FOREWORD

The usefulness of the sophisticated statistical techniques collectively known as Response Surface Methodology (RSM) has long been appreciated in some disciplines, particularly chemical-process control and metallurgical research. In other disciplines its use is not widespread, probably because its capability for describing complex interdependent relationships in relatively simple terms is not fully recognized. It is hoped that the following brief treatment of RSM will serve to demonstrate the same potential to other fields of endeavour as it did to the author's rather narrow field of flame research.

Much of the material has been thoroughly covered in the technical literature, and in such cases it has been deemed sufficient to indicate the classic references. The ridge-analysis technique, being relatively new, is not so well documented, and has therefore been given somewhat fuller treatment.


Ottawa, October 31, 1969

## AVANT-PROPOS

L'utilité des méthodes statistiques complexes communément désignées sous le nom de Méthodologie des"surfaces de réponse est reconnue depuis longtemps dans certaines disciplines, en particulier dans le controle des processus chimiques et la recherche métallurgique. Dans d'autres disciplines leur usage n'est pas très répandu, probablement parce qu'on n'est pas pleinement au courant de leurs possibilités pour décrire en termes relativement simples des relations interdépendantes complexes. Nous espérons que ce bref expọsé servira à démontrer que ces méthodes offrent les mêmes possibilités dans d'autres domaines d'exploration qu'elles ont values à l'auteur dans le domaine plutôt restreint de la recherche sur les flammes.

Une bonne partie du sujet ayant été traitée à fond dans des ouvrages techniques, l'auteur s'est contenté d'indiquer les références classiques pour ces éléments. La technique d'analyse des pointes, relativement plus récente, n'est pas aussi bien documentée et est donc exposée en plus grand détail.

Ottawa, le 31 octobre 1969


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SOME COMMENTS ON
THE INTERPRETATTON OF RESPONSE SURFACES

## by

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ABSTRACT

In the application of statistical analysis to industry and research, a response surface is the geometric rendition of an equation or set of equations describing the relationship between a dependent variable and a number of independent variables. The present report briefly outlines various techniques for determining the physical meaning of a response surface, assuming that the defining equations have already been obtained by statistical techniques.

Contour plots are briefly described, and an example shows how a computer can be used to extend them to three or more factors and three or more responses. The technique of ridge analysis is explained without mathematical proof. An example involving three independent variables is worked out. Finally, canonical analysis is discussed, and a brief example is given.

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## Direction des mines

Circulaire d'information IC 219
OBSERVATIONS SUR L'INTERPRETATION
DES SURFACES DE REPONSE

par<br>F. D. Friedrich*

## RÉSUME

Dans les applications de l'analyse statistique à l'industrie et à la recherche, on appelle surface de réponse la représentation géométrique d'une équation ou d'une série d'équations décrivant la relation entre une variable dépendante et un certain nombre de variables indépendantes. Le présent rapport expose brièvement diverses méthodes de détermination de la signification physique d'une surface de réponse, en supposant que les équations de définition ont déjà été obtenues par des méthodes statistiques.

L'auteur décrit brièvement les tracés équiscalaires et donne un exemple de l'utilisation d'un ordinateur pour les étendre à trois facteurs ou plus, età trois réponses ou plus. Il explique la technique d'analyse des pointes sans en faire la preuve mathématique, et traite un exemple à trois variables indépendantes. Enfin, il discute l'analyse canonique et en donne un bref exemple.

[^1]
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## INTRODUCTION

Response Surface Methodology (RSM) is an efficient experimental strategy, developed primarily by Box and Wilson (1), which finds wide application in empirically describing and optimizing systems and processes which cannot be readily treated from theoretical considerations. It is particularly advantageous to use RSM when it is desired to evaluate the effect of several independent variables or factors ( $x_{1}, x_{2}, \cdots-x_{k}$ ) on one or more dependent variables or responses $\left(y_{1}, y_{2}, \cdots y_{n}\right)$.

The method consists of four distinct steps, as follows:

1. A decision is made as to the number and range of factors to be investigated, and the number of responses to be measured. The levels of the factors are coded by denoting the highest experimental level or value by +1 , denoting the lowest experimental level by -1 , and denoting intermediate levels by a number which is proportional to the extremities. For example, if the highest experimental level of the factor $x_{1}=$ pressure were to be 150 psi , and the lowest level were to be 100 psi , then 150 psi would be coded as +1 , 100 psi would be coded as -1 , and 125 psi would be coded as 0. A suitable experimental design is then prepared (1, 2, 3 ). This may take the form of a $2^{k}$ factorial design in which tests are carried out at all combinations of +1 and -1 factor levels, i.e. $2^{k}$ tests are to be carried out, where $k$ is the number of factors or independent variables. It may be pointed out that such a design takes the form of a cube in $k$ dimensions, with the test points represented by the vertices. It is frequently desirable to add extra test points to the experimental design, such as the centre of each face of the cube, and the centre of the cube.
2. The experiment is carried out by setting up each combination of factor levels, preferably in randomized order, measuring the desired response or responses for each run, and repeating some or all of the runs to permit determination of variance.
3. Mathematical models are fitted to the measured data by applying the theory of least squares. Techniques for fitting a model may be found .. in a number of text books $(4,5)$. Common model forms are the firstorder polynomial
$y_{e}=b_{o}+b_{1} x_{1}+b_{2} x_{2}+\cdots+b_{k} x_{k}$
and the second-order polynomial

$$
\begin{aligned}
y_{e}= & b_{o}+b_{1} x_{1}+b_{2} x_{2}+\cdots+b_{k} x_{k}+b_{11} x_{1}^{2}+b_{22} x_{2}^{2}+\cdots+b_{k k} x_{k}^{2}+ \\
& b_{12} x_{1} x_{2}+b_{13} x_{1} x_{3}+\cdots+b_{k-1, k} x_{k-1} x_{k}
\end{aligned}
$$

where $y_{e}$ is the value estimated by the model for the true response $y$, and the coefficients $b_{o}, b_{1}$, etc, are parameters estimated from analys is of the data. Such a model must be fitted for each response being considered. The fitted mathematical model describes a surface in a $k+1$ dimensional space, which is called the response surface, and is a function of the factors $x_{1}, x_{2} \cdots-x_{k}$. Most response surfaces can be adequately represented by a carefully fitted second-order polynomial, but in some cases it may be necessary to use a third-order polynomial, or employ transformation of the variables (6).
4. The response surfaces represented by the mathematical models must be interpreted to establish, within the limits of the experimental region, the optimum conditions for the system or process, and to indicate in what region further experiments might be profitable. Interpretation is
an important step in response surface methodology. It is an often overlooked truism that an experimental study is only as useful as the use that is made of it, and, while it is relatively easy to interpret the results of an RSM study involving only 2 or 3 factors and one or two responses, accurately analyzing the results of a study involving 4 , 5 or more factors may require fairly intricate techniques.

It is the purpose of this report to discuss only the interpretation of response surfaces. It will be assumed that the foregoing steps 1,2 and 3 have been satisfactorily carried out, and it remains only to correctly interpret the meaning of a set of fitted mathematical models describing the response surfaces.

## RISSPONSE SURFACES FOR 1 AND 2 FACTORS

A trivial example of a response surface is the case of a single response evaluated with respect to a single factor. The fitted response function (e.g., $y_{1}=y i e l d$ ) takes the form of a single line, which can be plotted against the factor x (e.g., $\mathrm{x}=$ pressure) as shown in Figure 1, and the factor level which produces the most desirable response can readily be selected. Clearly a second response function (e.g., $y_{2}=\operatorname{cost}$ ) can be plotted as a second curve on the same graph, and a factor level can be arbitrarily selected at which both responses are satisfactory according to some additional criterion.

For the case of a single response (e.g., $y=y i e l d$ ) which is dependent on 2 factors (e.g., $x_{1}=$ pressure, $x_{2}=$ temperature), the response surface may be plotted in 2 dimensions as a series of contour lines, each representing a constant level of the response. This is exemplified in Figure 2. Each plotted response level can be achieved by a set of factor combinations, and response may be selected with an eye to optimum factor levels (e.g., satisfactory yield for minimum temperature and pressure). This approach can be extended to two or more responses by superimposing the contour plots of each response as shown in Figure 3, and then selecting factor levels which optimize both responses.

The problem of optimizing two or more responses can be approached in a more rigorous fashion by assigning a real-value function that is to be
optimized, that is, maximized or minimized, subject to given constraints. In the previous single-factor example, $z$ could be defined as $z=\frac{y_{2}}{y_{l}}$, the cost per unit yield, where $y_{1}=f(x)$ and $y_{2}=g(x)$. Standard techniques can then be used to minimize $z$. Or, if it were desirable to hold one res ponse (e.g., $y_{1}=y i e 1 d$ ) between certain limits, such as

$$
\mathrm{b} \leq \mathrm{y}_{1} \leq \mathrm{a}
$$

one could then define $z=g(x)=\cos t$, and by minimizing $z$ subject to $b \leq f(x) \leq a$ it is possible to minimize cost in the subset of $x$ where the specified inequality is satisfied.

## RESPONSE SURFACES FOR 3 FACTORS

When a single response depends on 3 factors, the response surface may be sketched in 3-dimensional space with the 3 factors as coordinates. If the response surface can be adequately described by a first-order polynomial, then a given response level will be represented by a plane, as shown in Figure 4. However, if the response function is a second, or higher, order of polynomial, the response surface may be cumbersome to draw and difficult to visualize. In such cases it may be advantageous to construct a 3-dimensional model of the response surface ( 7,8 ).

Three-factor response surfaces can also be handled reasonably conveniently by 2 -dimensional contour plots, and the tedium of drawing contours can be avoided by using tables prepared by a computer. This is well illustrated.in an example, from the food processing industry, given by Smith and Rose (9) and summarized below:

## Example 1. Optimizing a Pie-Crust Recipe

3 factors were considered:
$x_{1}=$ water content
$x_{2}=$ flour content
$x_{3}=$ shortening content
The factor levels were coded, and 32 experiments were carried out.
For each experiment, 3 responses were measured:

```
y
        panel, above }7\mathrm{ being considered acceptable.
y
        below 3.75 being considered acceptable.
y }=\mathrm{ specific volume, cc/g. Between 2.2 and 2.4 was desired.
```

Using least squares, a second-order polynomial was fitted for each response, thus providing mathematical models of the response surfaces.

The mathematical models were then programmed into a computer so as to obtain, for each response, 3 tables of response levels, each at the same 9 levels of $x_{1}$ and $x_{2}$, but one table at each of 3 levels of $x_{3}$. One table is shown in detail in Figure 5, and the entire set is shown schematically in Figure 6. On each table, the areas containing acceptable response levels were shaded. The tables corresponding to the same level of $x_{3}$ were then superimposed on each other, and the region where all three shaded areas overlapped contained the sets of factor levels providing a satisfactory recipe.

It must be kept in mind that tables such as those just described can only be superimposed if all factor coordinates are identical. If, for example, the table for $x_{3}=0$ had been the only one containing satisfactory levels of specific volume, it would have been necessary to either (a) conclude that a satisfactory recipe could not be obtained with the factor levels used in the experimental design, or (b) relax the criteria for the responses to the point where over1apping was achieved.

As shown schematically in Figure 7, the foregoing method can be applied to any number of responses and to several factors, but as the number of factors is increased the number of tables quickly becomes prohibitive. It then becomes desirable to employ a different approach.

RESPONSE SURFACES FOR k FACTORS

## a. Ridge Analysis

The advantage of ridge analysis in response optimization lies in
the fact that it permits the maxima and minima of the response to be plotted in two dimensions, regardless of the number of factors being considered. The basis for the method was laid by La Grange (10), and a mathematical derivation is given by Draper (11). A less rigorous but more readable account is given by Hoerl (12). Application of the ridge-analysis technique is probably best explained by the use of an example involving 3 factors. The extension to a larger number of factors will be obvious.

## Example 2. Application of Ridge Analysis

$$
\begin{align*}
& \quad \text { Consider the general second-order polynomial for } 3 \text { factors } \\
& y=b_{o}+b_{1} x_{1}+b_{2} x_{2}+b_{3} x_{3}+b_{11} x_{1}^{2}+b_{22^{x}}{ }^{2}+b_{33^{x}}{ }^{2}+b_{12} x_{1} x_{2}+ \\
& b_{13} x_{1} x_{3}+b_{23} x_{2} x_{3} \tag{2.1}
\end{align*}
$$

where the coefficients have been estimated by fitting the model to the data by means of least squares. The problem is to find maxima and minima on this surface. Essentially the ridge-analysis technique converts the problem to one of finding maxima and minima for the same surface on a sphere with origin at the centre of the experimental design, and radius R.

Let $\left.R=\left(x_{1}{ }^{2}+x_{2}{ }^{2}+x_{3}\right)^{2}\right)^{1 / 2}$
Then $x_{3}= \pm\left(R^{2}-x_{1}{ }^{2}-x_{2}\right)^{2 / 2}$
Consider only the positive root; i.e., $x_{3}=+\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{1 / 2}$
Substitute in (2.1)

$$
\begin{align*}
\text { Then } y= & b_{o}+b_{1} x_{1}+b_{2} x_{2}+b_{3}\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{1 / 2}+b_{11} x_{1}^{2}+b_{22^{x}}{ }^{2} \\
& +b_{33}\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)+b_{12} x_{1} x_{2}+b_{13} x_{1}\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{1 / 2} \\
& +b_{23} x_{2}\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{1 / 2} \tag{2.2}
\end{align*}
$$

Differentiate (2.2) with respect to $x_{1}$ and equate to 0 .

$$
\begin{aligned}
\frac{\partial y}{\partial x_{1}}= & b_{1}-b_{3} x_{1}\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{-1 / 2}+2 b_{11} x_{1}-2 b_{33^{x}}+b_{12} x_{2} \\
& +b_{13}\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{1 / 2}-b_{13^{x_{1}}}^{2}\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{-1 / 2} \\
& -b_{23^{x_{1}} x_{2}\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{-1 / 2}=0} \\
& \text { back-substitute } x_{3}=\left(R^{2}-x_{1}^{2}-x_{2}^{2}\right)^{1 / 2}
\end{aligned}
$$

Then $b_{1}-\frac{b_{3} x_{1}}{x_{3}}+2 b_{11} x_{1}-2 b_{33} x_{1}+b_{12} x_{2}+b_{13} x_{3}-\frac{b_{13} x_{1}}{x_{3}}$

$$
-\frac{\mathrm{b}_{23} \mathrm{x}_{1} \mathrm{x}_{2}}{\mathrm{x}_{3}}=0
$$

or $x_{1}\left[2 b_{11}-2 b_{33}-\left(\frac{b_{3}+b_{13} x_{1}+b_{23} x_{2}}{x_{3}}\right)\right]+b_{13} x_{3}+b_{12} x_{2}=-b_{1}$
let $\lambda=\frac{\mathrm{b}_{3}+\mathrm{b}_{13} \mathrm{x}_{1}+\mathrm{b}_{23} \mathrm{x}_{2}}{\mathrm{x}_{3}}$

Then

$$
\begin{equation*}
\left[2 b_{11}-2 b_{33}-\lambda\right] x_{1}+b_{12} x_{2}+b_{13} x_{3}=-b_{1} \tag{2.4}
\end{equation*}
$$

Similarly, if $\frac{\partial y}{\partial x_{2}}$ is evaluated, equated to zero, and $\lambda$ is substituted, the result is
$\mathrm{b}_{12} \mathrm{x}_{1}+\left[2 \mathrm{~b}_{22}-2 \mathrm{~b}_{33}-\lambda\right] \mathrm{x}_{2}+\mathrm{b}_{23} \mathrm{x}_{3}=-\mathrm{b}_{2}$
Also, Equation (2.3) can be rewritten as
$\mathrm{b}_{13} \mathrm{x}_{1}+\mathrm{b}_{23} \mathrm{x}_{2}-\lambda \mathrm{x}_{3}=-\mathrm{b}_{3}$
Equations (2.4), (2.5) and (2.6) now form a set relating $x_{1}, x_{2}$ and $x_{3}$ in terms of the parameter $\lambda$.

For purposes of this example, let it be assumed that the coefficients of Equation (2.1) have been evaluated and are as follows:

$$
\begin{aligned}
\mathrm{b}_{0}=6.89462 \quad \mathrm{~b}_{1} & =0.06323 & \mathrm{~b}_{11}=-0.11544 & \mathrm{~b}_{12}=0.09375 \\
\mathrm{~b}_{2} & =-0.12318 & \mathrm{~b}_{22}=-0.03997 & \mathrm{~b}_{13}=-0.34375 \\
\mathrm{~b}_{3} & =0.15162 & \mathrm{~b}_{33}=-0.11544 & \mathrm{~b}_{23}=-0.03125
\end{aligned}
$$

The set of simultaneous equations then reduces to

$$
\begin{gather*}
-\lambda \mathrm{x}_{1}+0.09375 \mathrm{x}_{2}-0.34375 \mathrm{x}_{3}=-0.06323  \tag{2.4a}\\
0.09375 \mathrm{x}_{1}+(0.15094-\lambda) \mathrm{x}_{2}-0.03125 \mathrm{x}_{3}=0.12318  \tag{2.5a}\\
-0.34375 \mathrm{x}_{1}-0.03125 \mathrm{x}_{2}-\lambda \mathrm{x}_{3}=-0.15162 \tag{2.6a}
\end{gather*}
$$

It is now necessary to determine the eigenvalues; that is, the values of $\lambda$ for which the simultaneous equations are not independent. This is done by equating the determinant of the coefficient matrix to zero, and solving the resulting equation for $\lambda$. For the example in question, the equation is

$$
-\lambda^{3}+0.15094 \lambda^{2}+0.12793 \lambda-0.01582=0
$$

and three eigenvalues exist. These are approximately

$$
\begin{aligned}
& \lambda=+0.37 \\
& \lambda=+0.11 \\
& \lambda=-0.35
\end{aligned}
$$

For the present purpose they do not have to be determined accurately. Some comments on the properties of this system are now in order. 1. For any assumed value of $\lambda$, the values of $x_{1}, x_{2}$ and $x_{3}$ are fixed, and can be evaluated by solving the simultaneous equations (2.4), (2.5) and (2.6). $\left[x_{1}, x_{2}, x_{3}\right]$ are coordinates of a point on a sphere at which $y$ has a maximum or minimum value. The radius of the sphere is $R$; and $R=\left(x_{1}^{2}+x_{2}^{2}+x_{3}^{2}\right)^{1 / 2}$.
2. The number of maximum and minimum ridges for $y$ corres ponds to the number of eigenvalues. Thus in this example $y$ has 3 maximum ridges and 3 minimum ridges.
3. The $y$ values along any one ridge can only go through one maximum or one minimum for increasing $R$.
4. $R$ approaches infinity as $\lambda$ approaches an eigenvalue from either side, as shown schematically in Figure 8.
5. The highest maximum ridge for $y$ will correspond to assumed values of $\lambda$ greater than the highest eigenvalue, the lowest minimum ridge for $y$ will correspond to assumed values of $\lambda$ less than the lowest eigenvalue, and intermediate maxima and minima will correspond to the numerical order of the assumed values of $\lambda$ relative to the eigenvalues. Thus, referring to Figure 8;

Curve 1 represents the highest maximum ridge,

| 1 | 2 | 11 | 11 | second-highest maximum ridge, |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| " | 3 | 11 | " | third | " | " | ' |
| " | 6 | 1 | 11 | lowest minimum ridge, |  |  |  |
| " | 5 | " | " | second-lowest minimum ridge, |  |  |  |
| 11 | 4 | 11 | 11 | third | , | mum | ge |

The profile of the highest maximum ridge for $y$ may be obtained as follows:

1. Assume 3 or 4 values for $\lambda$ higher than the highest eigenvalue.
2. For each $\lambda$, solve Equations (2.4), (2.5) and (2.6) to obtain $\left[x_{1}, x_{2}, x_{3}\right]$.
3. Calculate $R$ for each set $\left[x_{1}, x_{2}, x_{3}\right]$.
4. Calculate $y$ from Equation (2.1) for each set $\left[x_{1}, x_{2}, x_{3}\right]$.
5. Plot $x_{1}, x_{2}, x_{3}$ and $y$ versus $R$.

The same procedure, using appropriate values for $\lambda$, can be used to obtain the profiles of the lowest minimum ridge or any of the intermediate maximum or minimum ridges.

It must be kept in mind that while $y$ may increase (or decrease, in the case of a minimum) continuously as $R$ increases, the mathematical model of the response surface can only be expected to hold within the bounds of the experimental region. Thus, if in the experiment the highest
coded levels of $x_{1}, x_{2}$ and $x_{3}$ were all $1, R=(3)^{1 / 2}$ would represent the limit of the experimental region in the plot of $y$ versus R. For the numerical example, the highest maximum ridge was evaluated using the for egoing procedure. The results of the calculations are tabulated below, and the ridge profile and coordinates are plotted in Figure 9.

| $\lambda$ | $\mathrm{x}_{1}$ | $\mathrm{x}_{2}$ | $\mathrm{x}_{3}$ | R | y |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 1.0 | -0.0054 | -0.1515 | 0.1582 | 0.2191 | 6.934 |
| 0.6 | -0.1502 | -0.3304 | 0.3560 | 0.5084 | 6.985 |
| 0.5 | -0.3773 | -0.5074 | 0.5944 | 0.8678 | 7.060 |
| 0.42 | -1.4191 | -1.1390 | 1.6072 | 2.4278 | 7.599 |
| 0.37 | highest eigenvalue.root. |  |  |  |  |

It may now be explained that the numerical values assumed for the coefficients in Equation (2.1) are in fact the coefficients reported by Smith and Rose (9) for the "flakiness" response discussed in Example 1. Hence direct comparison between Figure 5 and Figure 9 should be possible. Figure 9 shows that, within the limits of the experimental region (in this case $R=\left(1.333^{2}+1.333^{2}+1^{2}\right)^{1 / 2}=2.135$ ), a maximum "flakiness" of 7.5 can be achieved by employing the following factor levels:

$$
\begin{aligned}
& x_{1}=-1.21 \\
& x_{2}=-1.05 \\
& x_{3}=+1.40
\end{aligned}
$$

But Figure 5 shows that a "flakiness" of 7.6 can be achieved with factor levels of

$$
\begin{aligned}
& x_{1}=-1.333 \\
& x_{2}=-1.333 \\
& x_{3}=+1.000
\end{aligned}
$$

However, substitution of these values into Equation (2.1) yields 7.4,
not 7.6. Further investigation demonstrated that the value of 7.6010 given by Smith and Rose (9) in Figure 5 is a typographical error. It should be 7.4010 .

For the same numerical example, all ridges were evaluated using the same procedure, taking $\lambda$ from -1.00 to +0.98 in steps of 0.03 . The results are summarized in Table 1 , and the ridge profiles are shown in Figure 10.

Other responses dependent on the factors $x_{1}, x_{2}$ and $x_{3}$ could be subjected to ridge analysis in the foregoing manner, and the results could all be plotted on the same graph against the common parameter R. This should simplify selection of factor levels which optimize all responses. A more rigorous procedure for optimizing multiple responses is described by Hoer1 (12).

While ridge analysis provides a reasonably quick way of obtaining the coordinates of a maximum or minimum on a response surface, it provides very little information about the general shape of the response surface. For this, another technique is more useful.

## b. Canonical Analysis

Canonical analysis provides another powerful tool for interpreting response surfaces regardless of the number of variables. The technique is fully described by Davies (4) and by Box and Wilson (1). It will suffice here to present a brief outline of the approach and give an example which demonstrates the potential of the method.

## Example 3. Application of Canonical Analysis

Consider a response surface described by a mathematical model of the form

$$
\begin{align*}
y= & b_{0}+b_{1} x_{1}+b_{2} x_{2}+b_{3} x_{3}+b_{11} x_{1}^{2}+b_{22} x_{2}^{2}+b_{33} x_{3}^{2} \\
& +b_{12} x_{1} x_{2}+b_{13} x_{1} x_{3}+b_{23} x_{2} x_{3} . \tag{3.1}
\end{align*}
$$

Conversion to canonical form consists of shifting the coordinate system so that Equation (3.1) is reduced to the form

$$
\begin{equation*}
\mathrm{Y}-\mathrm{y}_{\mathrm{s}}=\mathrm{B}_{1} \mathrm{X}_{1}^{2}+\mathrm{B}_{2} \mathrm{X}_{2}^{2}+\mathrm{B}_{3} \mathrm{X}_{3}{ }^{2} \tag{3.2}
\end{equation*}
$$

This can be accomplished as follows:

1. To determine $y_{s}$, carry out partial differentiation of Equation (3.1) with respect to $x_{1}, x_{2}$ and $x_{3}$, and equate each result to zero, thus getting the following 3 simultaneous equations:

$$
\begin{align*}
2 b_{11} x_{1}+b_{12} x_{2}+b_{13} x_{3} & =-b_{1}  \tag{3.3}\\
b_{12} x_{1}+2 b_{22} x_{2}+b_{23} x_{3} & =-b_{2}  \tag{3.4}\\
b_{13} x_{1}+b_{23} x_{2}+2 b_{33} x_{3} & =-b_{3} \tag{3.5}
\end{align*}
$$

Solving these for $x_{1}, x_{2}$ and $x_{3}$ yields the coordinates of the stationary point $y_{s}$, and these substituted in Equation (3.1) give the value of $y_{s}$. If, for example, the coefficients of Equation (3.1) are as follows:
$b_{0}=7.0418$
$\mathrm{b}_{1}=0.6985$
$b_{11}=2.9221$
$b_{12}=-2.9359$
$b_{2}=2.6844$
$b_{22}=1.5410$
$b_{13}=-1.1921$
$b_{3}=2.4410$
$b_{33}=1.0510$
$b_{23}=2.6637$

Substituting these values in Equations (3.3), (3.4) and (3.5) and solving yields

$$
\begin{aligned}
& x_{1}=-0.3365 \\
& x_{2}=0.2411 \\
& x_{3}=1.6576
\end{aligned}
$$

These are the coordinates of the point at which the response surface is stationary, i.e., has a maximum, a minimum, or a minimax. By substituting these values in Equation (3.1), $y_{s}$ is found to be 5.2247.
2. To determine $B_{1}, B_{2}$ and $B_{3}$, the determinant of the following matrix must be evaluated and the roots of the resulting cubic equation in B must be determined.

$$
\left.\begin{array}{lll}
b_{11}-B & \frac{b_{12}}{2} & \frac{b_{13}}{2} \\
\frac{b_{12}}{2} & b_{22}-B & \frac{b_{23}}{2} \\
\frac{b_{13}}{2} & \frac{b_{23}}{2} & b_{33}-B
\end{array} \right\rvert\,=0
$$

Substituting the assumed coefficients and evaluating the determinant yields

$$
\mathrm{B}^{3}-5.5141 \mathrm{~B}^{2}+4.9114 \mathrm{~B}+0.9290=0
$$

the roots of which are

$$
\begin{aligned}
& B_{1}=-0.1597 \\
& B_{2}=1.3434 \\
& B_{3}=4.3304
\end{aligned}
$$

Substituting in Equation (3.2) produces the canonical form
$Y-5.2247=-0.1597 X_{1}^{2}+1.3434 X_{2}^{2}+4.3304 X_{3}^{2}$
From inspection of Equation (3.6) it is clear that the response surface has the form of a hyperboloid of one sheet, and that $Y$ increases as the absolute values of $X_{2}$ and $X_{3}$ increase, but decreases as the absolute value of $X_{1}$ increases. Furthermore, plotting contours of $Y$ is considerably less tedious when the canonical form is used.

Box and Wilson (1) deal with the foregoing example at considerable length, and demonstrate the manner in which analysis of the canonical form can lead to further important conclusions about the nature of the response surface.

One further point bears mention. In canonical analysis, as always, the mathematical model of the response surface cannot be expected to hold beyond the limits of the experimental region. It may happen that the centre of the coordinate system which produces the canonical form lies outside the experimental region, and in this case' $y_{s}$ cannot be expected to be an actual maximum or minimum for the system. However, examination of that part of the canonical form which contains the experimental region is nonetheless useful, and can be particularly helpful in determining the area in which further experiments should be carried out.

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TABTE 1

## Coordinates and Response for a Range of Values of $\lambda_{2}$

## Example 2

| $\lambda$ | $\mathrm{x}_{1}$ | $\mathrm{x}_{2}$ | $\mathrm{x}_{3}$ | R | y |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $-1.00$ | -0.141462 | 0.113207 | -0.196710 | 0.035761 | 6.82424 |
| -0.97 | -0.149266 | 0.116646 | -0.205448 | 0.039048 | 6.82025 |
| -0.94 | -0.157905 | 0.120321 | -0.215042 | 0.042827 | 6.81576 |
| -0.91 | -0.167515 | 0.124261 | -0.225626 | 0.047205 | 6.81071 |
| -0.88 | -0.178263 | 0.128498 | -0.237366 | 0.052316 | 6.80496 |
| -0.85 | -0.190357 | 0.133074 | -0.250466 | 0.058339 | 6.79836 |
| -0.82 | -0.204058 | 0.138034 | -0.265184 | 0.065508 | 6.79072 |
| -0.79 | -0.219699 | 0.143440 | -0.281847 | 0.074140 | 6.78178 |
| -0.76 | -0.237709 | 0.149365 | -0.300874 | 0.084670 | 6.77119 |
| -0.73 | -0.258652 | 0.155902 | -0.322821 | 0.097710 | 6.75848 |
| -0.70 | -0.283286 | 0.163172 | -0.348428 | 0.114139 | 6.74295 |
| -0.67 | -0.312651 | 0.171336 | -0.378716 | 0.135266 | 6.72361 |
| -0.64 | -0.348218 | 0.180612 | -0.415118 | 0.163099 | 6.69897 |
| -0.61 | -0.392127 | 0.191310 | -0.459730 | 0.200857 | 6.66669 |
| -0.58 | -0.447630 | 0.203887 | -0.515726 | 0.253958 | 6.62288 |
| -0.55 | -0.519908 | 0.219050 | -0.588170 | 0.332116 | 6.56076 |
| -0.52 | -0.617753 | 0.237976 | -0.685646 | 0.454181 | 6.46742 |
| -0.49 | -0.757377 | 0.262793 | -0.823992 | 0.660821 | 6.31565 |
| -0.46 | -0.972329 | 0.297839 | -1.03598 | 1.05369 | 6.03902 |
| -0.43 | -1.34511 | 0.353678 | -1.40221 | 1.95030 | 5.43509 |
| -0.40 | -2.14773 | 0.464917 | -2.18844 | 4.80908 | 3.59822 |
| -0.37 | -5.11979 | 0.852234 | -5.09438 | 26.4456 | -9.59656 |
| -0.34 | 14.9070 | -1.67458 | 14.4716 | 217.226 | -115.444 |
| -0.31 | 3.11256 | -0.166124 | 2.94560 | 9.19608 | 2.25258 |
| -0.28 | 1.76375 | 0.020055 | 1.62606 | 2.87765 | 5.60228 |
| -0.25 | 1.24388 | 0.103422 | 1.11678 | 1.40256 | 6.33777 |
| -0.22 | 0.968933 | 0.158572 | 0.847303 | 0.840949 | 6.60055 |
| -0.19 | 0.799073 | 0.204012 | 0.681249 | 0.572119 | 6.71816 |

(Gontinued $\qquad$

TABLE 1 (Continued)

| $\lambda$ | $\mathrm{x}_{1}$ | $\mathrm{x}_{2}$ | $\mathrm{x}_{3}$ | R | y |
| :---: | :---: | :---: | :---: | :---: | :---: |
| -0.16 | 0.683728 | 0.247254 | 0.569617 | 0.426541 | 6.77746 |
| -0.13 | 0.600037 | 0.292809 | 0.490720 | 0.343294 | 6.80887 |
| -0.10 | 0.535954 | 0.344674 | 0.433856 | 0.297139 | 6.82490 |
| -0.07 | 0.484186 | 0.407769 | 0.393748 | 0.277874 | 6.83105 |
| -0.04 | 0.439453 | 0.489690 | 0.368628 | 0.284401 | 6.82926 |
| -0.01 | 0.396620 | 0.604302 | 0.360288 | 0.326148 | 6.81869 |
| 0.02 | 0.348113 | 0.781428 | 0.376804 | 0.436897 | 6.79393 |
| 0.05 | 0.276386 | 1.10111 | 0.444042 | 0.743002 | 6.73481 |
| 0.08 | 0.114052 | 1.88102 | 0.670404 | 2.00034 | 6.53138 |
| 0.11 | -0.997383 | 7.16942 | 2.45840 | 29.2196 | 3.07585 |
| 0.14 | 1.29067 | -3.51722 | -1.30096 | 7.86457 | 6.33870 |
| 0.17 | 0.852140 | -1.30043 | -0.592144 | 1.38394 | 6.87251 |
| 0.20 | 0.778689 | -0.725345 | -0.466937 | 0.675255 | 6.90766 |
| 0.23 | 0.791508 | -0.435862 | -0.464522 | 0.516121 | 6.91082 |
| 0.26 | 0.866421 | -0.231510 | -0.534529 | 0.545001 | 6.91161 |
| 0.29 | 1.03056 | -0.034854 | -0.694982 | 0.773131 | 6.92237 |
| 0.32 | 1.39863 | 0.241472 | -1.05220 | 1.56080 | 6.98329 |
| 0.35 | 2.59154 | 0.946549 | -2.19658 | 6.21850 | 7.49248 |
| 0.38 | -44.4554 | -24.5487 | 42.6324 | 2198.22 | 338.032 |
| 0.41 | -1.92964 | -1.42668 | 2.09638 | 5.07686 | 7.98978 |
| 0.44 | -0.899278 | -0.837436 | 1.10663 | 1.36731 | 7.28759 |
| 0.47 | -0.550300 | -0.622840 | 0.766486 | 0.639130 | 7.12652 |
| 0.50 | -0.377295 | -0.507433 | 0.594344 | 0.376542 | 7.06033 |
| 0.53 | -0.275300 | -0.433460 | 0.490188 | 0.251981 | 7.02514 |
| 0.56 | -0.208822 | -0.381089 | 0.420199 | 0.182701 | 7.00347 |
| 0.59 | -0.162552 | -0.341582 | 0.369782 | 0.139920 | 6.98880 |
| 0.62 | -0.128820 | -0.310450 | 0.331618 | 0.111472 | 6.97818 |
| 0.65 | -0.103365 | -0.285128 | $0.301633^{\circ}$ | 0.091482 | 6.97012 |
| 0.68 | -0.083638 | -0.264033 | 0.277384 | 0.076825 | 6.96376 |
| 0.71 | -0.068023 | -0.246124 | 0.257315 | 0.065708 | 6.95861 |
| 0.74 | -0.055448 | -0.230690 | 0.240390 | 0.05704 | 6.95434 |

(Continued

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TABLE 1 (Concluded)

| $\lambda$ | $\mathrm{x}_{1}$ | $\mathrm{x}_{2}$ | $\mathrm{x}_{3}$ | R | y |
| :--- | :---: | :---: | :---: | :---: | :---: |
| 0.77 | -0.045176 | -0.217223 | 0.225892 | 0.050127 | 6.95072 |
| 0.80 | -0.036683 | -0.205350 | 0.213308 | 0.044507 | 6.94760 |
| 0.83 | -0.029590 | -0.194790 | 0.202263 | 0.039865 | 6.94490 |
| 0.86 | -0.023614 | -0.185327 | 0.192475 | 0.035975 | 6.94251 |
| 0.89 | -0.018540 | -0.176791 | 0.183728 | 0.032677 | 6.94038 |
| 0.92 | -0.014204 | -0.169046 | 0.175853 | 0.029851 | 6.93848 |
| 0.95 | -0.010477 | -0.161983 | 0.168719 | 0.027407 | 6.93676 |
| 0.98 | -0.007257 | -0.155513 | 0.162218 | 0.025276 | 6.93520 |
|  |  |  |  |  |  |



FIGURE 1. RESPONSE-SURFAGE PLOT FOR 1 FAGTOR AND 2 RESPONSES.


FIGURE 2. RESPONSE-SURFAGE PLOT FOR 2 FAGTORS AND 1 RESPONSE.


FIGURE 3. RESPONSE-SURFACE PLOT FOR 2 FACTORS AND 2 RESPONSES.


FIGURE 4. RESPONSE-SURFAGE PLOT FOR 3 FACTORS AND 1 RESPONSE.
$\mathbf{Y}_{1}=$ Flakiness


FIGURE 5. PART OF A TABULAR RESPONSE-SURFAGE PLOT FOR 3 FAGTORS AND 1 RESPONSE.


FIGURE 6. SCHEMATIC DIAGRAM OF A TABULAR RESPONSE-SURFACE PLOT FOR 3 FACTORS AND 3 RESPONSES. (Shaded areas represent satisfactory response.)



FIGURE 8. SCHEMATIC PLOT OF R VS $\lambda$ FOR EXAMPLE 2 .


FIGURE 9. PLOT OF MAXIMUM RIDGE AND COORDINATES VS R FOR EXAMPLE 2.


FIGURE 10. PLOT OF MAXIMUH AND MINTMUM RIDGES VS R FOR EXAMPLE 2. (Dotted line shows limit of experimental region.)


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