Chapter 11

OPTIMAL DESIGN FOR THE EXPONENTIAL MODEL IN INDUSTRIAL APPLICATIONS

§11.1 Industrial Applications of the Exponential Model

While the exponential model is heavily used in impaired reproduction studies, it has many other applications. Responses in industrial processes often follow a Poisson distribution. Examples include the count of defects in a product or the yield from a process. Engineers are typically interested in finding the settings of equipment and/or the amount of additives which minimize the number of defects or maximizes the yield. However, these goals imply that certain regressors act as stimulants rather than toxicants as in impaired reproduction studies. For the purposes of industrial models, a *toxicant* is a design variable which causes a *decrease* in the expected response. In contrast, as the amount or setting of a *stimulant* increases it produces an *increase* in the expected count. Thus, designs for exponential models in industrial settings must accommodate regressors which function as stimulants. More importantly, the need exists to develop designs where some regressors function as stimulants and others function as toxicants.

The mixed toxicant-stimulant model is the most frequently encountered case in industry. Often some design variables in a process have negative effects on the final product whereas

others have positive effects. An example of this comes from the Chrysler Corporation. Increasing the amount of a chemical used in the molding of automobile grills creates small defects in the surface of the grill while increasing the amounts/settings of the other regressors tends to improve the quality of the grill. Chrysler was interested in finding the settings of all regressors which would minimize the count of these defects. Similarly, the textile industry is interested in minimizing the number of defects in quantities of cloth. These are just a few of the many applications that motivate the need for toxicant-stimulant models (Myers and Montgomery, 1997). In what follows, models are formulated and optimal designs are discussed.

§11.2 The Single Regressor Stimulant Model

Since no work has been done with exponential stimulant models, the single regressor case will be addressed first. The single regressor model takes on the same appearance as it did in impaired reproduction studies

$$y_{ij} = e^{\beta_0+\beta_1 x_i} + \varepsilon_{ij}. \qquad (11.2.1)$$

However, in this model, β_1 is positive so that the general form of the functions looks as it does in Figure 11.1.1.

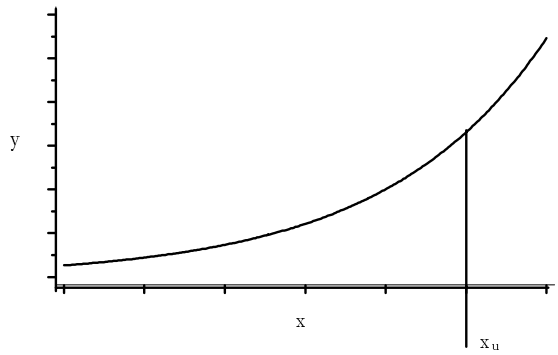

Figure 11.1.1 Graph of the Stimulant Model on a Restricted Region.

Of course, for these models the maximum response does not occur at x_i=0 which means there is no longer a control as defined in impaired reproduction studies. Instead, the maximum count occurs at $x_i = x_u$. However, it would be more convenient if this model could be parameterized

like the models for impaired reproduction studies. This can be accomplished using a coding scheme. Let

$$x_i^* = x_i - x_u . \tag{11.2.2}$$

Thus, $x_u^* = x_u - x_u = 0$. The model (11.2.1) in terms of the new coordinate system becomes

$$y_{ij} = e^{\beta_0^* + \beta_1 x_i^*} + \varepsilon_{ij} \tag{11.2.3}$$

where $\beta_0^* = \beta_0 + \beta_1 x_u$. The point of maximum response is now at $x_u^* = 0$. Define the expected value at this point as

$$E(y_u) = e^{\beta_0^* + \beta_1 x_u^*} = e^{\beta_0^*} = \lambda_u . \tag{11.2.4}$$

The quantity λ_u plays the same role as λ_c in impaired reproduction models. The expected value at any other point is denoted by

$$E(y_{ij}) = r_i \lambda_u = e^{\beta_0 + \beta_1 x_i} \tag{11.2.5}$$

where $r_i = e^{\beta_1 x_i^*}$ and $0 < r_i \leq 1$. Thus, r_i represents the proportion of the maximum response produced at the upper boundary of the region of operability, x_u. While r_i plays the same role as q_i in the impaired reproduction studies, it is important to notice the differences in the formulas associated with r_i and q_i especially in the transformation to natural units. The quantity r_i does represent an EC. However, the interpretation of this EC is slightly different. The point of reference for the EC is no longer the control, it is now the response produced at the upper extreme of the experimental region. Thus, for this model, an effective concentration represents the amount of stimulant necessary to illicit a particular proportion of the maximum amount produced at the upper extreme of the region of operability.

The same model and the similarity of the parameterization indicate that the single regressor stimulant model will have a similar determinant and thus a similar optimal design in

terms of this new effective concentration. Expression (11.2.6) shows the form of the determinant of the information matrix for the single regressor stimulant model.

$$|\mathbf{I}| = \lambda_1\lambda_2\left(x_1 - x_2\right)^2 = \frac{\lambda_u^2}{\beta_1^2} r_1 r_2 \left(\ln r_1 - \ln r_2\right)^2 \tag{11.2.6}$$

Maximizing the determinant apart from $\frac{\lambda_u^2}{\beta_1^2}$ indicates that 50% of the experimental units will be placed at the $EC_{13.53}$ and 50% will be placed at the EC_{100}. In terms of ECs, this design is the same as Chiacchierini's design for the single regressor impaired reproduction model. However, there is a difference in the conversion to natural units between the stimulant model and the toxicant model. Thus, design points for the stimulant model are converted to natural units using (11.2.7).

$$x_i = \frac{\ln r_i}{\beta_1} + x_u . \tag{11.2.7}$$

This should be contrasted with the single regressor impaired reproduction model in that $x_i = \frac{\ln q_i}{\beta_1}$. Basically, the value x_u in (11.2.7) adjusts the amount of the design variable in natural units to account for the fact that the control does not occur at x=0.

Of course, the same problems of impaired reproduction studies exist in the stimulant model. The single regressor stimulant model requires knowledge of parameters in order to convert it to natural units. In addition, these designs are saturated and thus provide no degrees of freedom to test for lack of fit. However, new research is not necessary to solve these problems. The Bayesian designs discussed in Chapters 3 and 4 of this work can be used to address cases of limited knowledge about parameters. In addition, Chiacchierini's three level designs can be used to test for lack-of-fit. Type I and Type II three level Bayesian designs can

also be used for this purpose. Note that the F-optimal design formulated by Minkin also applies to the stimulant model as well.

§11.3 Toxicant Models in the Industrial Context

A similar situation to that of the stimulant model occurs in the industrial toxicant model in the industrial world with regard to the idea of a restricted region. For example, if temperature functions as a toxicant, it is obvious that $0°$ is not likely to be in the range of operability for a particular process. In this case, the graph of the function and its region of operability may be more like Figure 11.1.1

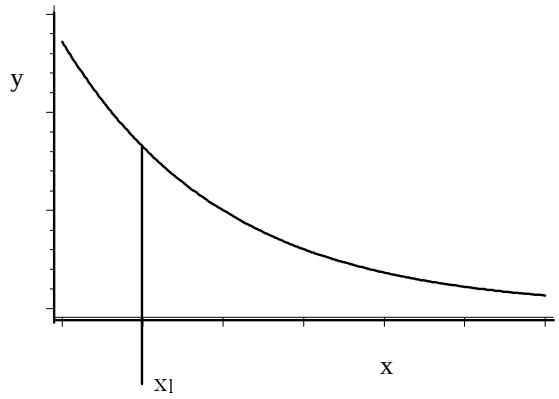

Figure 11.3.1 Graph of the Toxicant Model on a Restricted Region.

where x_l represents some lower bound on the regressor x_i. The same coding scheme is employed to make the model similar to the impaired reproduction study model. For this model, the value x_u in (11.2.2)-(11.2.7) would be replaced by x_l.

§11.4 The D-Optimal Design for *k*-regressor Stimulant Model

While the single regressor stimulant model provides a nice introduction to a broader use of the impaired reproduction designs for the exponential model, the real importance of this topic lies in the formulations of general designs for *k*-regressor industrial models. In order to develop designs for *k*-regressor toxicant-stimulant models, the *k*-regressor stimulant model must be explored first. The *k*-regressor stimulant model can be parameterized in terms of these

individual ECs like the *k*-regressor impaired reproduction model. The *k*-regressor stimulant model with no interaction takes on the same form as the IRS model as shown in (11.4.1).

$$y_{ij} = e^{\mathbf{x}_i'\boldsymbol{\beta}} + \boldsymbol{\varepsilon}_{ij}. \tag{11.4.1}$$

However, the expected value of the response takes on a slightly different form now that a model effective concentration or MEC represents the combination of stimulants required to illicit a proportion of the maximum response at the highest levels of all regressors. Expression (11.4.2) shows the expected value at a particular design point as a function of the MEC denoted by r_i and $\boldsymbol{\lambda}_u$, the expected value at the extreme of the region of operability, $\mathbf{x}_u' = \left(x_{1u}, x_{2u}, x_{3u}, \ldots, x_{ku}\right)$.

$$E(y_{ij}) = e^{\mathbf{x}_i'\boldsymbol{\beta}} = r_i\boldsymbol{\lambda}_u. \tag{11.4.2}$$

The same coding scheme is used in this model as in Section 11.2 the single regressor model meaning that the upper limit for each design variable is subtracted from its corresponding x-value. However, the asterisks are dropped for convenience in this case. This means that $\boldsymbol{\lambda}_u = e^{\boldsymbol{\beta}_0^*}$ where $\boldsymbol{\beta}_0^* = \boldsymbol{\beta}_0 + \boldsymbol{\beta}_1 x_{1u} + \cdots + \boldsymbol{\beta}_k x_{ku}$ and $r_i = e^{\boldsymbol{\beta}_1 x_{1i}^* + \boldsymbol{\beta}_2 x_{2i}^* + \cdots + \boldsymbol{\beta}_k x_{ki}^*}$. In the impairment model, an MEC is decomposed into a product of individual effective concentrations or IECs. The same decomposition can be performed in the stimulant model. However, one must be aware that an IEC is the quantity of a single stimulant that produces a particular proportion of the amount produced a the upper extreme of an individual regressor. The formula for an MEC in terms of its IECs is shown in (11.4.3).

$$r_i = r_{1i} r_{2i} \ldots r_{ki} \tag{11.4.3}$$

where $r_{mi} = e^{\boldsymbol{\beta}_m x_{mi}}$ and $0 < r_{mi} \leq 1$ for m=1,…,k. Thus,

$$E(y_{ij}) = r_{1i} r_{2i} \ldots r_{ki}\boldsymbol{\lambda}_u. \tag{11.4.4}$$

As in the single stimulant case, the determinant for the information matrix of a *k*-regressor stimulant model is that of the corresponding impairment model with the values of q_{mi}

replaced by r_{mi}. (Note that the x_{mu} cancel out in the determinants.) Hence the resulting D-optimal designs are composed of the same allocation percentages and the same design points in terms of IECs. The only difference is that the designs are found in terms of IEC_{100r} rather than IEC_{100q} so the appropriate formula must be used for the translation into natural units. This formula is shown in expression (11.4.5) for the m^{th} IEC.

$$x_{mi} = \frac{\ln r_{mi}}{\beta_m} + x_{mu}\,. \qquad (11.4.5)$$

Designs for k-regressor stimulant models with interaction are handled in the same way as those for IRS models discussed in Chapter 8. As before, convenient guesses of 0 are made for the interaction parameters so that designs can be found in terms of IECs. Recall that this helps eliminate the need for knowledge of all parameters in order to find optimal designs. Again, the form of the information matrix and determinant parallel that of the IRS models so the designs are the same. These designs also exhibit the same robustness properties with regard to positive and negative interaction parameters as discussed in Chapter 8.

§11.5 The *k*-regressor Toxicant-Stimulant Model

While stimulant models are very important, the most important model in the industrial setting is the combined toxicant-stimulant model as discussed in the introduction of this chapter. Very few industrial processes have additives or settings of equipment that function solely as toxicants or solely as stimulants. Usually, there is a mixture of the two types of regressors in the process.

This model takes on the same form as the multiple regressor models seen in previous chapters shown in (11.5.1).

$$y_{ij} = e^{\mathbf{x}_i'\boldsymbol{\beta}} + \boldsymbol{\varepsilon}_{ij} \qquad (11.5.1)$$

However, each of the *k* regressors fall into one of two groups: either toxicant or stimulant. Without loss of generality, the first k_1 of the regressors will be considered toxicants while the

remaining regressors k-k_1 regressors will be considered toxicants. Thus, the expected value at a particular design point becomes

$$E\left(y_{ij}\right) = q_i r_i \boldsymbol{\lambda}_{max} \tag{11.5.2}$$

where $\boldsymbol{\lambda}_{max}$ is the maximum achievable expected value at the point $\mathbf{x}'_{\mathbf{max}} = \left(x_{1l}, x_{2l}, \ldots, x_{kl}, x_{(k_1+1)u}, x_{(k_2+1)u}, \ldots, x_{ku}\right)$. In the vector, $\mathbf{x}'_{\mathbf{max}}$, the k_1 toxicants are set at the lower extremes of their experimental region where their individual maxima are achieved and the k-k_1 stimulants are set at the upper extremes of their regions respectively. In coded units, $\mathbf{x}'_{\mathbf{max}} = \mathbf{0}$ or the control since either the lower limit or the upper limit are subtracted accordingly. At these settings, the maximum response occurs. In (11.5.2), the quantity q_i represents the toxicant effective concentration and r_i represents the stimulant effective concentration. Each of these quantities can be decomposed into toxicant IECs and stimulant IECs respectively by the formulas

$$q_i = q_{1i} q_{2i} \ldots q_{k_1 i} \text{ where } q_{mi} = e^{\boldsymbol{\beta}_m x_{mi}} \tag{11.5.2}$$

and

$$r_i = r_{(k_1+1)i} r_{(k_1+2)i} \ldots r_{ki} \text{ where } r_{mi} = e^{\boldsymbol{\beta}_m \left(x_{mi} - x_{mu}\right)}.$$

As one might imagine, this parameterization results in a D-optimal design composed of a control, main effect points, and interaction points based on the $IEC_{13.53}$. Of course, one must be aware of whether the IEC is an IEC_{100q} associated with a toxicant or IEC_{100r} associated with a stimulant so that the appropriate conversion formulas are used to translate the design into natural units. Those conversion formulas are $x_{mi} = \dfrac{\ln q_{mi}}{\boldsymbol{\beta}_m} + x_{ml}$ and $x_{mi} = \dfrac{\ln r_{mi}}{\boldsymbol{\beta}_m} + x_{mu}$ for the m^{th} toxicant and the m^{th} stimulant respectively. Note that these design for interaction models are conditionally optimal under the convenient guess of zero for the interaction terms.

§11.6 Implications of the Stimulant and Toxicant-Stimulant Designs for the Exponential Model

As reasoned earlier, the same D-optimal designs, in terms of IECs, for the impaired reproduction model apply to both stimulant models and toxicant-stimulant models. This result stems from the similarity of the parameterization to IRS models in terms of the amount produced at the maximum and the concept of the IEC. However, the ability to parameterize stimulant and toxicant-stimulant models in a similar way has more far-reaching implications than just the D-optimal design. It means that the designs shown in Chapter 7 and 8 to test for lack of fit apply to these models as well. The interaction optimal design for the two regressor model and the D_s-optimal designs which allow us to estimate a model effective concentration as well as possible also remain the same. In addition, designs on restricted regions apply to these models as does the information presented on prediction variance, fractional factorials, and Bayesian designs. In conclusion, this means that the collection of theoretically optimal designs and practical enhancements presented in this work apply not only to the exponential model in the context of impaired reproduction studies but to the exponential model in general.