}+\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{bmatrix},\end{aligned} \tag{8}$$

and $\tau_{ij} \sim N(0,\sigma_{\tau_i}^2),\ i=0,1;\ j=1,\ldots,4,\ \varepsilon_i \sim N(0,\sigma^2),\ i=1,\ldots,4,$ where τ_0 represents the random effect of the transmitted error from stage 1 to stage 2 and τ_1 represents the random effect of the interactions between the stage-1 error and stage-2 factors. If the experiment is treated as completely randomized, an identity matrix should be used in front of the τ_0 vector.

Compared to Equation (6), the fixed effects of the factors are the same, while Equation (8) gives a better explanation of the random errors of the experiment. With the coded factor levels, $x_{i+}=1$, $x_{i-}=-1$, the random effects are confounded. The covariance matrix of the observational vector becomes the following:

$$V=\begin{bmatrix}\sigma^2+\sigma_{\tau_0}^2+\sigma_{\tau_1}^2 & 0 & 0 & 0\\ 0 & \sigma^2+\sigma_{\tau_0}{}^2+\sigma_{\tau_1}{}^2 & 0 & 0\\ 0 & 0 & \sigma^2+\sigma_{\tau_0}{}^2+\sigma_{\tau_1}{}^2 & 0\\ 0 & 0 & 0 & \sigma^2+\sigma_{\tau_0}{}^2+\sigma_{\tau_1}{}^2\end{bmatrix}. \tag{9}$$

where

$$\sigma_{total}^2=\sigma^2+\sigma_{\tau_0}^2+\sigma_{\tau_1}^2.$$

The variation of each observation is the same. The random effect cannot be separated from the disturbance due to the way the experiment is conducted. Therefore, if the experiment is carried out in a totally random order, the modeling strategies with and without consideration of the multistage nature are the same.

3.1.3. Modeling as a Single-Stage Split-Plot Design

When doing experiments for a multistage process, it is common and natural to treat the factors of one stage as hard-to-change factors to minimize costs (Mee and Bates [10]). In such a case, the experiment would have a split-plot structure.

Table 1. A 2^2 split-plot design.

Run Order	x_1	x_2
1	+	+
2		−
3	−	+
4		−

Suppose the two-stage process is inaccurately considered as a single-stage process and the experiment is conducted following the split-plot design shown in Table 1, i.e., factor x_1 is the whole-plot factor, and x_2 is randomized under x_1. The output of the experiment is then modeled as follows:

$$\mathbf{y}=\begin{bmatrix}y_1\\y_2\\y_3\\y_4\end{bmatrix}=\begin{bmatrix}1 & x_{1+} & x_{2+} & x_{1+}x_{2+}\\1 & x_{1+} & x_{2-} & x_{1+}x_{2-}\\1 & x_{1-} & x_{2+} & x_{1-}x_{2+}\\1 & x_{1-} & x_{2-} & x_{1-}x_{2-}\end{bmatrix}\begin{bmatrix}\beta_0\\\beta_1\\\beta_2\\\beta_3\end{bmatrix}+\begin{bmatrix}1&0\\1&0\\0&1\\0&1\end{bmatrix}\begin{bmatrix}\tau_{w1}\\\tau_{w2}\end{bmatrix}+\begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\end{bmatrix}, \tag{10}$$

and $\tau_w \sim N(0,\sigma_{\tau_w}^2)$, $\varepsilon \sim N(0,\sigma)$ where τ_w is the whole-plot random effect and ε is the experiment error of the whole system. Because the first two runs are carried out under the same and unchanged setting of x_1, these two runs share a common random effect; similarly, the second two runs share another random effect. In this design, the covariance matrix of the output becomes the following:

$$V=\begin{bmatrix}\sigma^2+\sigma_{\tau_w}^2 & \sigma_{\tau_w}^2 & 0 & 0\\ \sigma_{\tau_w}^2 & \sigma^2+\sigma_{\tau_w}^2 & 0 & 0\\ 0 & 0 & \sigma^2+\sigma_{\tau_w}^2 & \sigma_{\tau_w}^2\\ 0 & 0 & \sigma_{\tau_w}^2 & \sigma^2+\sigma_{\tau_w}^2\end{bmatrix}. \tag{11}$$

The split-plot model does not take the interaction between the first-stage error and the second-stage factors into account. Due to the restricted randomization, the random effect and the random error are now separable. Section 4 present example experiments and shows how to analyze such experiments.

3.1.4. Modeling as a Multistage Split-Plot Design

The formulation in Equation (10) does not consider the multistage nature of the experiment. If the multistage nature is taken into consideration, the output should be modeled as follows:

$$\mathbf{y}=\begin{bmatrix}y_1\\y_2\\y_3\\y_4\end{bmatrix}=\begin{bmatrix}1 & x_{1+} & x_{2+} & x_{1+}x_{2+}\\1 & x_{1+} & x_{2-} & x_{1+}x_{2-}\\1 & x_{1-} & x_{2+} & x_{1-}x_{2+}\\1 & x_{1-} & x_{2-} & x_{1-}x_{2-}\end{bmatrix}\begin{bmatrix}\beta_0\\\beta_1\\\beta_2\\\beta_3\end{bmatrix}+\begin{bmatrix}1 & 0\\1 & 0\\0 & 1\\0 & 1\end{bmatrix}\begin{bmatrix}\tau_{w1}\\\tau_{w2}\end{bmatrix}+\begin{bmatrix}x_{2+} & 0\\x_{2-} & 0\\0 & x_{2+}\\0 & x_{2-}\end{bmatrix}\begin{bmatrix}\tau_{11}\\\tau_{12}\end{bmatrix}+\begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\end{bmatrix}, \tag{12}$$

where τ_w represents the random effect of the whole plot and τ_1 represents the random effect between the factors at the second stage and the transmitted error from the first stage.

In Equation (12), the random effects $\sigma_{\tau_0}^2$ and $\sigma_{\tau_1}^2$ are now separable because the design matrices in front of τ_w and τ_1 are not identical.

The above analysis shows that for the same experiment, if the assumption about the way the data were collected changes, the model changes accordingly. The model is considered correct only if the assumption and model structure correctly reflect the way the experiment was carried out.

3.2. Unreplicated Experiments with Three Factors

In this section, we will consider a multistage process with three factors. In a single-stage process, an increase in the factor numbers does not change the model structure, but this is no longer true in a multistage process. Suppose the number of factors is increased from 2 to 3, and an unreplicated 2^3 design is carried out. In the following, we show how this experiment shall be modeled.

3.2.1. Modeling as a Randomized Factorial Design

If the experiment is considered a full factorial design with a single-stage process, when the number of factors increases, the output of the experiment is modeled in a manner similar to that shown in Equation (6):

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix} = \begin{bmatrix} 1 & x_{1+} & x_{2+} & x_{3+} \\ 1 & x_{1+} & x_{2+} & x_{3-} \\ 1 & x_{1+} & x_{2-} & x_{3+} \\ 1 & x_{1+} & x_{2-} & x_{3-} \\ 1 & x_{1-} & x_{2+} & x_{3+} \\ 1 & x_{1-} & x_{2+} & x_{3-} \\ 1 & x_{1-} & x_{2-} & x_{3+} \\ 1 & x_{1-} & x_{2-} & x_{3-} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \\ \varepsilon_7 \\ \varepsilon_8 \end{bmatrix}. \tag{13}$$

The effects of all factors can be estimated as usual.

3.2.2. Modeling as a Randomized Multistage Design

If the experiment is modeled with its multistage nature taken into consideration, the model structure depends on the stage in which the third factor appears. If the factor is added to the first stage, the model becomes the following:

$$\begin{aligned} \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix} &= \begin{bmatrix} 1 & x_{1+} & x_{2+} & x_{3+} \\ 1 & x_{1+} & x_{2+} & x_{3-} \\ 1 & x_{1+} & x_{2-} & x_{3+} \\ 1 & x_{1+} & x_{2-} & x_{3-} \\ 1 & x_{1-} & x_{2+} & x_{3+} \\ 1 & x_{1-} & x_{2+} & x_{3-} \\ 1 & x_{1-} & x_{2-} & x_{3+} \\ 1 & x_{1-} & x_{2-} & x_{3-} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \tau_{01} \\ \tau_{02} \\ \tau_{03} \\ \tau_{04} \\ \tau_{05} \\ \tau_{06} \\ \tau_{07} \\ \tau_{08} \end{bmatrix} \\ &+ \begin{bmatrix} x_{3+} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & x_{3-} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & x_{3+} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & x_{3-} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & x_{3+} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & x_{3-} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & x_{3+} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & x_{3-} \end{bmatrix} \begin{bmatrix} \tau_{11} \\ \tau_{12} \\ \tau_{13} \\ \tau_{14} \\ \tau_{15} \\ \tau_{16} \\ \tau_{17} \\ \tau_{18} \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \\ \varepsilon_7 \\ \varepsilon_8 \end{bmatrix}. \end{aligned} \tag{14}$$

Compared with Equation (8), this model structure is the same, except that the dimension becomes higher. If the third factor appears at the second stage, the number of random effects increases because the interactions between the first-stage error and the factors at the second stage increase. The output now can be expressed as follows:

$$
\mathbf{y}=\begin{bmatrix} y_1\\ y_2\\ y_3\\ y_4\\ y_5\\ y_6\\ y_7\\ y_8 \end{bmatrix}=\begin{bmatrix} 1 & x_{1+} & x_{2+} & x_{3+}\\ 1 & x_{1+} & x_{2+} & x_{3-}\\ 1 & x_{1+} & x_{2-} & x_{3+}\\ 1 & x_{1+} & x_{2-} & x_{3-}\\ 1 & x_{1-} & x_{2+} & x_{3+}\\ 1 & x_{1-} & x_{2+} & x_{3-}\\ 1 & x_{1-} & x_{2-} & x_{3+}\\ 1 & x_{1-} & x_{2-} & x_{3-} \end{bmatrix}\begin{bmatrix} \beta_0\\ \beta_1\\ \beta_2\\ \beta_3 \end{bmatrix}+\begin{bmatrix} 1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&0&0&0&1 \end{bmatrix}\begin{bmatrix} \tau_{01}\\ \tau_{02}\\ \tau_{03}\\ \tau_{04}\\ \tau_{05}\\ \tau_{06}\\ \tau_{07}\\ \tau_{08} \end{bmatrix}+ \qquad (15)
$$

$$
\begin{bmatrix} x_{2+}&0&0&0&0&0&0&0\\ 0&x_{2+}&0&0&0&0&0&0\\ 0&0&x_{2-}&0&0&0&0&0\\ 0&0&0&x_{2-}&0&0&0&0\\ 0&0&0&0&x_{2+}&0&0&0\\ 0&0&0&0&0&x_{2+}&0&0\\ 0&0&0&0&0&0&x_{2-}&0\\ 0&0&0&0&0&0&0&x_{2-} \end{bmatrix}\begin{bmatrix} \tau_{11}\\ \tau_{12}\\ \tau_{13}\\ \tau_{14}\\ \tau_{15}\\ \tau_{16}\\ \tau_{17}\\ \tau_{18} \end{bmatrix}+\begin{bmatrix} x_{3+}&0&0&0&0&0&0&0\\ 0&x_{3-}&0&0&0&0&0&0\\ 0&0&x_{3+}&0&0&0&0&0\\ 0&0&0&x_{3-}&0&0&0&0\\ 0&0&0&0&x_{3+}&0&0&0\\ 0&0&0&0&0&x_{3-}&0&0\\ 0&0&0&0&0&0&x_{3+}&0\\ 0&0&0&0&0&0&0&x_{3-} \end{bmatrix}\begin{bmatrix} \tau_{21}\\ \tau_{22}\\ \tau_{23}\\ \tau_{24}\\ \tau_{25}\\ \tau_{26}\\ \tau_{27}\\ \tau_{28} \end{bmatrix}+\begin{bmatrix} \varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \varepsilon_4\\ \varepsilon_5\\ \varepsilon_6\\ \varepsilon_7\\ \varepsilon_8 \end{bmatrix}.
$$

Therefore, the modeling structure of a multistage process, as opposed to that of a single-stage process, depends on the location of the factors, because the multistage structure of the process makes the roles of the factors different. The factors at a downstream stage interact with the errors transmitted from the upstream stages, making the relationships among the factors complicated.

3.2.3. Modeling as a Split-Plot Design

The split-plot design is also sensitive to new factors. If a new factor is added to the first stage, the number of whole-plot blocks will increase. The output of the experiment is now modeled as follows:

$$
\mathbf{y}=\begin{bmatrix} y_1\\ y_2\\ y_3\\ y_4\\ y_5\\ y_6\\ y_7\\ y_8 \end{bmatrix}=\begin{bmatrix} 1 & x_{1+} & x_{2+} & x_{3+}\\ 1 & x_{1+} & x_{2+} & x_{3-}\\ 1 & x_{1+} & x_{2-} & x_{3+}\\ 1 & x_{1+} & x_{2-} & x_{3-}\\ 1 & x_{1-} & x_{2+} & x_{3+}\\ 1 & x_{1-} & x_{2+} & x_{3-}\\ 1 & x_{1-} & x_{2-} & x_{3+}\\ 1 & x_{1-} & x_{2-} & x_{3-} \end{bmatrix}\begin{bmatrix} \beta_0\\ \beta_1\\ \beta_2\\ \beta_3 \end{bmatrix}+\begin{bmatrix} 1&0&0&0\\ 1&0&0&0\\ 0&1&0&0\\ 0&1&0&0\\ 0&0&1&0\\ 0&0&1&0\\ 0&0&0&1\\ 0&0&0&1 \end{bmatrix}\begin{bmatrix} \tau_{w1}\\ \tau_{w2}\\ \tau_{w3}\\ \tau_{w4} \end{bmatrix}+\begin{bmatrix} \varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \varepsilon_4\\ \varepsilon_5\\ \varepsilon_6\\ \varepsilon_7\\ \varepsilon_8 \end{bmatrix}, \qquad (16)
$$

and the covariance matrix of $\mathbf{y}$ becomes the following:

$$
V=\begin{bmatrix} \sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} & 0&0&0&0&0&0\\ \sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} & 0&0&0&0&0&0\\ 0&0&\sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} &0&0&0&0\\ 0&0&\sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} &0&0&0&0\\ 0&0&0&0&\sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} &0&0\\ 0&0&0&0&\sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} &0&0\\ 0&0&0&0&0&0&\sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w}\\ 0&0&0&0&0&0&\sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} \end{bmatrix}. \qquad (17)
$$

We see in Equation (17) that there are more "blocks" than in the matrix in Equation (11). These blocks correspond to the whole-plot random effects in the experiment.

In the split-plot design, if the new factor is added to the second stage, the number of whole-plots does not change, so, the output is expressed as follows:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix} = \begin{bmatrix} 1 & x_{1+} & x_{2+} & x_{3+} \\ 1 & x_{1+} & x_{2+} & x_{3-} \\ 1 & x_{1+} & x_{2-} & x_{3+} \\ 1 & x_{1+} & x_{2-} & x_{3-} \\ 1 & x_{1-} & x_{2+} & x_{3+} \\ 1 & x_{1-} & x_{2+} & x_{3-} \\ 1 & x_{1-} & x_{2-} & x_{3+} \\ 1 & x_{1-} & x_{2-} & x_{3-} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \tau_{w1} \\ \tau_{w2} \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \\ \varepsilon_7 \\ \varepsilon_8 \end{bmatrix}. \tag{18}$$

The covariance matrix now becomes the following:

$$V = \begin{bmatrix} \sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & 0 & 0 & 0 & 0 \\ \sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & 0 & 0 & 0 & 0 \\ \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} & 0 & 0 & 0 & 0 \\ \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} \\ 0 & 0 & 0 & 0 & \sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} \\ 0 & 0 & 0 & 0 & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} & \sigma^2_{\tau_w} \\ 0 & 0 & 0 & 0 & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2_{\tau_w} & \sigma^2+\sigma^2_{\tau_w} \end{bmatrix}. \tag{19}$$

A new factor at the second stage does not change the number of blocks, but it increases the number of runs in each block. This again shows that an experiment with a multistage process is rather different from an experiment with a single-stage process. If the multistage process is wrongly treated as a single-stage process, erroneous conclusions may be drawn from the analysis.

3.2.4. Modeling as a Multistage Split-Plot Design

For the split-plot design, if the third factor appears at the first stage, the experiment will be modeled as follows:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \end{bmatrix} = \begin{bmatrix} 1 & x_{1+} & x_{2+} & x_{3+} \\ 1 & x_{1+} & x_{2+} & x_{3-} \\ 1 & x_{1+} & x_{2-} & x_{3+} \\ 1 & x_{1+} & x_{2-} & x_{3-} \\ 1 & x_{1-} & x_{2+} & x_{3+} \\ 1 & x_{1-} & x_{2+} & x_{3-} \\ 1 & x_{1-} & x_{2-} & x_{3+} \\ 1 & x_{1-} & x_{2-} & x_{3-} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \tau_{w1} \\ \tau_{w2} \\ \tau_{w3} \\ \tau_{w4} \end{bmatrix} + \begin{bmatrix} x_{2+} & 0 & 0 & 0 \\ x_{2+} & 0 & 0 & 0 \\ 0 & x_{2-} & 0 & 0 \\ 0 & x_{2-} & 0 & 0 \\ 0 & 0 & x_{2+} & 0 \\ 0 & 0 & x_{2+} & 0 \\ 0 & 0 & 0 & x_{2-} \\ 0 & 0 & 0 & x_{2-} \end{bmatrix} \begin{bmatrix} \tau_{11} \\ \tau_{12} \\ \tau_{13} \\ \tau_{14} \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \\ \varepsilon_7 \\ \varepsilon_8 \end{bmatrix}. \tag{20}$$

Compared with Equation (12), we can see that the number of blocks has increased, while the number of runs in each block remains the same.

If the new factor appears at the second stage, as in the case of a split-plot design, the number of whole-plot blocks remains the same, but the number of random effects of the interactions between the new factors and the first-stage error increases:

$$\mathbf{y}=\begin{bmatrix}y_1\\y_2\\y_3\\y_4\\y_5\\y_6\\y_7\\y_8\end{bmatrix}=\begin{bmatrix}1&x_{1+}&x_{2+}&x_{3+}\\1&x_{1+}&x_{2+}&x_{3-}\\1&x_{1+}&x_{2-}&x_{3+}\\1&x_{1+}&x_{2-}&x_{3-}\\1&x_{1-}&x_{2+}&x_{3+}\\1&x_{1-}&x_{2+}&x_{3-}\\1&x_{1-}&x_{2-}&x_{3+}\\1&x_{1-}&x_{2-}&x_{3-}\end{bmatrix}\begin{bmatrix}\beta_0\\\beta_1\\\beta_2\\\beta_3\end{bmatrix}+\begin{bmatrix}1&0\\1&0\\1&0\\1&0\\0&1\\0&1\\0&1\\0&1\end{bmatrix}\begin{bmatrix}\tau_{w1}\\\tau_{w2}\end{bmatrix}+\begin{bmatrix}x_{2+}&0\\x_{2+}&0\\x_{2-}&0\\x_{2-}&0\\0&x_{2+}\\0&x_{2+}\\0&x_{2-}\\0&x_{2-}\end{bmatrix}\begin{bmatrix}\tau_{11}\\\tau_{12}\end{bmatrix}+\begin{bmatrix}x_{3+}&0\\x_{3-}&0\\x_{3+}&0\\x_{3-}&0\\0&x_{3+}\\0&x_{3-}\\0&x_{3+}\\0&x_{3-}\end{bmatrix}\begin{bmatrix}\tau_{21}\\\tau_{22}\end{bmatrix}+\begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\\\varepsilon_5\\\varepsilon_6\\\varepsilon_7\\\varepsilon_8\end{bmatrix}.\quad(21)$$

3.3. Replicated Experiments with Two Factors

Replication is a basic means of improving estimation accuracy in experimental design. In this section, we study a case in which the experiment is carried out with replicates. We want to see how different the models may become. The process still has two stages, with one factor at each stage.

If the experiment is totally randomized within each replicate and is modeled as a factorial design, the model structure is similar to that shown in Equation (6), except that more observations are included. If the experiment is modeled as a multistage design, the model structure is similar to that shown in Equation (8). In both cases, in a manner similar to that discussed in Section 3.1.1, only the main effects can be estimated. Therefore, in the following section, we only focus on the cases in which the split-plot design is used.

3.3.1. Modeling as a Split-Plot Design

Replication in a split-plot design adds another blocking factor to the model. The structure of the experiment is shown in Table 2.

The model of the split-plot design with replication is a slightly different from that shown in Equation (10). With the blocking factor B being considered, the output of the experiment is given as follows:

$$\mathbf{y}=\begin{bmatrix}y_1\\y_2\\y_3\\y_4\\y_5\\y_6\\y_7\\y_8\end{bmatrix}=\begin{bmatrix}\beta_0\\\beta_0\\\beta_0\\\beta_0\\\beta_0\\\beta_0\\\beta_0\\\beta_0\end{bmatrix}+\begin{bmatrix}1&0\\1&0\\1&0\\1&0\\0&1\\0&1\\0&1\\0&1\end{bmatrix}\begin{bmatrix}B_1\\B_2\end{bmatrix}+\begin{bmatrix}x_{1+}&x_{2+}\\x_{1+}&x_{2-}\\x_{1-}&x_{2+}\\x_{1-}&x_{2-}\\x_{1+}&x_{2+}\\x_{1+}&x_{2-}\\x_{1-}&x_{2+}\\x_{1-}&x_{2-}\end{bmatrix}\begin{bmatrix}\beta_1\\\beta_2\end{bmatrix}+\begin{bmatrix}1&0&0&0\\1&0&0&0\\0&1&0&0\\0&1&0&0\\0&0&1&0\\0&0&1&0\\0&0&0&1\\0&0&0&1\end{bmatrix}\begin{bmatrix}\tau_{w1}\\\tau_{w2}\\\tau_{w3}\\\tau_{w4}\end{bmatrix}+\begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\\\varepsilon_5\\\varepsilon_6\\\varepsilon_7\\\varepsilon_8\end{bmatrix}.\qquad(22)$$

Now, we see a new factor "block" in the model, and more blocks in the matrix correspond to the random effects.

Table 2. A 2^2 replicated split-plot design.

	Replicate A		Replicate B	
Factors	x_1	x_2	x_1	x_2
1	+	+	+	+
2	+	−	+	−
3	−	+	−	+
4	−	−	−	−

3.3.2. Modeling as a Multistage Split-Plot Design

If the multistage nature of the process is considered, the replication in the design increases the number of whole plots and adds the effect of blocking into the model:

$$\mathbf{y}=\begin{bmatrix}y_1\\y_2\\y_3\\y_4\\y_5\\y_6\\y_7\\y_8\end{bmatrix}=\begin{bmatrix}\beta_0\\\beta_0\\\beta_0\\\beta_0\\\beta_0\\\beta_0\\\beta_0\\\beta_0\end{bmatrix}+\begin{bmatrix}1&0\\1&0\\1&0\\1&0\\0&1\\0&1\\0&1\\0&1\end{bmatrix}\begin{bmatrix}B_1\\B_2\end{bmatrix}+\begin{bmatrix}x_{1+}&x_{2+}\\x_{1+}&x_{2-}\\x_{1-}&x_{2+}\\x_{1-}&x_{2-}\\x_{1+}&x_{2+}\\x_{1+}&x_{2-}\\x_{1-}&x_{2+}\\x_{1-}&x_{2-}\end{bmatrix}\begin{bmatrix}\beta_1\\\beta_2\end{bmatrix}$$
$$+\begin{bmatrix}1&0&0&0\\1&0&0&0\\0&1&0&0\\0&1&0&0\\0&0&1&0\\0&0&1&0\\0&0&0&1\\0&0&0&1\end{bmatrix}\begin{bmatrix}\tau_{01}\\\tau_{02}\\\tau_{03}\\\tau_{04}\end{bmatrix}+\begin{bmatrix}x_{2+}&0&0&0\\x_{2-}&0&0&0\\0&x_{2+}&0&0\\0&x_{2-}&0&0\\0&0&x_{2+}&0\\0&0&x_{2-}&0\\0&0&0&x_{2+}\\0&0&0&x_{2-}\end{bmatrix}\begin{bmatrix}\tau_{11}\\\tau_{12}\\\tau_{13}\\\tau_{14}\end{bmatrix}+\begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\\\varepsilon_4\\\varepsilon_5\\\varepsilon_6\\\varepsilon_7\\\varepsilon_8\end{bmatrix}. \quad (23)$$

We see that compared to Equation (12), there is an extra blocking effect, while the metrics corresponding to the random effects have larger dimensions.

4. A Comparison of Different Modeling Strategies

In this section, we first apply the different modeling techniques to a set of simulated data and compare their performance. Then, a real case study is presented using data from a wafer fabrication process.

4.1. A Simulated Example

We first use simulated data to see whether the model is able to identify the factors and the sources of variation correctly. We assume a two-stage system with one factor at each stage. The experiment has 8 blocks and 32 runs in total.

We assume that the first stage of the simulated process is dominated by the following model:

$$y' = 10 + 5x_1 + \varepsilon' ,$$

where $\varepsilon' \sim N(0,1)$ is the experiment error. A random effect is also added to y' to simulate the blocking effect. Stage 2 is assumed to follow the following model form:

$$y = 10x_2 + y' + y'x_2 + \varepsilon ,$$

where $\varepsilon \sim N(0,1)$, which is equivalent to the following:

$$y = 10 + 5x_1 + 20x_2 + 5x_1x_2 + x_2\varepsilon' + \varepsilon' + \varepsilon .$$

The simulated data are shown in Table 3.

Table 3. A simulated experiment.

Run order	Replicate	x_1	y'	x_2	y
1	1	1	15.24119	1	41.18
2	1	1	15.24119	-1	-10.77
3	1	-1	3.767793	1	17.72
4	1	-1	3.767793	-1	-10.29
5	2	1	15.82919	1	40.36
6	2	1	15.82919	-1	-9.230
7	2	-1	3.780316	1	17.56
8	2	-1	3.780316	-1	-10.72
9	3	1	14.74322	1	40.79
10	3	1	14.74322	-1	-8.680
11	3	-1	3.742470	1	16.62
12	3	-1	3.742470	-1	-10.54
13	4	1	16.33879	1	44.07
14	4	1	16.33879	-1	-11.20
15	4	-1	4.440861	1	17.14
16	4	-1	4.440861	-1	-11.59
17	5	1	15.58961	1	41.52
18	5	1	15.58961	-1	-9.030
19	5	-1	4.729086	1	20.82
20	5	-1	4.729086	-1	-9.280
21	6	1	14.23056	1	37.35
22	6	1	14.23056	-1	-7.920
23	6	-1	3.591119	1	17.72
24	6	-1	3.591119	-1	-11.00
25	7	1	15.83576	1	42.96
26	7	1	15.83576	-1	-12.21
27	7	-1	5.456556	1	18.56
28	7	-1	5.456556	-1	-8.710
29	8	1	13.95306	1	38.65
30	8	1	13.95306	-1	-9.980
31	8	-1	4.329408	1	19.10
32	8	-1	4.329408	-1	-9.860

The following R code is used to prepare the data for further analysis:

- *response=c(41.18,-10.77,17.72,-10.29,40.36,-9.23,17.56,-10.72,40.79,-8.68,16.62,-10.54, 44.07,-11.20,17.14,-11.59,41.52,-9.03,20.82,-9.28,37.35,-7.92,17.72,-11.00,42.96,-12.21, 18.56,-8.71,38.65,-9.98,19.10,-9.86)*

- *block=c(1,1,1,1,2,2,2,2,3,3,3,3,4,4,4,4,5,5,5,5,6,6,6,6,7,7,7,7,8,8,8,8)*
- *x1=c(1,1,-1,-1,1,1,-1,-1,1,1,-1,-1,1,1,-1,-1,1,1,-1,-1,1,1,-1,-1,1,1,-1,-1,1,1,-1,-1)*
- *x2=c(1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1)*
- *simdata=data.frame(response=response, x1=x1,x2=x2,block=block)*

In the following section, three different models are used to analyze the data.

4.1.1. Modeling as a Randomized Factorial Design

If the experiment is treated as a randomized factorial design, the data are analyzed as follows:

- *model1=lm(response~ x1*x2, data= simdata)*
- *summary(model)*

The output of the above code is shown in Figure 4. The estimated intercept and coefficients of x_1 and x_2 and the interaction are close to the true parameters used in the simulation (the parameters are 10, 5, 20 and 5, respectively, in the simulation). However, the model can only estimate the total error as 1.53.

```
Call:
lm(formula = response ~ x1 * x2, data = test)

Coefficients:
             Estimate Std. Error  t value  Pr(>|t|)
(Intercept)   9.7222     0.2704   35.95   <2e-16
x1            5.7691     0.2704   21.33   <2e-16
x2           19.7853     0.2704   73.17   <2e-16
x1:x2         5.5834     0.2704   20.65   <2e-16

Residual standard error: 1.53 on 28 degrees of freedom
Multiple R-squared: 0.9955,     Adjusted R-squared: 0.9951
F-statistic:  2078 on 3 and 28 DF,  p-value: < 2.2e-16
```

Figure 4. Model summary when the experiment is analyzed as a factorial design.

```
Linear mixed-effect model fit by REML
Data: test
       AIC      BIC    logLik
  131.1271     140.4526  -58.56357

Random effects:
Formula: ~1 | block
        (Intercept)
StdDev: 3.35086e-05

Formula: ~1 | x1 %in% block
         (Intercept) Residual
StdDev: 3.765274e-05  1.52969

Fixed effects: response ~ x1 * x2
                  Value Std.Error DF   t-value    p-value
(Intercept)   9.722188 0.2704135 14  35.95304       0
x1            5.769062 0.2704135  7  21.33422       0
x2           19.785313 0.2704135 14  73.16687       0
x1:x2         5.583437 0.2704135 14  20.64777       0
```

Figure 5. Model summary when the experiment is analyzed as a split-plot design.

4.1.2. Modeling as a Split-Plot Design

If the same experiment is treated as a split-plot design, the following code can be used to analyze the data:

- *library(nlme)*
- *model2=lme(response~x1*x2,data=simdata, random=list(block=pdDiag(~1),x1=pdDiag(~1)))*
- *summary(model2)*

The restricted maximum likelihood (REML) algorithm is used for this model. The output is given in Figure 5. The estimates of the intercept and coefficients are nearly the same as those shown in Figure 4. All the factors are identified. One significant difference is that the split-plot design can separate and estimate the error of each single stage (the whole-plot factor and the sub-plot factor). However, the estimate of the first-stage error is much smaller than its true value, although the second-stage error is estimated to be 1.53, which is quite close to the value in the factorial design in Figure 4.

4.1.3. Modeling as a Multistage Split-Plot Design

Alternatively, if the multistage nature of the process is taken into consideration, we can analyze the same dataset as follows:

- *library(nlme)*
- *model3=lme(response~x1*x2,data=simdata, random=list(block=pdDiag(~1),x1=pdDiag(~x2)))*
- *summary(model3)*

The results are shown in Figure 6. Once again, the estimates of the coefficients are nearly the same. The block does not affect the response either. However, it is clearly that this model can separate the errors from both stages more precisely.

```
Linear mixed-effect model fit by REML
Data: test
       AIC      BIC    logLik
  131.7819   142.4395  -57.89094

Random effects:
Formula: ~1 | block
         (Intercept)
StdDev: 0.0001030876

Formula: ~x2 | x1 %in% block
Structure: Diagonal
        (Intercept)       x2   Residual
StdDev:   0.9027694 1.234197  0.04136634

Fixed effects: response ~ x1 * x2
                Value Std.Error DF   t-value    p-value
(Intercept)   9.722187 0.2258108 14  43.05457       0
x1            5.769063 0.2258108  7  25.54821       0
x2           19.785312 0.3086359 14  64.10568       0
x1:x2         5.583438 0.3086359 14  18.09070       0
```

Figure 6. Model summary when the experiment is analyzed as a multistage split-plot design.

4.2. Case Study

We next use the wafer rinsing process as an example. In the silicon chip production system, the cleanness and roughness of the surface could significantly affect the quality and failure rate of the final product. A multi-cavity rinsing device is used to remove the grain, metal contamination, organic contamination and oxidation film from the wafers (Cady and Varadarajan [3]). The process has two stages, with different solutions used at each stage. The density of the solution and the time spent at each stage may affect the rinsing effect. Therefore, in this experiment, four factors, the solution density at stage 1 (x_1), the rinsing time at stage 1 (x_2), the solution density at stage 2 (x_3) and the rinsing time at stage 2 (x_4) are studied. The response variable is the cleanness of the finished wafer, which is measured by the amount of metal ion left on the wafer surface. Considering the limitations of time and cost, 16 runs were conducted in the experiment.

As illustrated in the previous section, we may analyze the experiment as a factorial design, a split-plot design, or a multistage split-plot design. The data and the R code used to analyze the experiment are shown in Appendix A, and the summary of the three models are presented in Appendix B. If the experiment is analyzed as a single-stage factorial design, after removing all insignificant two-factor interactions, we noticed that factors x_2 and x_4 are significant in this model (using $\alpha = 0.10$ here and later); if the experiment is analyzed as a split-plot design, only the factor x_4 is significant. If the experiment is analyzed as a multistage split-plot design, both x_3 and x_4 are significant. In addition, this model can estimate all the random effects and show that the variability of the first stage is small and the variability of the second stage is much larger. This piece of information is important to further process diagnosis and improvement.

5. Conclusions

Multistage processes are widely observed in industrial processes. When designed experiments are conducted with a multistage process, it is crucial to consider the nature of the data generation process in the analysis of the data.

In this paper, we develop a mixed-effect model for analyzing experiments with multistage processes. Compared with cases in which an experiment is wrongly analyzed as a factorial design or a single-stage split-plot design, the proposed model can identify the random effects caused by the transmission of errors from upstream stages. If the experiment is correctly designed, the mixed-effect model can also separate the errors associated with the multiple stages and provide information for further process improvement. Performance studies based on simulated data and real data show that if the same experiment is modeled in different ways, different conclusions about factor significance may be drawn.

Because multistage processes are widely observed in practice, we believe that experimental design strategies for such processes, with the consideration of real constraints, deserve more attention in future research.

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Appendix A: R Code for Analyzing the Wafer Rinse Example

```
#real data
response=c(0.11,0.13,-0.65,0.47,-0.10,-0.26,0.89,-0.15,0.25,-0.32,0.61,5.64,1.01,1.47,0.40,-0.01)
x1=c(-1,-1,-1,-1,1,1,1,1,-1,-1,-1,-1,1,1,1,1)
x2=c(-1,-1,-1,-1,-1,-1,-1,-1,1,1,1,1,1,1,1,1)
x3=c(-1,1,1,-1,1,-1,-1,1,-1,1,1,-1,1,-1,-1,1)
x4=c(-1,-1,1,1,1,1,-1,-1,1,1,-1,-1,-1,-1,1,1)
waferdata=data.frame(response=response, x1=x1,x2=x2,x3=x3,x4=x4)

#analyze as a factorial design
model1=lm(response~x1+x2+x3+x4+x1:x3+x1:x4+x2:x3+x2:x4,data=waferdata)

#remove insignificant two-factor interactions
model1=lm(response~x1+x2+x3+x4,data=waferdata)
summary(model1)

#analyze as a split-plot design
library(nlme)
K=x1+2*x2
model2=lme(response~x1+x2+x3+x4+x1:x3+x1:x4+x2:x3+x2:x4,data=waferdata, random=~1|K)

#remove insignificant two-factor interactions
model2=lme(response~x1+x2+x3+x4,data=waferdata, random=~1|K)
summary(model2)

#analyze as a multistage split-plot design
library(nlme)
K=x1+2*x2
model3=lme(response~x1+x2+x3+x4+x1:x3+x1:x4+x2:x3+x2:x4,data=waferdata,
random=list(K=pdDiag(~x3+x4)))

#remove insignificant two-factor interactions
model3=lme(response~x1+x2+x3+x4,data=waferdata, random=list(K=pdDiag(~x3+x4)))
summary(model3)
```

Appendix B: Model Summary Generated from the Wafer Rinse Example

```
#summary of model 1
Coefficients:
            Estimate Std. Error t value   Pr(>|t|)
(Intercept)   0.5931     0.2997   1.979   0.0734
x1           -0.1869     0.2997  -0.624   0.5456
x2            0.5381     0.2997   1.796   0.1000
x3           -0.5281     0.2997  -1.762   0.1057
x4           -0.6206     0.2997  -2.071   0.0627

#summary of model 2
Linear mixed-effects model fit by REML
 Data: waferdata
       AIC      BIC    logLik
  63.06708 65.85234 -24.53354

Random effects:
Formula: ~1 | K
         (Intercept) Residual
StdDev: 5.760578e-05 1.198714

Fixed effects: response ~ x1 + x2 + x3 + x4
                Value Std.Error DF    t-value  p-value
(Intercept)  0.593125 0.2996785 10  1.9792043  0.0760
x1          -0.186875 0.2996785  1 -0.6235849  0.6450
x2           0.538125 0.2996785  1  1.7956743  0.3235
x3          -0.528125 0.2996785 10 -1.7623052  0.1085
x4          -0.620625 0.2996785 10 -2.0709693  0.0652

#summary of model 3
Linear mixed-effects model fit by REML
Data: waferdata
       AIC      BIC    logLik
  66.97258 70.55364 -24.48629

Random effects:
Formula: ~x3 + x4 | K
Structure: Diagonal
         (Intercept)        x3        x4 Residual
StdDev: 7.146907e-05 0.1202379 0.3381592 1.138594

Fixed effects: response ~ x1 + x2 + x3 + x4
                Value Std.Error DF    t-value  p-value
(Intercept)  0.593125 0.2846485 10  2.0837101  0.0638
x1          -0.186875 0.2846485  1 -0.6565114  0.6302
x2           0.538125 0.2846485  1  1.8904894  0.3097
x3          -0.528125 0.2909279 10 -1.8153121  0.0995
x4          -0.620625 0.3310781 10 -1.8745578  0.0903
```

Authors' Biographies:

Kaibo Wang is an Associate Professor in the Department of Industrial Engineering, Tsinghua University, Beijing, China. He received his B.S. and M.S. degrees in Mechatronics from Xi'an Jiaotong University, Xi'an, China, and his Ph.D. in Industrial Engineering and Engineering Management from the Hong Kong University of Science and Technology, Hong Kong. He has published papers in journals such as *Journal of Quality Technology*, *IIE Transactions*, *Quality and Reliability Engineering International*, *International Journal of Production Research*, and others. His research is devoted to statistical quality control and data-driven complex system modeling, monitoring, diagnosis, and control, with a special emphasis on the integration of engineering knowledge and statistical theories for solving problems from real industry. He is a member of ASQ, INFORMS and IIE.

Chenxu Dai received his B.S. and M.S. degrees in Industrial Engineering from Tsinghua University, Beijing, China, in 2011 and 2013, respectively. His research focuses on the statistical modeling, monitoring and control of engineering systems.