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Fundamental Principles of Response Curves and Surfaces

Yi Liu[1], Yulin Ye[1,2], Zhangdong Wei[2,3], Chongyang Wang[1,2], Chuhan Wang[4], Yanzhou Li[5], Chengcheng Shen[1], Haojie Zang[1], Luhang Li[1], Yile Pan[1], Lin Wang[1,3,*]

[1]Miami College, Henan University, Kaifeng, Henan, 475002, China;

[2]School of Mathematics and Statistics, Henan University, Kaifeng, Henan, 475002, China;

[3]School of Environment and Planning, Henan University, Kaifeng, Henan, 475002, China;

[4]College of International Education, Henan University, Kaifeng, Henan, 475002, China;

[5]College of Chemistry and Chemical Engineering, Henan University, Kaifeng, Henan, 475002, China.

*Corresponding Author's E-mail: wanglin@henu.edu.cn

Abstract

Optimization refers to improving the performance of a system, process or product in order to get the maximum benefit from it. The term optimization is often used in analytical chemistry as a means of finding conditions under which a program is applied to produce the best possible response. Traditionally, optimization in analytical chemistry is achieved by monitoring the effect of one factor on the experimental response at a time. When only one parameter changes, the other parameters remain unchanged. This optimization technique is called one variable at a time. Its main drawback is that it does not take into account the interaction between the research variables. Therefore, this technique does not describe the complete effect of parameters on the response. Another disadvantage of single factor optimization is that the number of experiments needed to carry out the research increases, which leads to the increase of time and cost, as well as the increase of reagent and material consumption. In order to overcome this problem, the multivariate statistical technique is used to optimize the analysis method. Response surface methodology (RSM) is one of the most relevant multivariate techniques. Response surface method is a set of mathematical and statistical techniques based on polynomial equation fitting experimental data. It must describe the behavior of data set for statistical prediction. When one or a group of interesting answers are affected by multiple variables, it can be well applied. The goal is to optimize the levels of these variables at the same time to achieve the best system performance. Before applying RSM method, we need to select an experimental design to determine which experiments should be carried out in the experimental area. There are some experimental matrices for this. When the data set does not show curvature, the experimental design of first-order model (such as factorial design) can be used. However, in order to make the response function approximate to the experimental data that cannot be described by linear function, quadratic response surface design should be used, such as third-order factorial, Box Behnken, central composite and Doehlert design. This paper discusses the basic principle of response curve and response surfaces.

Keywords

Response Surface Methodology; Response Curves; Response Surfaces; Optimization.

1. Introduction

Response surface methodology (RSM) is an optimization analysis method based on the principle of statistics [1,2]. Constructing the functional relationship between the response value

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of the system and multiple factors, it evaluates the interaction between various factors and accurately determines the optimal conditions [3]. RSM, a comprehensive application of experimental design, mathematical statistics and optimization technology, has advantages such as less test times, excellent prediction performance, and high precision [4]. As the combination of mathematics and statistics, RSM constructs the function between the target response value and factors (single or multiple), displays the functional relationship through multi-dimensional graphics, and finally optimizes the response value. It applies an explicit mathematical model to replace the implicit function between test factors and response values, so as to optimize the calculation and predict the results [5]. Response surface methodology generally has the following main steps: (a) experimental design, (b) model establishment, (c) model validation, (d) optimization of various factors, (e) prediction results, (f) and results verification [6-8]. The advantage of response surface method is to establish a mathematical model including the first-order term, the square term and the interaction term of any two factors through the design of limited reasonable experiments [9]. Expressing the functional relationship between each factor and the response value, RSM optimizes and evaluates the level of each factor and its interaction through the analysis of functional response surface and contour, facilitating optimum conditions of multi-factor system [10]. Response surface method overcomes the defect that orthogonal test only analyzes isolated test points and lacks intuitive graphics, resulting to its widely application in experimental design and process optimization [11]. RSM is an effective statistical method, which investigates the combination of factors in a wide range, as well as the impact on the response value [12]. Compared with the traditional design method, the response surface method is more effective than the single factor analysis method, more comprehensive than the uniform design method, and more simplified than the orthogonal design method [13]. Moreover, the obtained relationship can be used to predict the response value of any test point within the domain of the experiment, thus showing outstanding superiorities [14]. Therefore, response surface methodology is a practical and significant technique in chemical industry, food industry, material chemistry and bioengineering [1,15-17].

2. Elements and Notation

The *i*th type of factor is denoted as X_i and the response value by Y. Whether we are using X_i to refer to the factor in general or to a specific quantity of the factor will be apparent from given context. If Y contains n factors, the *i*th subscript on X runs from 1 to i. Y and all the Xs must be non-negative quantities.

Response value is determined by the function of n inputs.

Y depends on $X_1, X_2, X_3, \ldots\ X_i, \ldots\ X_n$

or, more briefly,

$$Y = F(X_l, X_2, X_3, \ldots X_i, \ldots X_n) \quad (1)$$

Where Y is some unspecified mathematical function of the quantity of Xs, with the exact algebraic form of this function being left unspecified [1,18].

3. Theory of Response

In general, it is impossible to numerate all the independent variables involved in producing a particular alloy, material, or food product [19,20]. To simplify the problem, *Theory of Response* is initiated based on the more important input factors. As already noted, response theory is concerned with the dependent variable achieved in relation to various independent variables [21].

Under present conditions of knowledge, within the reasonable domain, the basic theory is that:

(i) Graph of Function (1.1) is continuous and smooth

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(ii) Beyond some peak yield, additional units of X_i have a deleterious effect on yield

(iii) An equal proportionate increase in all independent variables results in a less than proportionate increase in dependent variables

(1) Assumption (i) implies that the first derivatives $\frac{\partial Y}{\partial X_i}$ exist.

(2) Assumption (ii) implies $\frac{\partial Y}{\partial X_i}$ decreases as X_i increases, which in turn implies that the second derivatives $\frac{\partial^2 Y}{\partial^2 X_i}$ of response exist and are negative.

(3) Assumption (iii) implies that: $\sum(\frac{X_i}{Y})(\frac{\partial Y}{\partial X_i}) < 1 \quad (\mathrm{i} = 1, 2, \ldots, \mathrm{n})$.

Compared to other variables, time exerts a much more pervasive influence in response [22,23]. A suitably modified version of theory of response will be described in the end of this paper.

4. Variable, Fixed and Unimportant Input Factors

Function (1.1) implies all n independent variables are changeable. We will be concerned with the situation in which only k independent variables are changeable, the other (n –k) independent variables being held fixed. Supposing that (n –k) factors are fixed or unimportant, Function (1.1) is revised as

$$Y = f(X_1, X_2, X_3, \ldots, X_k, X_{k+1}, \ldots, X_n) \quad (2)$$

or briefly as

$$Y = f(X_1, X_2, X_3, \ldots, X_k) \quad (3)$$

5. Single Variable Input

We have

$$Y = f(X_1) \quad (4)$$

which can be depicted as a Response Curve [24,25]. According to the theory of response, it is a smooth, continuous curve, and turning point exists.

5.1. Deductions Derived from Y=f(X$_i$)

From algebraic form of $Y = f(X_1)$, four quantities are derived:

(i) the **Average Yield** of X_1, written AY_1

(ii) the **Marginal Yield** of X_1, written MY_1

(iii) the **Maximum Level** of Y, written Y_{max}

(iv) the **Elasticity of Response** of X_1, written E_1.

Average Yield of X_1 is defined as

$$AY_1 = \frac{Y}{X_1} \quad (5)$$

Average Yield must decrease as X_1 increases since it is simply average yield per unit of the factor involved. Marginal Yield is defined as the slope of the response curve [26].

$$MY = \frac{\partial Y}{\partial X_1} \quad (6)$$

Marginal Yield tells us what happens to Y at any level of X_1 as marginal changes occur in X_1. $\frac{\partial Y}{\partial X_1}$ is measured in units of Y per unit of X_1 since it is a rate of change. Maximum Yield occurs where marginal yield is zero [27].

Elasticity of Response with respect to X_1 is defined as the relative change in Y divided by the relative change in X_1.

Algebraically, in incremental units, we have

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$$E_1 = \frac{\frac{\Delta Y}{Y}}{\frac{\Delta X_1}{X_1}} \tag{7}$$

At a particular point on the response curve, Equation (7) can be revised as

$$E_1 = \left(\frac{\partial Y}{\partial X_1}\right)\left(\frac{X_1}{Y}\right) = \frac{MY_1}{AY_1} \tag{8}$$

Since MY_1 and AY_1 are measured in the same units, E_1 is a dimensionless number. As a result, it is usually simplified as the percentage change in Y corresponding to a 1 percent growth in X_1. To summarize, we have discussed the single-variable relationship as a continuous function within the domain of a well-designed and empirically practical response theory. The single-variable response function has 2 shortcomings. Firstly, it indicates nothing about the dynamic relation between X_1 and the other Xs. In addition, it gives nothing of the relation between Y and the rest factors.

6. Two Variable Inputs

For the two-variable condition, we obtain

$$Y = f(X_1, X_2) \tag{9}$$

Different from the single-variable function, this two-variable function cannot be described as a single curve. It depicts a surface in the three-dimensional space.

Theoretical deductions from Y=f(X₁, X₂)

As long as we know the algebraic form of Y=$f(X_1, X_2)$, we can derive all the conclusions available from the single variable functions Y=$f(X_1)$ and Y=$f(X_2)$. To investigate single variable functions contained, we simply take X_1 or X_2, respectively, as fixed at some level.

Based on the factor - yield relationship, we enter the field of factor-factor relationship through the input of two variables. These consist of:

(i) Family of equivalent equations

(ii) the Rate of Technical Substitution of X_i for X_j, written RTS_{ij}

(iii) the Elasticity of Substitution of X_i for X_j, written ES_{ij}

(iv) the family of Isocline equations

(v) the Ridge - Line equations

By rearranging the response function, taking one variable as the function of another variable, the equivalent equation of the trajectory of the input combination with fixed output level is obtained. Therefore, if Y* represents the fixed level of Y, the equivalent function of output Y* is

$$X_1 = f(X_2; Y^*) \tag{10}$$

For different levels of Y, this function gives a series of equivalent equations. Obviously, the shape and position of the quantum dots depend on the form of the parent response function.

The technical substitution rate of X_1 for X_2 is given by the equivalent slope. We have

$$RTS_{12} = \frac{\partial X_1}{\partial X_2} = \frac{1}{RTS_{21}} \tag{11}$$

The technical substitution rate of X_1, for X_2, tells us that if we reduce X_2 by an infinitesimal amount and want to keep the output unchanged, we must use X_1 to replace the rate of X_2. It can go from negative infinity to positive infinity. As the rate, the unit of RTS_{12} is X_1 per unit of X_2.

The elasticity of substitution of X_1 for X_2 is defined as the relative change of X_1 divided by the relative change of X_2, if we use X_1 to replace X_2 while keeping the production unchanged. We thus have

$$ES_{12} = \frac{\frac{\Delta X_1}{X_1}}{\frac{\Delta X_2}{X_2}}, (Y = Y^*) \tag{12}$$

ISSN: 2710-0588 DOI: 10.29556/FSE.202110_1(7).0021

which, estimated at a particular point on the isoquant, is

$$ES_{12} = \left(\frac{\partial X_1}{\partial X_2}\right)\left(\frac{X_2}{X_1}\right) = RTS_{12}\left(\frac{X_2}{X_1}\right) = \frac{1}{ES_{21}} \quad (13)$$

Expressed as an elasticity, ES_{12} is a pure number. It goes from negative infinity to positive infinity, and it can be explained that if X_j changes by 1%, the percentage change of X_i needs to keep Y unchanged.

Isoclines are defined as the loci of all combinations of X_1 and X_2 which have the same rate of technical substitution. Hence they constitute paths up or down the response surface joining points of equal curvature on the isoquants.

The family of isocline equations is derived by solving

$$\frac{\partial X_1}{\partial X_2} = k \quad (14)$$

We obtain X_1 as a function of X_2, where k is the value of RTS_{12}, specifying a specific contour.

Ridge-lines are those two special isoclines for which RTS_{12} is equal to zero or infinity, as implied respectively by their equations:

$$\frac{\partial X_1}{\partial X_2} = 0 \quad (15)$$

$$\frac{\partial X_2}{\partial X_1} = 0 \quad (16)$$

As long as the response function exhibits a specific maximum, the ridge divides the surface into four parts. As will be mentioned later, since the ridge marks the boundary between reasonable and unreasonable combinations of inputs, these features have different meanings. Technology substitution rate is the most basic and important concept among the above factors. Therefore, we will study this concept in more detail [6,28].

7. n Variable Inputs

For n larger than two, the advantage of the n-variable response function

$$Y = f(X_1, X_2, \dots, X_n) \quad (17)$$

In addition to providing extra information about Y, it also provides information about the factor-factor relationship of more than one pair of factors. However, these additional information can only be obtained at a certain cost. The size of n is usually determined by the size of these costs, which are related to the importance of understanding the role of X_1, X_2,..., X_n determines Y. For n greater than 2, the description and analysis of the response process must be algebraic. The algebra involved is only a generalization of two variable input algebras. For i or j = 1, 2, ..., n, we have the following relationships:

$$AY_i = \frac{Y}{X_i} \quad (18)$$

$$MY_i = \frac{\partial Y}{\partial X_i} \quad (19)$$

$$RTS_{ij} = -\left(\frac{MY_j}{MY_i}\right) \quad (20)$$

$$ES_{ij} = RTS_{ij}\left(\frac{X_j}{X_i}\right) \quad (21)$$

The isoquant surface for a particular level of output is specified by the function:

$$X_1 = f(X_2, X_3, \dots, X_n; Y^*) \quad (22)$$

Isoclines joining all combinations of Xi and A^-which have the same rate of technical substitution, say k-, are given by:

$$RTS_{ij} = k_{ij} \quad (23)$$

Ridge-lines or surfaces on which RTS» equals zero or infinity are derived by solving the isocline equation for k- values of zero and infinity, respectively. [22,29-31]

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Diminishing returns to X_i implies

$$\frac{\partial(MY_i)}{\partial X_i} < 0 \quad (24)$$

At any point on the response surface, the total response elasticity for diminishing returns to scale must be less than 1, given by the sum

$$\sum\left(\frac{\partial Y}{\partial X_i}\right)\left(\frac{X_i}{Y}\right) \quad (25)$$

According to the algebraic form of the parent response function, all the above relationships may involve up to n variables. That is to say, for (n + 1) – dimensional space, factor and factor product relation may correspond to up to n or (n + l) dimensional space.

Obviously, the power function is a very special response function. Because of its multiplicative property, if x is zero, the output must also be zero. It does not show a finite maximum, as the fact that MY_i is always positive indicates. Accordingly, its ridge (like all isometric lines) is emitted from the origin and does not converge. In fact, the ridge is the input axis. By contrast, the negative growth rate of technology substitution among factors is gradually decreasing, which is dominant on the whole surface. In addition, the response elasticity and overall response elasticity of X_i are constant, and they do not change in the whole response surface with the change of independent variable.

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