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Optimization of Products and Processes

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1 Introduction

One of the definitions of the verb 'to optimize' in Chambers Dictionary is 'to make as efficient as possible especially by the use of analysing and planning processes'. Clearly the objective of anybody concerned with product and process development is to obtain the best or most efficient product or process possible. The purpose of this contribution is to consider some of the planning and analysing processes which can be used to achieve this objective.

An optimization problem can be defined in the following terms. We wish to maximize some parameter y, which we shall term the *objective function*. y will be a function of a series of variables,

$$y = f(x_1, x_2, x_3, \cdots)$$

which can be termed the *decision variables*. In general there will be *constraints* which place limitations on the values of x_i which are allowed.

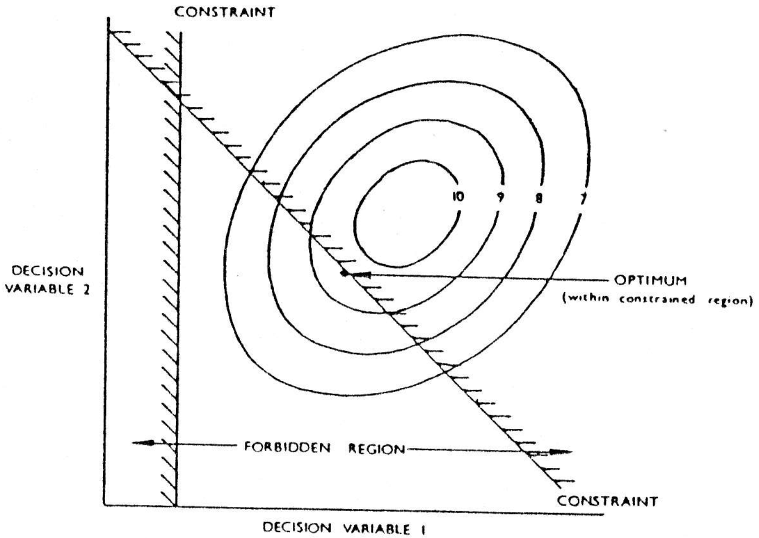

Figure 1 *The elements of a static optimization problem for two decision variables presented as a contour plot. In this case the constraints are active since, if they were omitted, the optimum would be located at a different point.*

We can distinguish between *static* and *dynamic* optimization problems. In a static problem the solution is a series of single values of x_i. In a dynamic problem the decision variables themselves are functions of another variable, most frequently time (t). In this case the solution to the problem will be a series of functions, $x_i(t)$, which maximizes y. An example of a dynamic optimization problem is the determination of the retort temperature as a function of time which maximizes nutrient retention in a thermal process within the constraint that the f_0 value should exceed the minimum required for commercial sterilization.[1] Methods for the solution of dynamic optimization problems have been discussed by Saguy.[2] In this short chapter we will confine ourselves to the simpler static optimization problem. The elements of this problem are illustrated in the case of two decision variables in Figure 1.

There are two ways in which this general problem can be tackled systematically. The first is what we shall term the *mathematical model method*. In this approach the function $y = f(x_i)$ is represented by an equation which is an approximation of the true relationship. The equation is then examined to find the maximum value of y within the constraints on x_i.

The second approach will be termed the *sequential or evolutionary method*. Here a series of measurements are made for different values of the vector $x = [x_i]$. An algorithm is then used to predict the next set of decision variables at which a measurement of y should be made. In this way it is possible to move iteratively or sequentially towards the optimum. In practice these two approaches can overlap. Thus the algorithm used to drive an experimental programme can equally well be used to examine a mathematical model with the advantage that the value of y can be calculated from the mathematical model in a fraction of the time taken to determine it experimentally. Conversely a mathematical model can be used to predict where the next experiment should be carried out, or a model can be fitted to a set of data obtained from a series of experiments driven by a sequential algorithm.

In this chapter we will outline these two different approaches to the static optimization problem. In the case of the mathematical model method it will be possible to illustrate the approach with examples relating to baked products. In the case of sequential methods this is more difficult since this approach has been discussed less frequently in the food technology literature. One reason for this is that sequential methods are directed at finding a single point optimum whereas published research is more concerned with obtaining an overall understanding of the system. Mathematical model methods are more appropriate if this is the objective.

2 The Mathematical Model Approach

This method is often called *response surface methodology* (RSM) since the relationship between the response y and the 'n' decision variables x_i is a surface in $(n + 1)$ dimensions. The stages in an optimization exercise using this approach are shown in Figure 2.

[1] D. B. Lund, *Food Technol.*, 1982, **36** (7), 97.
[2] I. Saguy, in 'Computer-aided Techniques in Food Technology', ed. I. Saguy, Marcel Dekker, New York, 1983, Chapter 11.

Identify important variables (x_i) and ranges over which they are to be varied

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Identify parameters to be measured and method of measurement

|

Decide form of equation relating measured parameters to variable levels

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Devise an appropriate experimental design

|

Carry out the experiment

|

Fit model to data

|

Determine if fit satisfactory and model appropriate

|

If above conditions hold, determine optimum within constrained range from inspection of equations

Figure 2 *Stages in an optimization process using the mathematical model method*

It has been assumed in the above that the response surface has to be obtained predominantly by experimental methods. For food systems it is extremely unlikely that a model of the process can be obtained from engineering first principles, though of course a knowledge of these principles is essential in selecting the important variables. In this procedure the critical stage is obtaining a suitable mathematical model.

The prediction of the optimum from the model is generally straightforward. In the case of a product optimization exercise, defining what properties of the product are required, and what the constraints should be, may be as much a marketing as a technical decision.

We will now discuss some of the stages listed in Figure 2 and then consider some examples where the mathematical model approach has been applied to baked products.

Selection of Variables.—The number of experimental trials required increases rapidly with the number of variables and with the complexity of the model to be fitted. From these considerations a decision can be made on the number of variables that it is possible to handle. In many cases it is obvious which variables to choose. If, however, there are a large number of variables which may be important it is necessary to select a few for detailed examination, and the use of a fractional factorial design as a screening experiment may be valuable. Examples of such designs for 2^{n-k} fractional factorial experiments for up to fifteen variables have recently been given by Mullen and Ennis.[3] For example if there are twelve variables, a full factorial experiment where each variable can be held at two levels and all possible combinations are examined would require 4096 (2^{12}) treatments. A fractional factorial experiment consisting of 32 treatments (2^{12-7}) is given by Mullen and Ennis including a blocking scheme. Although the main effects will be aliased with higher-order interactions (since the latter can almost certainly be neglected) it will be possible from the analysis of such an experiment to decide on the relative importance of the variables and in a subsequent experimental design keep the variables of lesser importance at a constant level.

[3] K. Mullen and D. M. Ennis, *Food Technol.*, 1985, **39** (5), 90.

In an optimization exercise one is generally attempting to improve on an existing situation. The logical centre point of the design is, therefore, the current product or process. It is easier to analyse the experiment in terms of coded levels and the values of the variables at this centre point would be coded as zero. The range over which the variables will be changed is governed by the conflicting requirements of obtaining sufficient data in the critical region to predict an optimum precisely and making the experimental net large enough to avoid missing the optimum region altogether. The actual levels of the variables are converted into coded levels (-1, $+1$, $+2$, *etc.*) by an appropriate transformation which can be linear or non-linear. A non-linear form may be suggested by a theoretical knowledge of the process; for an example of this see the brief discussion below of the work of Keagy *et al.*[4] on vitamin retention in biscuits.

Form of Model.—Polynomial models are most frequently employed. These have the advantage of being easy to fit using multiple regression. They are however notoriously untrustworthy when extrapolated outside the experimental range. The use of a second-order polynomial of the form shown in equation (1) is often chosen. It is a good compromise between the conflicting requirements of providing a good fit to a complex surface, keeping the total number of experimental points down to an acceptable level, and using terms whose meaning can be readily appreciated.

$$y = a_0 + \sum_i a_i x_i + \sum_j b_j x_j^2 + \sum_{\substack{i,j \\ i>j}} a_{ij} x_i x_j \qquad (1)$$

A preliminary examination of the appropriateness of the model can be made by plotting the residuals [y(predicted) $-$ y(measured)] against the values of each of the variables. The analysis of variance will give information about the overall goodness of fit.

Experimental Designs.—*Central Composite Designs.* It is obvious that no information about the squared terms in equation (1) can be obtained from a 2^n factorial experiment where the variables are only examined at two levels. Some information about non-linearity can be obtained if a centre point is added to such a design, so in addition to the $+1$ and -1 levels of the coded variables the (0, 0, $\cdots$) treatment is also investigated. This centre point is generally replicated to give information on the error associated with an individual measurement. Information about non-linearity can also be obtained from full or fractional 3^n experiments. An example of such a design is given by Henika.[5] However, only a poor estimate of quadratic terms can be obtained when the variables are held at three levels. The design most frequently applied to baked products is the central composite type discussed by Box and Hunter[6] and by Cochran and Cox.[7] In addition to the centre

[4] P. M. Keagy, M. A. Connor, and T. F. Schatzki, *Cereal Chem.*, 1979, **56**, 567.
[5] R. G. Henika, *Cereal Sci. Today*, 1972, **17**, 309.
[6] G. E. P. Box and J. S. Hunter, *Ann. Math. Stat.*, 1957, **28**, 195.
[7] W. G. Cochran and G. M. Cox, 'Experimental Designs', 2nd Edn., Wiley, New York, 1957, Chapter 8.

point and the 2^n factorial points, measurements are made at the star points (α, 0, 0, $\cdots$) ($-\alpha$, 0, 0, $\cdots$) (0, α, 0, $\cdots$) (0, $-\alpha$, 0, $\cdots$), *etc.* By choosing an appropriate value for α and repeating the centre point a number of times the design can be given the property of rotatability. This means that the standard error of y will be the same for all points that are the same distance from the centre of the region (the coded 0, 0, 0, $\cdots$ point). If this condition is to hold, then $\alpha = 2^{n/4}$. As the number of variables (n) increases, it may be desirable to replicate fractionally the factorial part of the design. If this is the case, then the value of α is reduced. For example, for a half replicate design it becomes $2^{(n-1)/4}$. Very often the standard error in y is kept roughly constant within a circle (thinking in two-dimensional terms) of radius 1 from the centre. Mullen and Ennis[8] give a number of examples of designs of this type.

Constant Weight Mixture Designs. Where the objective of the work is to find an optimum blend of ingredients, the constraint that the total weight of the components is a constant impinges on the design, *i.e.* $\Sigma w_i x_i$ = a constant, where w_i is the weight of one unit of component x_i. Clearly there are no longer n independent variables. One approach to this problem is to use $n-1$ sets of ratios of the true variables and use these ratios as the actual variables in a central composite design. From a knowledge of the $n-1$ ratios the n true variables can be evaluated. Examples of this approach are given later in this section under Cakes.

Specific designs for handling constant-weight mixtures are discussed by Draper and Lawrence,[9,10] Scheffe,[11,12] and McLean and Anderson.[13] The extreme vertices design of McLean and Anderson seems particular pertinent since it allows constraints to be put on the allowed levels of the individual values of x_i. An example of its application to a cake formulation problem will be given below.

Examination of Model to Find the Optimum.—In general, for a polynomial model the maximum will lie outside the region of interest. Setting the partial derivative of y with respect to each variable equal to zero, and solving the resultant simultaneous equations to determine the stationary point, will not often be useful. Where the number of variables is reasonably small the use of contour plots obtained by keeping all but two of the variables constant is a useful way of visualizing the surface. In a situation where there is a large number of variables the best approach is to use one of the optimization routines in major software libraries, such as the Numerical Algorithms Group (NAG) or the National Physical Laboratory (NPL). The available software is listed and discussed by Saguy *et al.*[14] Where a number of y values have been measured, a decision is made on the one to maximize or minimize and then the remainder are used to define constraints. For example, the cost of a process might be minimized subject to certain constraints regarding the quality of the product. The cost function would be a straightforward linear function,

[8] K. Mullen and D. M. Ennis, *Food Technol.*, 1979, **33** (7), 74.
[9] N. R. Draper and W. E. Lawrence, *J. R. Statis. Soc., Ser. B*, 1965, **27**, 450.
[10] N. R. Draper and W. E. Lawrence, *J. R. Statis. Soc., Ser. B*, 1965, **27**, 473.
[11] H. Scheffe, *J. R. Statis. Soc., Ser. B*, 1958, **20**, 344.
[12] H. Scheffe, *J. R. Statis. Soc., Ser. B*, 1963, **25**, 235.
[13] R. A. McLean and V. L. Anderson, *Technometrics*, 1966, **8**, 447.
[14] I. Saguy, M. A. Mishkin, and M. Karel, *CRC Crit. Rev. Food Sci. Nutr.*, 1984, **20**, 275.

whereas various quality attributes could be represented by second-order polynomials obtained using response surface analysis. An example of this approach is given in the Appendix to this chapter.

Examples of Modelling of Baked Products and Processes.—*Cakes.* The response surface approach has frequently been used to determine the effect of a wide range of variables on cake quality (cake volume, structure, and top contour being the major parameters measured). An early but interesting example is given by Donelson and Wilson.[15] They fractionated soft white flour into four components, water solubles, gluten, tailings, and prime starch. To determine the role of these components, cakes were then baked from reconstituted flours containing different proportions of the flour ingredients. Cake volume was measured by a seed displacement method. Cake structure was scored on a 0—15 scale composed of the sum of separate evaluations of cell wall size, cell wall thickness, and uniformity of cell distribution. The weight of reconstituted flour in the formulation remained constant so a four-variable design would be inappropriate since the ingredient levels could not be varied independently. Instead three variables were used which were the following ratios of the ingredient levels.

$$x_1 = \frac{\text{water solubles}}{\text{gluten + tailings + starch}}$$

$$x_2 = \frac{\text{gluten}}{\text{tailings + starch}}$$

$$x_3 = \frac{\text{tailings}}{\text{starch}}$$

Each of these ratios could be varied independently but the specification of all three defined the levels of the four components in the flour. The coded levels of the variables were selected so that the components were kept within the range of interest (1—7% for water solubles, 5—17% for gluten, 3—20% for tailings, 65—82% for prime starch). Thus, for example, the ratio x_1 was transformed to the coded variable X_1 by the relationship

$$X_1 = \frac{-0.0430 + x_1}{0.0165}$$

The central composite design consisted of the 2^3 factorial, the centre point, the six star points (2,0,0; -2,0,0; 0,2,0, *etc.*) and the centres of the faces of the cube (1,0,0; -1,0,0; 0,1,0, *etc.*). A second-order polynomial was fitted to the data. Because ratios were used as the variables, interpretation of the model was slightly awkward. However, by using three-dimensional representations of sections of the surface it was possible to illustrate the major features of the model. One such three-dimensional representation is shown in Figure 3.

A very similar approach to the problem of handling a constant-weight mixture was used by Kissell and Marshall.[16] In this case the total recipe contained five ingredients, baking powder, shortening, flour, sugar, and water. In addition to

[15] D. H. Donelson and J. T. Wilson, *Cereal Chem.*, 1960, **37**, 241.
[16] L. T. Kissel and B. D. Marshall, *Cereal Chem.*, 1962, **39**, 16.

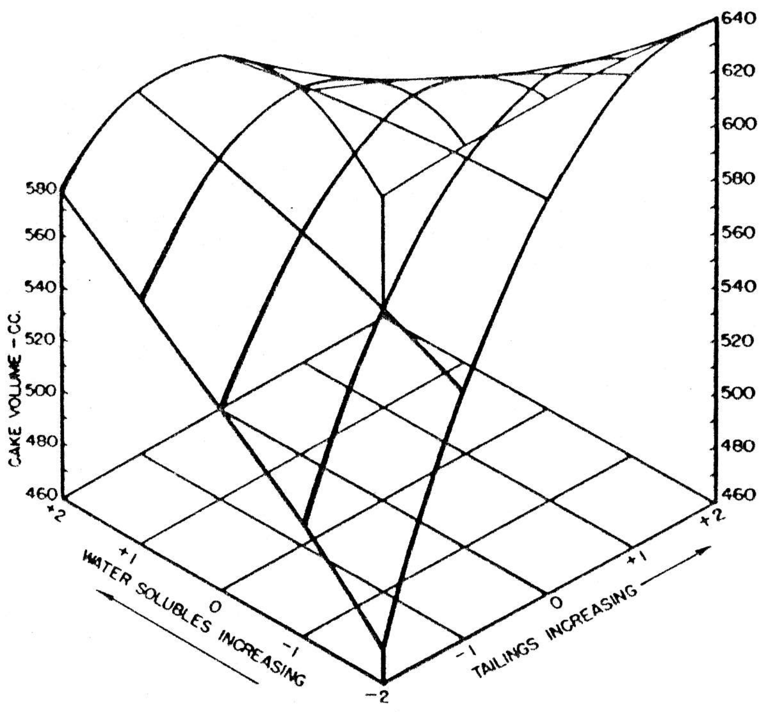

Figure 3 *Example of a second-order polynomial response surface for cake volume. The axes 'water solubles increasing' and 'tailings increasing' are the coded variables for X_1 and X_3 which are defined in the text; X_2 was fixed at the median of its range*
(Reproduced with permission from *Cereal Chem.*, 1960, **37**, 241)

volume, top contour appearance was evaluated subjectively on a 1—10 scale. A central composite design was used giving 25 formulations (16 from the 2^4 factorial, 8 star points, and the centre point); again the results were fitted by a second-order polynomial. In a later paper Kissel[17] investigated a more commercial formulation containing egg albumen and milk powder as additional ingredient variables plus constant low levels of salt and vanilla. This gave seven ingredient variables and therefore six ratio variables. The central composite design thus had 77 treatments ($2^6 + 12 + 1$). Volume, top contour, and total internal score were measured and the usual second-order polynomial model was used.

It may sometimes be helpful to transform the model to a canonical form (*e.g.* Wilson and Donelson[18]). That is to say the response is given by

$$Y = f(v_i)$$

where the vectors v_i correspond to the principal component vectors. One advantage of this approach is that variables with little influence on the property to be

[17] L. T. Kissel, *Cereal Chem.*, 1967, **44**, 253.
[18] J. T. Wilson and D. H. Donelson, *Cereal Chem.*, 1965, **42**, 25.

optimized may be easily detected and omitted from the subsequent analysis. The dimensionality of the problem may thus be reduced with consequent reduction in the number of experiments needed.

A more recent example of the use of second-order polynomial models applied to cakes is the work of Lee and Hoseney,[19] who optimized the fat–emulsifier system and the gum–egg–water system for a laboratory single-stage cake mix. The two systems were treated separately in individual three-variable experiments. The variables in the fat–emulsifier system were the levels of shortening, propylene glycol monostearate, and a mono-diglyceride emulsifier. Specific gravity, viscosity of mix, volume, top contour, shrinkage, and cake structure were measured. Splitting the design in this way reduces the amount of work and simplifies the interpretation, but implies that there is no interaction between the two systems; *i.e.* the optimum level for the emulsifier–shortening system is independent of the levels of the gum–egg–water system.

An example of the application of the extreme vertices design of McClean and Anderson[13] to cakes is given by Johnson and Zabik.[20] They were interested in the effect of the levels of five egg proteins, in a blend, on the properties of angel food cakes. The procedure for selecting the treatments consisted of initially defining the admissible ranges for proteins in the blend; *e.g.* the minimum and maximum values for ovomucin were 0 and 2.50%, whereas the corresponding figures for ovalbumin were 30% and 89%.

The vertices were constructed by considering all possible treatments with five of the proteins at the maximum and minimum of their range and adjusting the level of the sixth protein (ovalbumin) to make up the blend to 100%. In view of the large allowed range for ovalbumin all 32 formulations calculated in this way were feasible. The design was completed by including the centroids of the three-dimensional faces. This was achieved by averaging the vertices.

The authors used a technique described by Becker[21] to detect components with a linear blending behaviour. This resulted in a model containing terms of the form

$$\frac{x_i . x_j}{x_i + x_j}$$

as well as linear, second-order, and third-order terms.

Bread. A simple fractional 3^3 factorial design has been used by Henselman *et al.*[22] to investigate breads fortified with added protein from different sources. The variables were the type of added protein (soya, milk, or fish) and the protein level (0, 4, and 8%). Bread volume, specific volume, structure, and flavour were determined. The results were fitted by a second-order polynomial.

Paloheimo *et al.*[23] investigated the effect of oven variables on bread quality using a half replicate 2^{5-1} factorial design with four replicates at the centre point. Variables were baking temperature, the height of the bread in the oven, humidity, air circulation velocity, and the presence or absence of a separate heatable hearth.

[19] C. C. Lee and R. C. Hoseney, *Cereal Chem.*, 1982, **59**, 392.
[20] T. M. Johnson and M. E. Zabik, *J. Food Sci.*, 1981, **46**, 1226.
[21] N. G. Becker, *J. R. Statis. Soc., Ser. B*, 1968, **30**, 349.
[22] M. R. Henselman, S. M. Donatoni, and R. G. Henika, *J. Food Sci.*, 1974, **39**, 943.
[23] M. Paloheimo, Y. Malcki, and S. Kaijaluoto, in 'Thermal Processing and Quality of Foods', ed. P. Zeuthen *et al.*, Elsevier Applied Science, London, 1984.

Measured parameters included theoretical energy consumption, volume and specific volume, and thickness and colour of the crust. The results were expressed in terms of a linear model only, as it was considered that there were insufficient experimental data to justify determining cross-product (interaction) terms.

Biscuits. A good example of the transformation of variables can be found in the studies of Connor and Keagy on vitamin retention during the baking of vitamin-fortified biscuits.[4,24] Here the primary objective of the work was to study the retention of thiamin or folacin. The variables were biscuit thickness, baking time, temperature, rest time, and levels of sodium bicarbonate and ammonium bicarbonate. Rest time was defined as the time from the end of mixing to the beginning of baking.

It has been shown that the thermal destruction of the vitamins follows first-order kinetics, *i.e.*

$$\ln C_0/C = Kt$$

where C_0 is the initial vitamin concentration and C the concentration at time t. In the above equation

$$K = A\exp(-E_a/RT)$$

Where E_a is the activation energy. Substituting and taking logs gives

$$\ln \ln (C_0/C) = \ln A - E_a/RT + \ln t$$

Thus the measured vitamin retention is expressed as $\ln \ln (C_0/C)$ and time and temperature are expressed in terms of $\ln t$ and $1/T$ respectively.

The centre point of the design and an appropriate value for the +1 level were decided by the investigator. It was then possible to generate the transformation equation. For example in the case of baking time the real value at the centre point was 9.7 min and the +1 level was 12.2 min.

The transformation equation takes the general form

$$X = B + C \ln t$$

where X is the coded level of the time variable which will be used in the design and subsequent analysis. B and C are constants. We thus have

$$0 = B + C \ln 9.7$$
$$\text{and } 1 = B + C \ln 12.2$$

Solving these two equations gives the appropriate transformation relationship:

$$X = -9.84 + 4.33 \ln t$$

Extrusion. A large proportion of the recent extensive research on extrusion cooking utilizes response surface methods (RSM). Space precludes a detailed examination of specific examples. A very good discussion of the applicability of central composite rotatable designs to extrusion cooking is given by Olkku and Hagqvist.[25] This paper includes examples of the use of RSM to model the extrusion processing of barley, wheat, and rye flours. Another excellent example of the use of RSM to optimize extrusion process variables is given in the case of soya extrusion by Frazier *et al.*[26]

24 M. A. Connor and K. P. M. Keagy, *Cereal Chem.*, 1981, **58**, 239.
25 J. Olkku and A. Hagqvist, *J. Food Eng.*, 1983, **2**, 105.
26 P. J. Frazier, A. Crawshaw, N. W. R. Daniels, and P. W. Russell-Eggit, *Food Eng.*, 1983, **2**, 79.

3 Evolutionary and Sequential Methods

Evolutionary Operation (EVOP).—Evolutionary operation (generally termed EVOP for convenience) is as much a management philosophy as a statistical technique. It is described in detail in the book by Box and Draper.[27] An optimization exercise carried out in the laboratory or pilot plant will normally be only partly applicable to a full-scale process. The EVOP approach is to make small systematic changes in the full-scale process. The results are then analysed and decision variables are altered in the direction which it is predicted will most improve the process. The changes are sufficiently small to preclude the production of unsaleable product. The statistical designs used are very straightforward so production personnel are directly involved in the exercise, which is a continuous process rather than a project of limited duration.

Most frequently 2^2 or 2^3 factorial designs are used with the current process being taken as the centre point. In view of the fact that the 'experiment' is run by process operators it is generally considered that a design involving more than two variables will be too demanding and result in a negative reaction from the personnel involved. The experimental cycle is repeated a number of times, the exact number depending upon the significance of the changes that are being detected.

The approach can also be applied to the case where the responses are ranked rather than evaluated quantitatively.[28,29]

Simplex Methods.—A simplex is a figure in n dimensions with $n + 1$ vertices. Thus in two dimensions it is a triangle and in three dimensions a tetrahedron. In the basic simplex approach the responses are measured at the vertices and a new simplex is created by elimating the worst vertex by reflection through the centroid of the remaining vertices. A simple example of the early stages of this approach is shown in Figure 4.[30] Here the gel strength of a blend of the three polysaccharides guar, locust bean gum, and carrageenan is being measured. Although there are three ingredients the dimensionality of the problem is reduced to two by giving all formulations tested the same total cost. That is to say the relationship

$$4X_1 + 2X_2 + X_3 = 27$$

is obeyed where X_1, X_2, and X_3 are the concentrations of carrageenan, locust bean gum, and guar gum respectively in g l^{-1}. (At the time of writing these relative costs would not be realistic.) It is clear that a quantitative evaluation of the response at the vertices is not required; all that is necessary is that the worst response is identified. It has been suggested that for this reason the simplex approach would be useful in product development since it is far easier for a sensory panel to select one product from a series than quantitatively to evaluate or rank all of them.[31] However, an attempt in our laboratory to hit a target ice cream formulation starting

27 G. E. P. Box and N. R. Draper, 'Evolutionary Operation', Wiley, New York, 1969.
28 A. Kramer, *Food Technol.*, 1964, **19** (1), 37.
29 A. Kramer and B. A. Twigg, 'Quality Control for the Food Industry', 3rd Edn. AVI, Connecticut, 1970, Chapter 16.
30 J. Y. Y. Lee, 'Optimisation of a Gel Formulation by Simplex and Response Surface Methods', BSc. Thesis, University of Nottingham, Faculty of Agricultural Science, 1984.
31 J. R. Mitchell, *Food Manuf.*, 1983, **58** (8), 27.

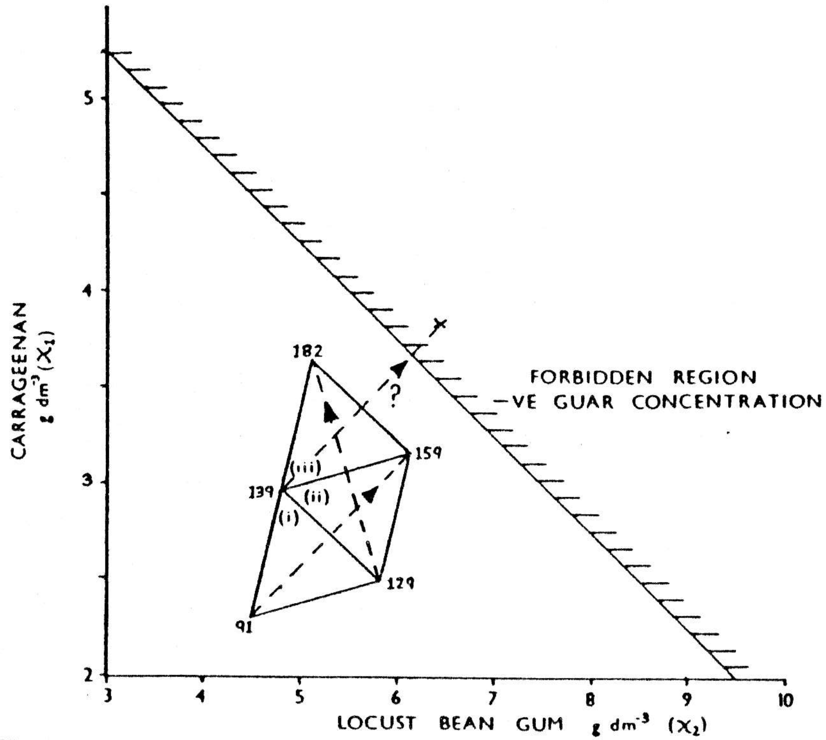

Figure 4 *The early stages of a simplex, run experimentally, to determine an optimum gel blend formulation. Although the blend contains the three polysaccharides, carrageenan, locust bean gum, and guar gum, the use of the constant-cost constraint discussed in the text reduces the dimensionality of the problem to 2. The numbers* (i)—(iii) *correspond to the progress of the optimization procedure and the arrowed lines show the successive reflections. The next move will trespass into a region of negative guar concentration, which is experimentally inaccessible, so a decision is now required. The numbers at the vertices are F.I.R.A. gel strengths obtained for a* 30° *paddle turn. The blends have been autoclaved at* 121.1 °C *for* 60 min *prior to measurement*
(Adapted from J. Y. Y. Lee, BSc. Thesis, University of Nottingham, 1984)

from random levels of four ingredient variables using this approach was not successful.

There have been extensive modifications of the basic simplex idea. These have aimed at speeding up the search and dealing with the problem, illustrated in Figure 4, of what to do when the next vertex requested by the algorithm trespasses into a forbidden region. Examples include the modified simplex of Nelder and Mead,[32] where expansion and contraction steps are included if the reflected vertex is respectively the best or the worst of the new simplex. Trespassing into forbidden regions is handled by assigning a very unfavourable value of y to that region, when a contraction into the allowed area will automatically follow. In the super modified simplex of Routh *et al.*[33] a second-order polynomial is fitted to the responses at the

[32] J. A. Nelder and R. Mead, *Comput. J.*, 1965, 7, 308.
[33] M. W. Routh, P. A. Swartz, and M. B. Denton, *Anal. Chem.*, 1977, 49, 1422.

centroid, the worst, and the reflected vertices. If the maximum of this curve lies between the worst and reflected vertices, then this is taken at the new simplex vertex; if, however, the curve is concave upward then the vector joining the worst and reflected vertices is extended by an appropriate interval. If a boundary is transgressed then the point where the vector crosses the boundary is taken as the new vertex. Nakai[34] compared a number of different optimization techniques by evaluating the efficiency with which they found the maxima or minima of surfaces described by second-order polynomials containing three or five variables. Overall, a modified super simplex algorithm performed best. This algorithm followed the approach by Routh *et al.*[33] described above, with the addition of a subprogram of quadratic factorial regression analysis to calculate new vertices at various stages in the process. To improve the efficiency further Nakai *et al.*[35] added a graphical mapping procedure. It is claimed that the mapping super simplex procedure has been applied to more than 20 food processing experiments and has markedly improved the efficiency of research. Most experiments on food analysis and processing have been optimized within 25—35 iterative experiments depending on the number of factors.

One of the few examples of the application of the simplex method to a baked product is reported by MacDonald and Bly.[36] The objective of the investigation was to determine optimum combination of four emulsifiers (monoglycerides, sorbitan monostearate, polysorbate 60, and glyceryl lactopalmitate) for cake mix shortenings. Initially a designed experiment was carried out in which the four emulsifiers could take one of three levels where each level was a percentage of the total weight of the shortening–emulsifier mixture. This latter total weight was kept constant. Cakes were evaluated for volume (measured by seed displacement), volume index (the sum of cake height measured at three points), symmetry index, grain, and texture. Total score was obtained as sum of grain, volume, and texture. A second-order polynomial [equation (1)] was fitted for each of the responses. Initially an attempt to determine the optimum ingredient combination region was made by constructing a series of two-way tables for each of the responses, *i.e.* two of the independent variables were kept constant and the response was tabulated for a range of combinations of the other two independent variables. Minimum standards for each response were decided on and areas of unacceptable results were eliminated in turn. Hence a region of acceptable formulations suitable for further examination was attained. (This is a manual method of solving the problem discussed in the Appendix.) Having determined a near optimum formulation in this way, a simplex design was then employed to refine the optimum further. Thus a decision was made as to the scale length for each of the four emulsifiers and the size of the simplex was defined. A five-point simplex was then constructed and five cakes were baked corresponding to the emulsifier levels at the vertices. The worst cake as judged by total score was eliminated and a new formulation predicted. Clearly at this stage each additional experimental run consisted of baking one cake alone since data for four of the simplex points were known. An optimum formulation was arrived at after eight experimental trials.

[34] S. Nakai, *J. Food Sci.*, 1982, 47, 144.
[35] S. Nakai, K. Koidei, and K. Eugster, *J. Food Sci.*, 1984, 49, 1143.
[36] I. A. MacDonald and D. A. Bly, *Cereal Chem.*, 1966, 43, 571.

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Appendix: An Example of the Determination of the Optimum Parameters from the Response Surface Model Using Standard Numerical Algorithms

A number of standard numerical packages are now available for the minimization or maximization of a non-linear function involving several variables, with constraints (Saguy *et al.*[14]). One such routine which appears particularly well suited to the problem is the NAG (FORTRAN) routine E04UAF.[37] In this study this routine is used to optimize a dry mix formulation.

The NAG routine E04UAF employs a method using sequential augmented Lagrangian multipliers[38,39] which are successively iterated with the aid of a 'penalty parameter' until a minimum is found. The gradient of the augmented Lagrangian functions is estimated by finite differences during the iterations.

Mather[40] used a conventional central composite design to model a commercial dry cake mix. In addition to volume (which was measured as an averaged height), air cell size, air cell size consistency, colour, and firmness were evaluated on a 1—5 scale. The results were expressed in terms of second-order polynomial models, non-significant terms being eliminated. The optimization approach used was to maximize *one* response within constraints placed on the coded levels of the ingredient variables and the other responses. The question considered was: what is the formulation for the sponge mix that gives the greatest volume for the same total ingredient cost as the current formulation? The appearance and texture of the sponge must be satisfactory. We now seek to obtain the optimum formulation using the standard package E04UAF.

The constraints

$$-1 \leqslant X_i \leqslant 1 \; (i = 1\text{—}6) \qquad \text{(A1)}$$

(where X_1, X_2, X_3, X_4, X_5, and X_6 are the coded levels of flour, sugar, fat, dextrose, salt, and cornflour respectively) confine the six ingredient variables to a range where the second-order polynomial might be expected to give a reasonable representation of the true response. The centre point of the design $(X_i = 0)_{i=1-6}$ corresponds to the currently used formulation.

Cost will be a linear function of the coded ingredient levels and the condition that the cost of the new optimum formulation is the same as the original formulation is given by

$$0.375X_1 + 0.88X_2 + 0.52X_3 + 0.0277X_4 + 0.0017X_5 + 0.040X_6 = 0 \qquad \text{(A2)}$$

[37] NAG Fortran Library Manual, 1978. Numerical Algorithms Group, Banbury Road, Oxford, UK.
[38] P. E. Gill and W. Murray, 'Numerical Methods for Constrained Minimisation', Academic Press, New York, 1974.
[39] W. Murray, in 'Optimisation in Action', ed. L. C. W. Dixon, Academic Press, New York, 1976, Chapter 12.
[40] S. Mather, 'Optimisation of a Sponge Mix Formulation', BSc. Thesis, University of Nottingham, Faculty of Agricultural Science, 1985.

It was decided that the product would be satisfactory if the following conditions held:

air cell size $\geqslant$ 3.0
3.0 $\leqslant$ air cell size consistency $\leqslant$ 4.5
firmness $\geqslant$ 3.0
colour $\geqslant$ 3.0

In terms of the response surface model these conditions can be expressed respectively by equations (A3)—(A6):

$$0.056 + 0.27X_2 + 0.42X_6 - 0.34X_3X_6 \geqslant 0 \qquad \text{(A3)}$$

$$3.0 \leqslant 4.01 - 0.32X_1^2 - 0.23X_4^2 - 0.32X_5^2 - 0.41X_3X_5 + 0.34X_4X_6 \leqslant 4.5 \qquad \text{(A4)}$$

$$0.22 + 0.72X_1 - 0.39X_2 \geqslant 0 \qquad \text{(A5)}$$

$$0.17 + 0.22X_2 + 0.23X_4 - 0.28X_1X_3 \geqslant 0 \qquad \text{(A6)}$$

The volume response y_V (measured as an averaged height) is given by

$$y_V = 1.057 + 0.098X_1 + 0.053X_3 - 0.092X_1^2 - 0.067X_2^2 + 0.113X_1X_2 - 0.052X_2X_5 \qquad \text{(A7)}$$

The problem is thus defined as maximizing y_V subject to the conditions A1—A6.

For the NAG routine E04UAF, equation (A1) for i = 1—6 is supplied as the fixed bounds, (A2) as an equality constraint, equations (A3), (A5), and (A6) as inequality constraints and (A4) as a range constraint. Equation (A7) has to be rearranged slightly since E04UAF minimizes rather than maximizes a function *FC*; this is simply done by changing positive coefficients for negative (and *vice versa*):

$$FC = -1.057 - 0.098X_1 - 0.053X_3 + 0.092X_1^2 + 0.067X_2^2 - 0.113X_1X_2 + 0.052X_2X_5$$

The user has to supply standard workspace parameters *etc.*, a starting point (for this case a value for the X_i of 0 was chosen, corresponding to the original formulation), and also has to specify the accuracy in the variables X_i to which the solution is required (for this example, to two decimal places).

A satisfactory minimization was obtained after less than 2 seconds CPU time on the Cambridge University IBM 3081 Model B. The following values for the parameters were obtained:

y_V (volume)	=	1.112
X_1 (flour)	=	0.044
X_2 (sugar)	=	−0.588
X_3 (fat)	=	0.893
X_4 (dextrose)	=	−0.145
X_5 (salt)	=	1.000
X_6 (cornflour)	=	1.000

where the value for y_V corresponds to an increase in volume (averaged height) of *ca.* 5.2% as compared with the original formulation.

Although we have used a numerical package (E04UAF) originally designed for mainframe computers, it is to be expected that such routines will be available on popular microcomputers in the near future: indeed many NAG routines are already available for the IBM Personal Computer. This availability will no doubt enhance the general application of such procedures to similar optimization problems in the food industry.

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The Way Ahead: Wheat Breeding for Quality Improvement

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1 Introduction

At a time of cereal surplus in the UK, wheat producers face the challenge of increasing efficiency and reducing costs, and of providing a product finely tuned to the needs of the marketplace and the end user. Quality wheat is used principally by the breadmaking industry, which sets the standards that plant breeders strive to meet. Breadmaking currently uses 3.8 mt, biscuits 0.6 mt, and other 1.0 mt of grain per year. Millers and bakers require a stable, assured supply of inexpensive grain of high specific weight and good milling texture that is low in α-amylase. This grain must have a high content of endosperm proteins that give bread doughs the crucial visco-elastic properties that bakers depend on. At the same time, breeders have to attend to the producers' need for high grain yield, resistance to lodging, and ability to resist the depredation of pests, diseases, and climatic extremes. Until fairly recently, UK breadmaking grists were very dependent on imports of high quality North American hard red wheat. For example, in 1970 home-produced wheat made up less than 30% of the grists. Progress in breeding and growing better UK wheat varieties,[1] and improvements in breadmaking technology, have reduced imports so that in 1984 they made up only 20% of UK grists, and several bakeries are regularly producing white bread from 100% home-grown flour. North American wheat is now used principally to make wholemeal bread, although even the need for this may be reduced by gluten supplementation. In this paper, we review the major problems faced by breeders whose objective is to increase the quality of home-produced grain. We discuss work in progress to find solutions and speculate on the likely shape of the developments to come.

2 The Basis of Quality

Milling Texture.—For breadmaking, millers require wheat with a hard endosperm which resists fracturing across the dehydrated protoplasm because of strong adhesion between protein and starch. When cleavage occurs mainly along the lines of the cell walls, large, regular shaped particles are formed which make for a free-running flour. During milling, the starch granules tend to remain embedded in the protein matrix, and so become damaged, more so than in a soft milling wheat.

[1] J. Bingham, J. A. Blackman, and R. A. Newman, 'Wheat. A guide to varieties from the Plant Breeding Institute,' National Seeds Development Organisation, 1985, 80 pp.