OPTIMIZATION OF COAGULANT VARIABLES BY THE SEQUENTIAL SIMPLEX METHOD

By

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CHAPTER I

INTRODUCTION

Since most water treatment plants are subject to fluctuations of some uncontrollable variables in their raw water supply at various times, the dynamic aspect of optimization is always present. By "dynamic optimization" it is meant the establishing of how best to change the controlled variables in order to correct for fluctuation or suddenly changing values of the uncontrolled variables. But dynamic optimization is not always justified; for example, it is not justified when normal operation is smooth and no serious effects occur if major changes are made in a non-optimal manner. But if conditions necessarily fluctuate, there may be much to be gained from superimposing an optimal controlled function on the optional steady-state procedure.

After reviewing several articles (1, 2, 3, 4, 5) and text books (6, 7) on coagulation and the jar test procedure, it became apparent that there was no good procedure for determining the optimum dose of several controlled coagulant variables. At best it seems that the only method now used in obtaining the optimal dose is the one-variable-at-a-time method. Since the trend in recent years has been for water treatment plants to use more controlled variables (coagulant

aids, pH regulation, and alkalies) in the unit operation of chemical coagulation, the one-variable-at-a-time optimization procedure will prove to be very inefficient for the rapid determination of the optimum dose of several controlled coagulant variables.

At the present time there are a number of investigators (2, 3, 4, 5) studying the basic relationship between the optimum coagulation conditions and a measurable property of the raw water or of the system during treatment. Many attempts have been made to develop such relationships, but none has proven capable of wide application. Until a better understanding of the relationships is known, the only method for obtaining the optimum dose of the controlled coagulant variables will be - in spite of its known shortcomings - the jar test procedure.

In the past the jar test procedure has proved valuable in water plant operation, particularly in the hands of an experienced individual. An improvement of the basic procedure has been reported by Jesse M. Cohen (8) which has proven to be a much better procedure than the one used in the past.

Even with this improved procedure it is known and has been reported by A. P. Black, J. E. Singly, G. P. Whittle, and J. S. Maulding (3) that in plant operation the time required to run the jar test is one of the main disadvantages. The time lag between the change of an uncontrolled coagulation variable in plant operation and the determination

of the optimum dose of the controlled coagulant variable will seldom be less than three hours and may be as long as eight to ten hours.

Various methods have been developed for determining the optimum level of several variables which have proven to be very useful; therefore it is felt by this author that one of these methods could be utilized and applied to the jar test procedure to decrease the time lag mentioned above and make the jar test procedure more expedient when studying several control variables.

Purpose of Study

The purpose of this particular study was to select a method of empirical optimization and apply it to the jar test procedure.

CHAPTER II

REVIEW OF MAXIMUM-SEEKING METHODS

The object of many endeavors is to achieve some maximum response by an examination of the effects of various combinations of the factors that more or less determine the response. If the functional relation between the response and the factors is not known, an estimate of the optimal factor combination is made from the responses determined by trying various combinations experimentally. The methods that have been used for making such estimates are one-variable-at-a-time method, factorial designs, methods of steepest ascent, and random experimentation. The most recently developed procedure is the Sequential Simplex Method.

It will be convenient to describe optimization procedures first in terms of two variables, and to use the topological analogies introduced by Box in which the optimum is assumed to be a maximum. Reaching the optimum corresponds to climbing a hill. The hill is not in practice usually found to be of simple shape: ridges are much more common. The criterion to be optimized is called the "response;" it may be the yield or output of the plant or some derived economic criterion, such as profitability. Fig. 1 shows a contour map of a response surface summit. From this map can be read

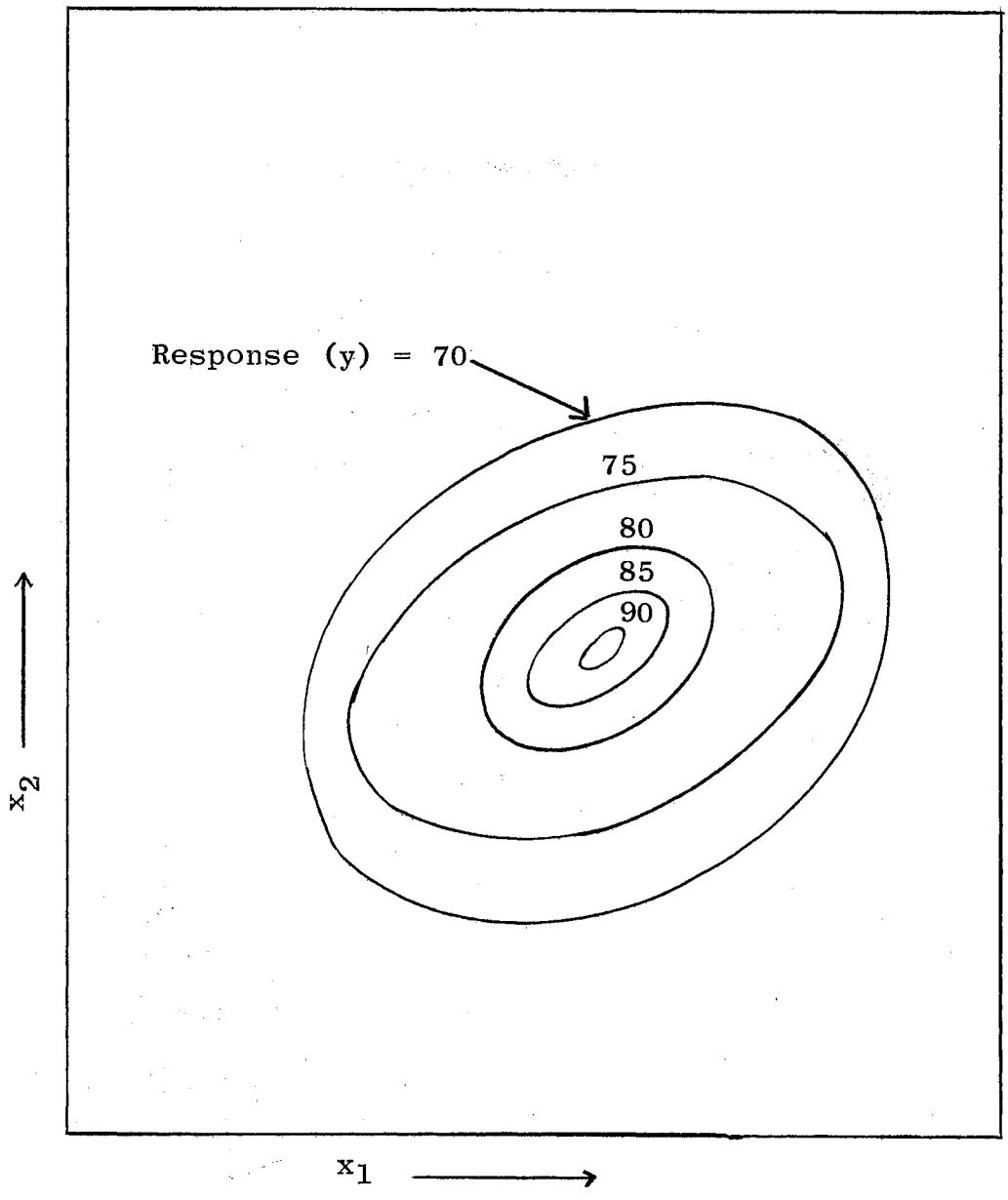

Fig. 1 - RESPONSE CONTOUR MAP

off the response, y, for any pair of values of the process variables, x_1 and x_2. The problem is to climb the hill from any starting point. To do this requires at least two observations to determine whether a given move leads uphill or downhill.

One-Variable-at-a-time

In the 'one-variable-at-a-time' method (9) all variables except one are held constant, and the optimum value of this one for a given value of the remainder is found by trial and error. The procedure is repeated for each variable in turn until all have been sub-optimized for a particular set of values of the remaining variables. It will usually be necessary to repeat the cycle several times before a stable solution is found, and it is by no means certain that this is a true optimum. Even if it is, the method is wasteful of effort in that it requires many more trials than other methods which study all variables simultaneously, especially when the number of variables is more than two.

Fig. 2 shows a map of the response contours and the experimental points for a univariate-experiment example. The first set of points (points 1, 2, 3, 4, 5 and 6) is where x_1 is held constant and x_2 is varied. The value of x_2 which gives the maximum response is found. Point 5 on the map represents the maximum for the first set of trials. The second set of trials, represented by points 7, 8, 5, 9, 10 and 11 are those where x_2 is held constant and x_1 is varied along a line containing the maximum response from the first set of

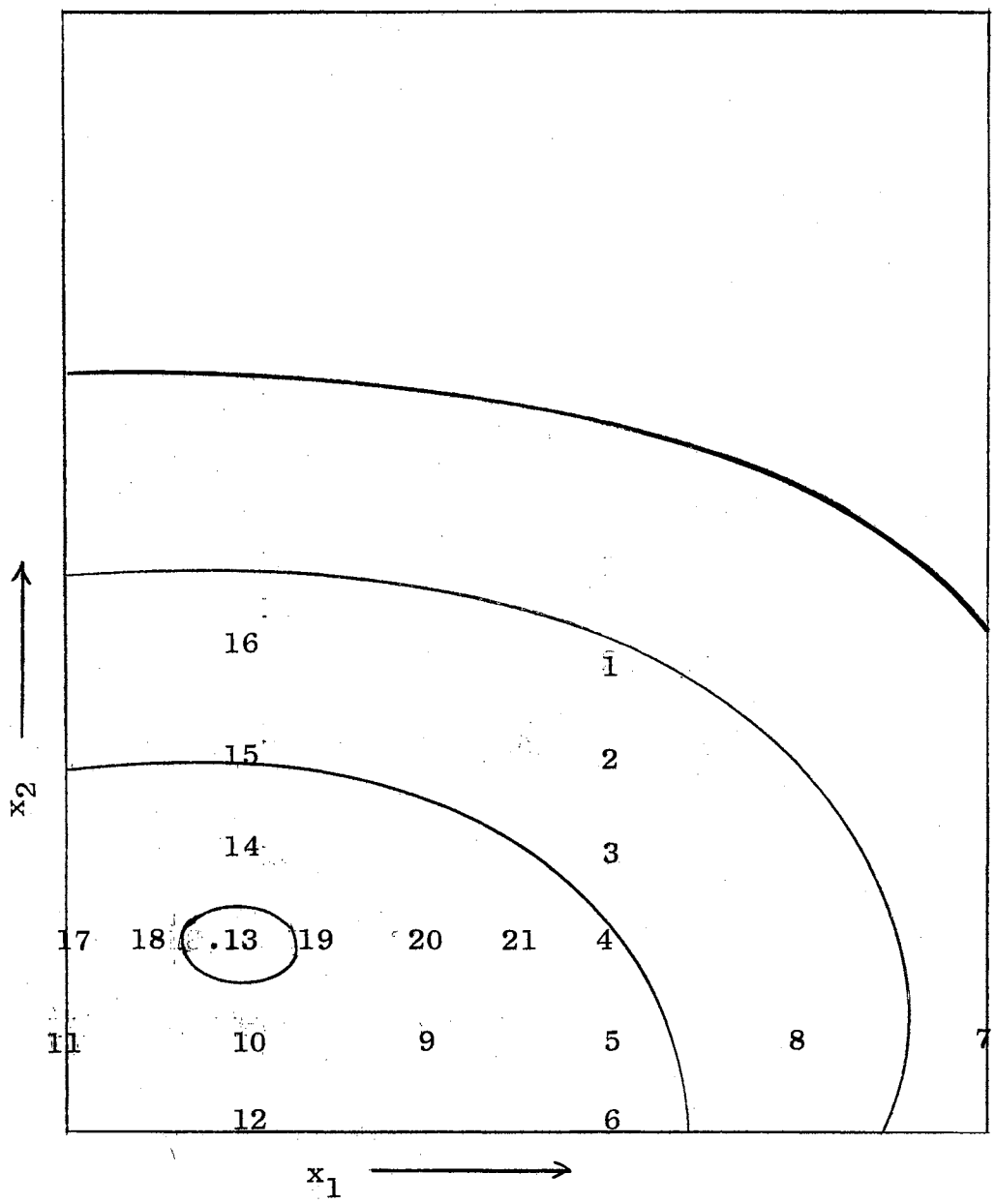

Fig. 2 - UNIVARIATE-EXPERIMENT MAP

trials. The third set of trials is represented by points 12, 10, 13, 14, 15 and 16. The maximum of this set is point 13. The fourth set of trials is represented by points 17, 18, 13, 19, 20 and 21. The maximum from this set is point 13; therefore the co-ordinants of the optimum response are located at point 13.

Although this method is simple and easy to apply for two variables, the number of trials for three or more variables becomes excessive.

Factorial Method

The factorial method (10, 11, 12) is characterized by the use of a single factorial design, either fractional, complete, or replicated. Although the results of a complete factorial experiment provide a systematic over-all picture of the response surface, which may be a highly desirable but secondary objective of the experiment, it usually requires a large number of factor combinations when the number of control variables is more than three. Also for the "best" design it will require a large number of levels of each factor.

Fig. 3 represents a factorial experiment example, two factors each at four levels. It is seen from this example that it would require sixteen trials. If three variables each at four levels were to be investigated, it would require sixty-four combinations. From this map it is suggested that points 2 or 6 may be the optimum combination of the two factors. Taking the region of points 2 and 6 to be close to

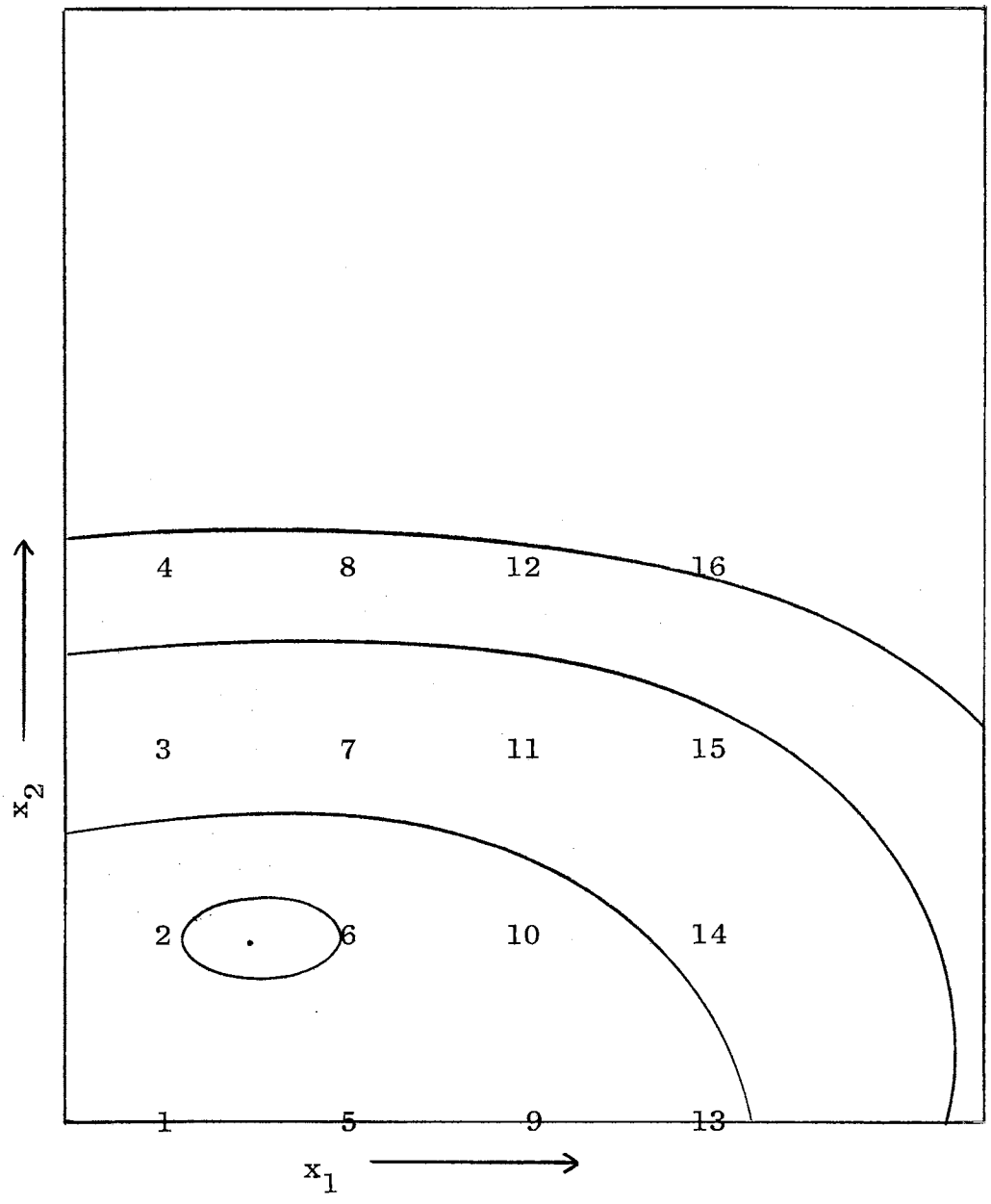

Fig. 3 - FACTORIAL EXPERIMENT MAP

the summit, another factorial experiment would have to be run in this region with smaller differences between levels.

Steepest Ascent Method

The principle of the method of steepest ascent (12, 13, and 14) is to determine the slope of the response surface in the neighborhood of the starting point and to move in the "direction of steepest ascent." This is not necessarily the most direct route to the summit, but enables the maximum advantage to be gained from the first move. Subsequent trials are made at points along the path, until no further improvement is found. A further set of trials is made to determine the new direction of steepest ascent and so on until no further progress is possible, when it is assumed that the summit has been reached. In experimentation, the direction of steepest ascent is deduced from a set of trials, usually in the form of a factorial experiment. Statistical tests of significance are used to decide whether the direction of steepest ascent has been reasonably well defined, taking into account the effect of experimental errors, or whether the trials should be repeated until this is so.

For optimization by means of test procedures this method has the disadvantage that considerable time may be spent in experimenting in one region before a move is made. There is also the risk that the operating personnel may tire of repeating a quite elaborate pattern of changes before making a purposeful move.

In maximizing a mathematical function, the direction of steepest ascent is found by calculating the derivatives of the function by any suitable method. Fig. 4 shows a contour map of the method of steepest ascent. The contour map represents a two factor response surface. After the initial set of trials is run (represented by points 1, 2, 3, and 4) the line of steepest ascent is calculated. This line is represented by points 5, 6, and 7. Further trials along this line show a decrease; therefore another set of trials is run, letting the last point showing an increase be one corner of the new square. From the second square (represented by points 7, 8, 9, and 10), the second path of steepest ascent is calculated. This line is represented by points 11 and 12. Further points along this line show a decrease; therefore a new square has to be constructed and a new path of steepest ascent has to be calculated. The third line is represented by point 17 on the map. Further points along this line would show a decrease. The same procedure is carried out until no further improvement is made or the last set of trials shows the same response.

Random Experimentation

There are three possible situations in random experimentation. They are simple random sampling (9), stratified random sampling (9), and random search (15).

Simple random sampling is characterized by making trials at points selected completely at random over the entire ex-

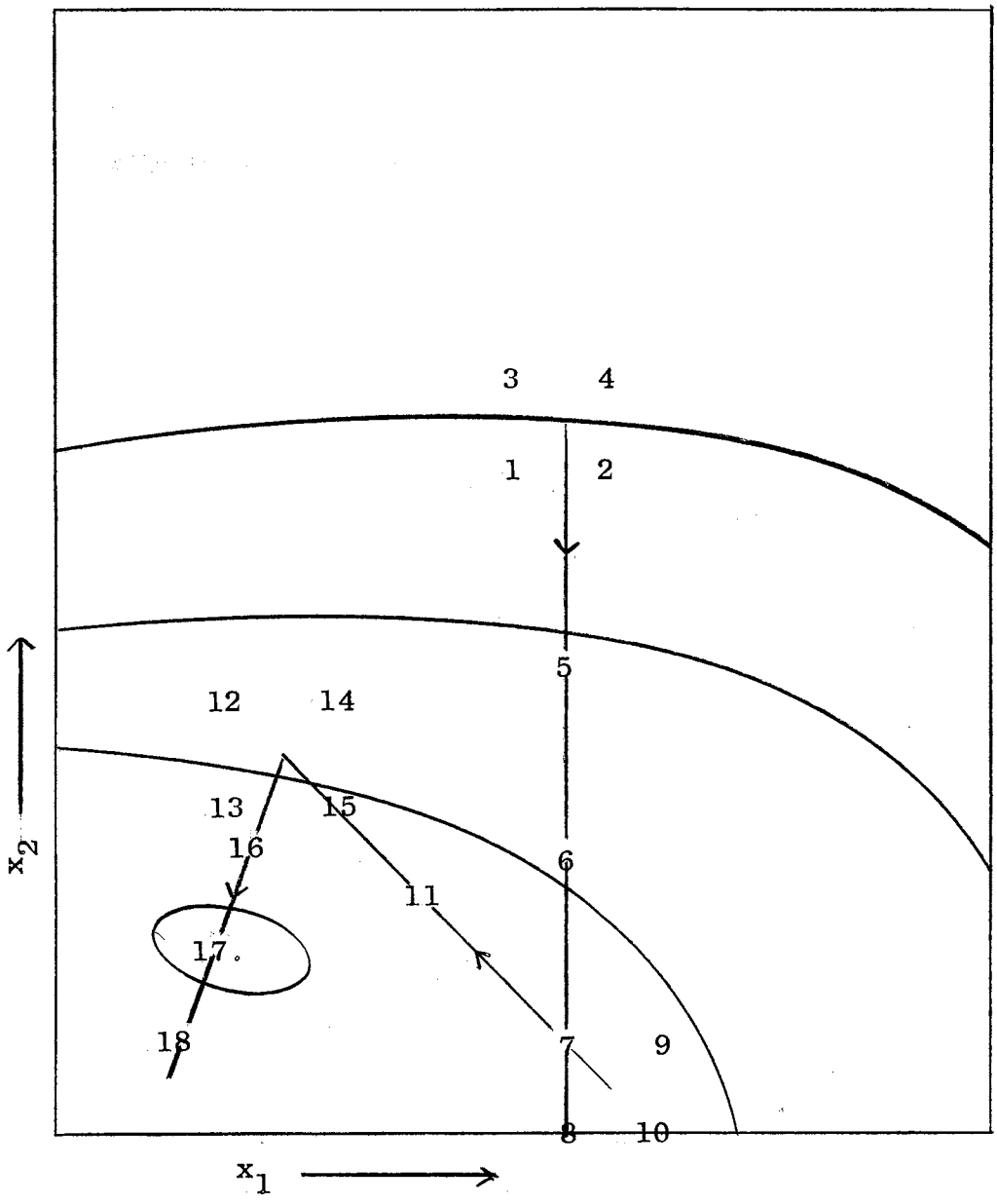

Fig. 4 - STEEPEST ASCENT EXPERIMENT MAP

perimental region. Fig. 5 represents a possible selection of points. It is seen that if one were real lucky he might pick the "winner" (point 15).

Fig. 6 shows a possible stratified random-experiment example. Here the experimental region is divided up in a grid, and points are selected at random in each grid. Also here the selection of the optimum combination is by chance alone.

The third possible procedure, mentioned by Spendley, Hext, and Himsworth (15) is to start at some arbitrary point in the space of the variables, and then to move in a randomly chosen direction to a second point. If the second point gives a better response than the first, it is used as the starting point for a fresh random move. If the second point gives a worse response than the first, it is assumed that a move in the opposite direction would have been more favorable and this point is used as the starting point for the next random move. Thus, so long as the response surface does not have a maximum in the immediate neighborhood, and ignoring the effect of experimental error, every move will lead to some improvement and the optimum will be reached by a torturous path.

Such a procedure has obvious drawbacks for use in plant experimentation. Only a plant manager with strong gambling instincts would approve of a change in conditions which all the evidence suggested would be in quite the wrong direction - as must sometimes happen if the direction is chosen at

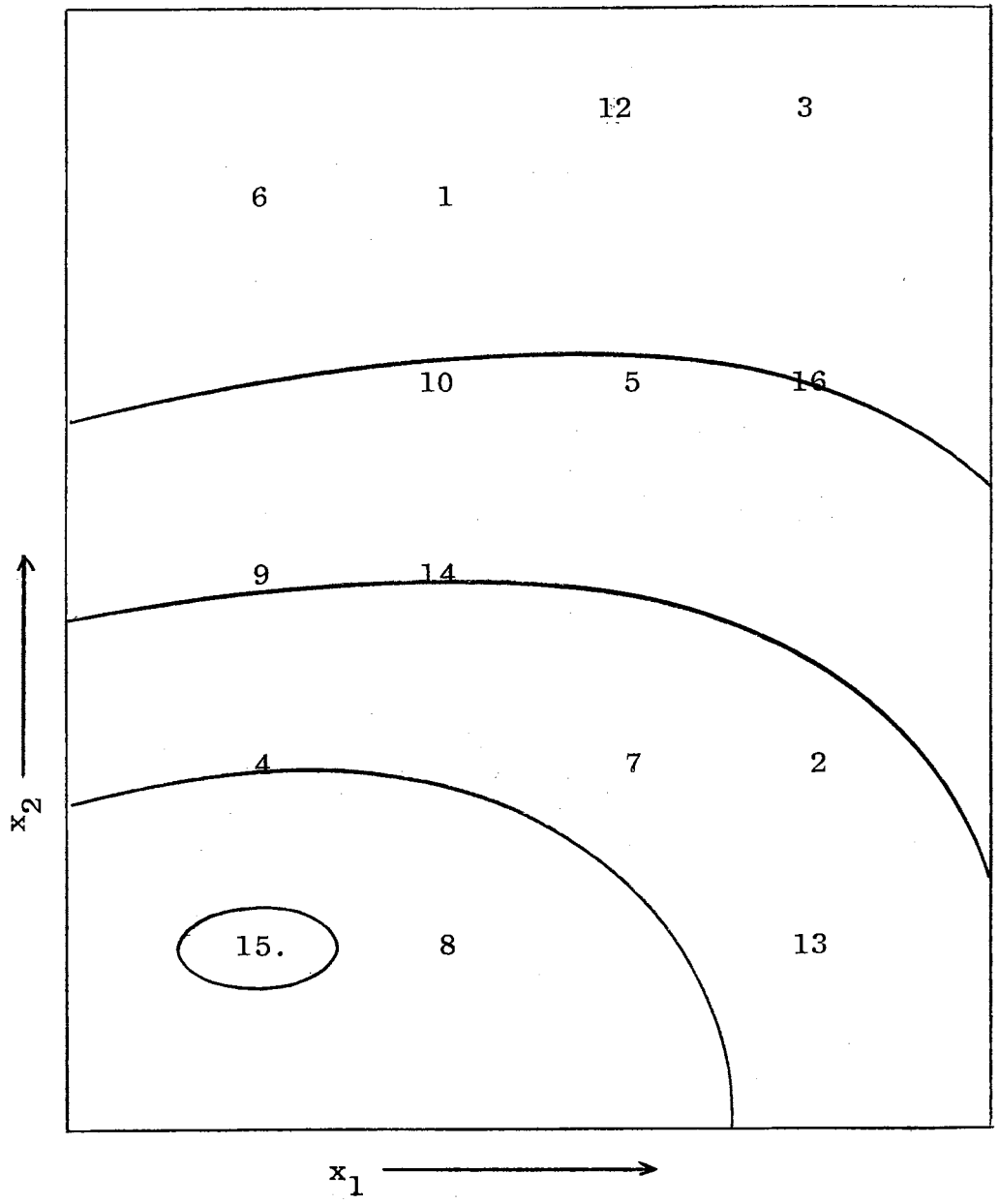

Fig. 5 - SIMPLE RANDOM EXPERIMENT MAP

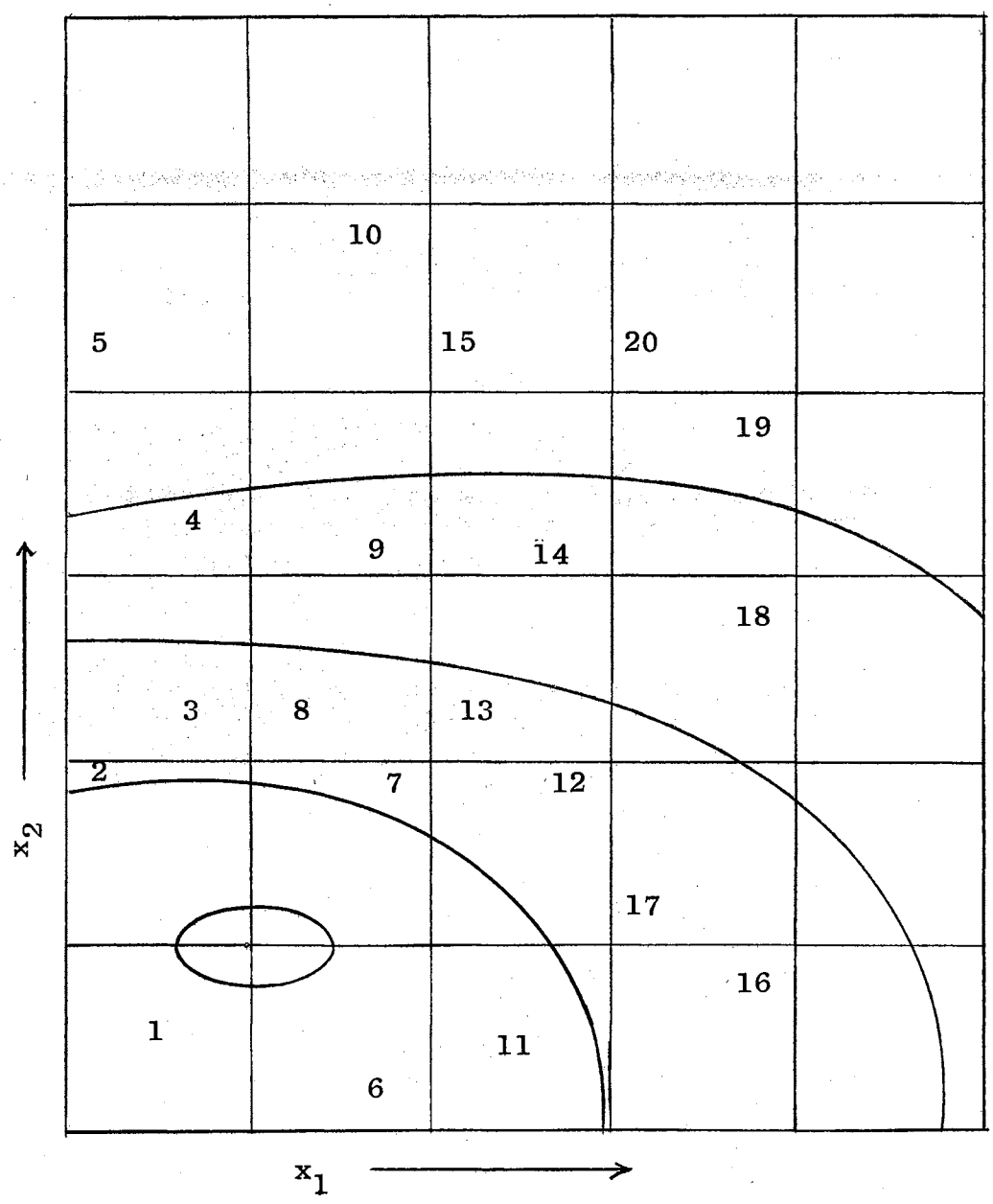

Fig. 6 - STRATIFIED RANDOM EXPERIMENT MAP

random. There would obviously be a preference for a procedure which made some use of previous data in planning the next move. Random Search ignores everything except the current and the immediately previous results.

Fig. 7 represents such a procedure. The original starting point is taken at point 1. The next point, selected at random, is point 2. It is seen that this point gives a lower response than point 1; therefore the next point would be selected in the opposite direction from point 2. This combination is shown by point 3. This procedure is carried out until a move in every direction gives a lower response than the point in question. This point could be taken as the optimum, but it could be very misleading. The point could be riding a ridge which is not the true optimum, but only a high response in the immediate vicinity of the factor space one is experimenting in.

Sequential Simplex Method

The Sequential Simplex Method (15) has some resemblance to the methods of steepest ascent, the main difference being that no attempt is made to find the best direction in which to move. A rapid determination is made of a direction which is steep, though not steepest, so that frequent moves are made in directions which are at least favorable, though not in general most favorable. The procedure with two variables is as follows:

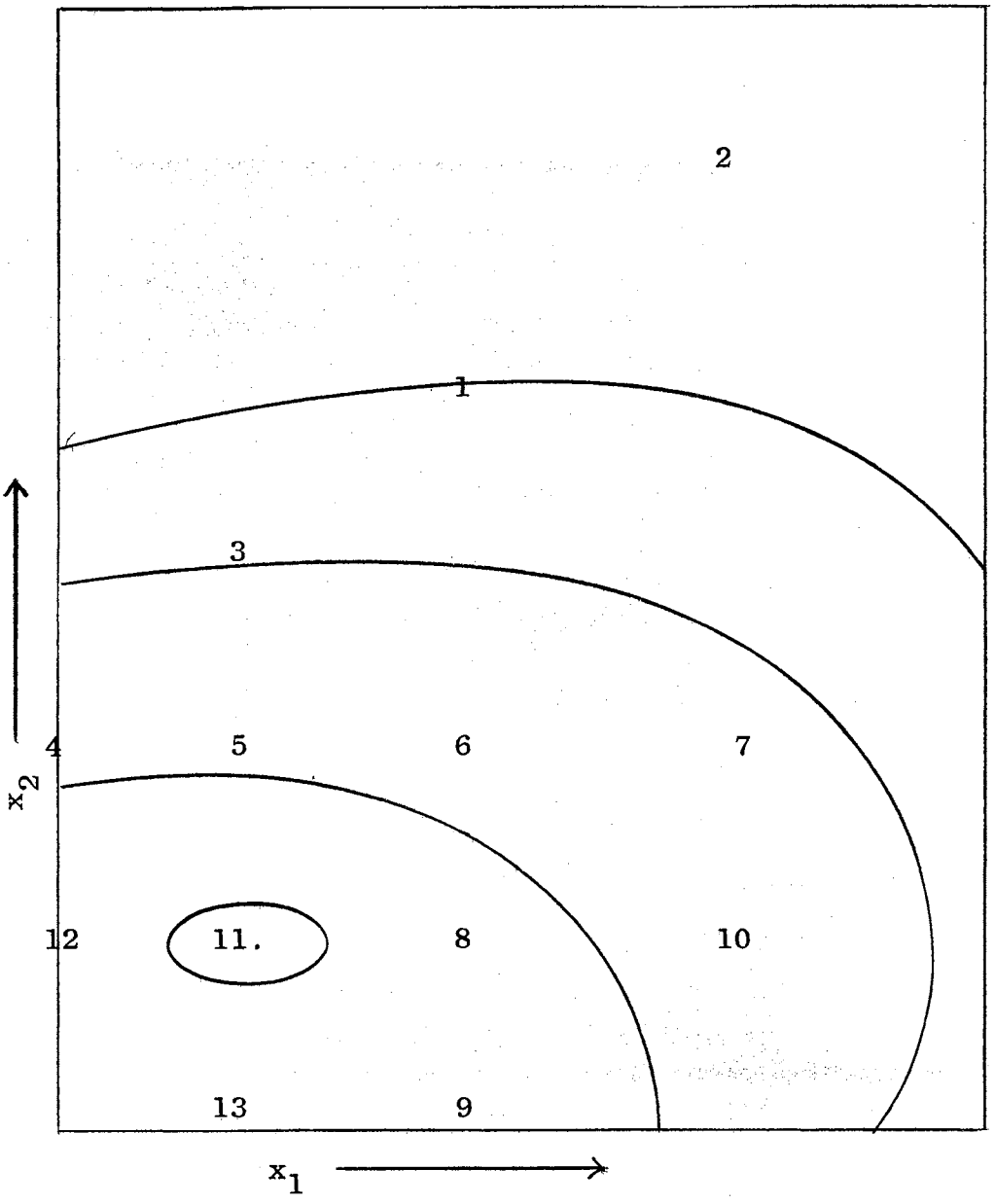

Fig. 7 - RANDOM SEARCH MAP

Three trials are made, the values of the two variables being such that the three points correspond to the vertices of an equilateral triangle; for example, points 1, 2, 3, on Fig. 8. (It is convenient to think in terms of an equilateral triangle, but this is not necessary. Any triangle can be made equilateral by adjusting the scales of the variables, and in the conventional scales it is unnecessary to form an equilateral triangle.) A move is then made to a new point which is constrained to be such that, together with two of the points of the original triangle, it forms a second equilateral triangle. (See point 4 on Fig. 8.) If the response surface is locally a plane or nearly so, one of the three permitted new points will give a higher result than the other two, and it is easy to see that this new point is the "mirror image" of the lowest of the first three points. Thus, after the first three trials have been made, the point giving the worst result is discarded, and replaced by its mirror image to form a second triangle. This is repeated, and so long as the surface is sloping and reasonably plane over the area of the triangle, every move leads to a more favorable region and eventually the "summit" is reached.

The path taken is a zigzag one, but oscillates about the line of steepest ascent. Points 1 to 12 on Fig. 8 show this path leading to the summit. Experimental errors may lead to some move being downhill instead of uphill, but these false moves are rapidly corrected, and simply slow down the average rate of climb.

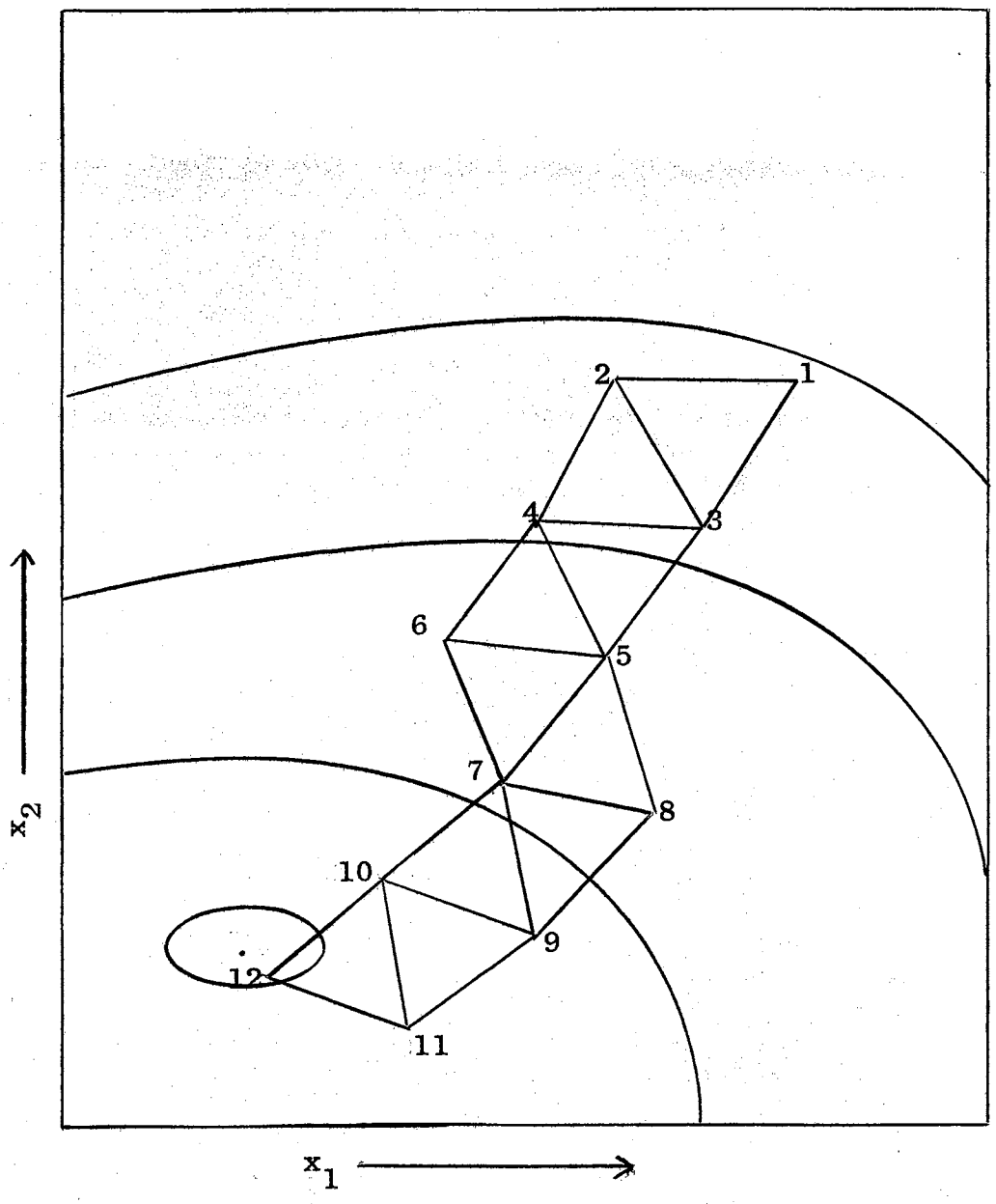

Fig. 8 - SEQUENTIAL SIMPLEX MAP

For more than two variables the procedure is the same, except that the first set of trials consists of (k + 1) points, where k is the number of variables. Thereafter a move is made after every point. The (k + 1) points correspond to the vertices of a regular simplex in k dimensions. (A simplex is a geometrical figure. A simplex in three dimensions would require four points and would form a tetrahedon; in two dimensions a simplex has three points arranged in a triangle. In more than three dimensions the analogous figure is called simply a "simplex.") Thus, after the initial set of trials, which for k variables could not be smaller, the number of variables does not matter. The simplex method has other attractive features: the calculations involved are trivial, calling for no mathematical or statistical knowledge, and each move is completely determined by the previous results, so that judgement or extrapolation is not required.

The method is thus ideally suited for operation by plant staff with no knowledge of statistics, or by a computer where fast or automatic operation is required.

It is easy to add an extra variable at any time. It is only necessary to add one point, which completes a simplex in (k + 1) instead of k dimension, to give a starting simplex for optimizing the (k + 1) variables. For example, one point is added to an equilateral triangle to form a regular tetrahedon.

In this method it is not necessary to have a numerical measure of the response. It is only necessary to rank the results and discard the worst. This is useful when it is impossible to measure quality numerically, and also where there are several responses which cannot be maximized simultaneously, and a judgement may have to be made as to the relative importance of the various responses.

If it is required to fit a second degree equation in order to estimate the form of the surface - say in the region of the optimum where the surface is not even approximately a plane - it is easy to add further points to the current simplex and obtain a set of points which efficiently estimate the second degree surface which fits the results. This is also true for the method of steepest ascent.

It may be noted that Brooks and Mickey (16) have shown that the most efficient experimental design for estimating the slope of a plane (i.e., the design giving most information per observation in the presence of experimental error) is the regular simplex.

The problem of restraints is easily dealth with. If it is specified that some function of the input variables or of the response, or a subsidiary response, must not exceed a stated value, it is only necessary to calculate this function, compare it with the specified value, and if this is exceeded, to replace the response by some large negative constant which ensures that the offending point is the worst in the simplex and is immediately discarded. In experimentation the restraint

might be simply an upper limit on one variable - a maximum permissible pH for example. In this case the trial need not - indeed, must not - be made; the response can at once be set equal to a negative constant. The same would apply to a function of several variables; for example, if a high dosage of alum and a high mixing speed must not occur together. The restraint may be limited to a second response, say a condition that the cost must not be above a given limit, the object being to make turbidity removal a maximum subject to this condition. In this case the trial would have to be done, and if the cost were too high, the main response - turbidity removal - would be set at a negative value, so that the offending point would be immediately discarded. Since the responses in a simplex need only be ranked, this procedure is valid.

Summary of the Literature

The literature can be summarized as follows:

1. The "one-variable-at-a-time" method is only expedient when the number of variables is not more than two.

2. Factorial experiments should be used only when an overall picture of the response surface is needed. Also, the number of trials for three or more variables become quite excessive.

3. The steepest ascent method is the best known and currently most used optimization procedure. Considerable knowledge of statistics is required for correct application

of this procedure. Another disadvantage is that considerable time may be spent in experimenting in one region before a move is made to another region. Also, numerical responses are needed for this procedure.

4. Although random experimentation is easy to program and can be made automatic, it has the main disadvantage in that the selection of the optimum combination of the levels of each variable is by chance alone.

5. The Sequential Simplex Method has these attractive features: the calculations involved are trivial, calling for no mathematical or statistical knowledge; each move is completely determined by a previous result so that judgement or extrapolation is not required; it is easy to add an extra variable at any time; and it is not necessary to have a numerical measure of the response.

Based on the above review of the literature, the Sequential Simplex Method seems to be the method best suited for application to the jar test procedure. The next chapter will develop and outline the formal procedure of this method.

CHAPTER III

FORMAL PROCEDURE OF THE SEQUENTIAL SIMPLEX METHOD

The basic design (15) of the scheme is the regular simplex in k dimensions, where k is the number of factors currently under investigation. Relative to a chosen origin, a regular simplex of unit edge is conveniently specified by the (k + 1) x k design matrix.

$$D_o = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ p & q & q & \cdots & q \\ q & p & q & \cdots & q \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ q & q & q & \cdots & p \end{bmatrix}$$

Where $p = \frac{1}{1.414k}\left[(k-1) + (k+1)^{\frac{1}{2}}\right]$

And $q = \frac{1}{1.414k}\left[(k+1)^{\frac{1}{2}} - 1\right]$

The rows of the matrix give k coordinates of each of the (k + 1) vertices of the simplex. D_o is suggested as a convenient starting simplex once the origin and scales of measurement have been defined.

"Regularity" is, of course, one of those metrical concepts which is not scale-invariant, and therefore cannot be

strictly applied in a multidimensional factor space in which scaling is inherently arbitrary. Regularity in some sense, however, is preserved if the scales for the separate factors are chosen in such a way that the unit change in each is of equal interest to the experimenter. Therefore it will be assumed in what follows that "regular" has its customary geometrical meaning. It is noted, nevertheless, that by a suitable linear transformation of co-ordinates any simplex can be made regular, so that regularity in a specified co-ordinate system is not essential to the application of the technique.

In the most general case we can consider a "regular" simplex S_o with vertices $V_1, V_2, \ldots V_{k+1}$ and center C_o. On each face of the S_o it is possible to construct a new simplex S_j with center C_j, which has k vertices $V_1, V_2, \ldots V_{j-1}, V_{j+1} \ldots V_{k+1}$ in common with S_o and is completed by one new vertex V_j^*, the mirror image of V_j in common face. To find any one co-ordinate of V_j^* we take twice the average of the corresponding co-ordinates for the common vertices $V_1, V_2, \ldots V_{j-1}, V_{j+1} \ldots V_{k-1}$ and subtract the corresponding co-ordinate of V_j. In vector notation

$$V_j^* = \frac{2}{k} (V_1 + V_2 + \ldots + V_{j-1} + V_{j+1} \ldots + V_{k+1}) - V_j$$

Suppose now that S_o is a simplex in the factor space and that the responses n_j $(j = 1, 2, \ldots k+1)$ at the vertices of S_o are known or have been estimated by experimental readings y_j. Then we move through the factor space in that direction $C_o \longrightarrow C_p$ which is "nearest" to the direction of

steepest ascent by applying

Rule 1 - Ascertain the lowest reading y_p of y_1 . . . y_{k+1}, complete a new simplex S_p by excluding the point V_p corresponding to y_p and replacing it by V_p^* defined as above.

When the procedure is used on observations which are subject to error, there is the possibility that the system of simplexes may become anchored to some spuriously high result which is treated as if it were a genuine optimum. To reduce the risk of this, we apply

Rule 2 - If a result has occurred in (k+1) successive simplexes and is not then eliminated by application of Rule 1, do not move in the direction indicated by Rule 1 or at all, but discard the result and replace it by a new observation at the same point. If the point is a genuine optimum, the repeat observation will also tend to be high. If, however, the result was high only by reason of errors of observation, it is unlikely that the repeat observation will also give so high a result, and the point will be eliminated in due course.

When the responses are not subject to error (i.e., when the procedure is used for numerical optimization) a different Rule 2 is required, and a different criterion for deciding when the system is no longer progressing. For a discussion of this different Rule 2 reference should be made to Hext and Himsworth's original paper (15).

Less difficulty will be caused by spuriously low results, since these will tend to be eliminated from the system fairly rapidly. However, there are advantages to be gained by also applying

Rule 3 - If y_p is the lowest reading in S_o, and if the next observation made, y_p^*, is the lowest reading in the new simplex S_p, do not apply Rule 1 and return to S_o from S_p. Move out of S_p by rejecting the second lowest reading (which is also the second lowest reading in S_o).

This will go some way toward reducing wandering caused by spuriously low results, but its chief purpose is that it forces the simplexes to circle continuously about an indicated optimum rather than oscillate over a limited range. It also makes progress possible if by chance the system of simplexes should straddle a "ridge" in the factor space.

The three rules given above may be summarized briefly as: move by rejecting the lowest observation unless (a) another observation is too old - in which case we renew the latter, or (b) such a move would cause us to return to the previous simplex, in which case we try the next most favorable direction. Between them these rules define an evolutionary procedure capable of indefinite application. Given a fixed optimum, the system of simplexes will approach this with a closeness determined by the basic step size, and will then circle continuously around it, any straying caused by observational errors being corrected by later observation.

If the optimum should move with time, the continuous circling will ensure that information is generated enabling the moving optimum to be followed. Only the most trivial calculations are involved, so that the procedure is as suited to manual application as to electronic computation.

It must be realized, however, that this method is intended as a permanent mode of operation, and not as a short-term investigational technique.

CHAPTER IV

APPLYING THE PROCEDURE

The best way to describe the procedure is by considering a hypothetical example. The example will involve several simple calculations; therefore Fig. 9 represents a sample calculation sheet for use in these calculations.

The hypothetical example will involve a water treatment plant which is using two control variables in their unit operation of chemical coagulation. The control variables are ferric sulfate and a coagulant aid. The present dosage of the variables is 20 ppm of ferric sulfate and 0.2 ppm of coagulant aid. For some reason a change in the raw water supply occurs and the above dosage does not give good results. The problem is to find the combination of the control variables that will give the optimum response. The optimum response would be the levels of each factor that will give the greatest turbidity removal at the lowest cost.

The first step in the technique is the selection of the levels of the variables to use in combination with one another. From Chapter II it is seen that a convenient starting simplex is given by

Simplex No._____

Line No.			Run No.	Rank	x_1	x_2	x_3	.	.	x_k
(1)	Co-ordinates of Points									
(2)										
(3)										
.										
.										
(k+1)										
(k+2)	Sum of Retained Co-ordinates	Sum of k Numbers								
(k+3)	2x(Average of Retained Points)	Line(k+2) x $\frac{2}{k}$								
(k+4)	Co-ordinate of Discarded Point	-								
(k+5)	Co-ordinate of New Point	Line(k+3)-Line(k+4)								
Remarks:										

Fig. 9 - FORM OF CALCULATION SHEET FOR SEQUENTIAL SIMPLEX METHOD

$$D_o = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ p & q & q & \cdots & q \\ q & p & q & \cdots & q \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ q & q & q & \cdots & p \end{bmatrix}$$

Where $p = \frac{1}{1.414k}\left[(k-1) + (k+1)^{\frac{1}{2}}\right]$

And $q = \frac{1}{1.414k}\left[(k+1)^{\frac{1}{2}} - 1\right]$

The restrictions placed on this simplex are:

1. It must have one combination of levels more than the number of variables under study.

2. It must conform to "regularity;" that is, it must have the scales of each variable chosen in such a manner that a unit change in each variable is of equal interest to the investigator.

Since there are two control variables (k = 2), the first simplex will require three combinations (k + 1) of the two factors. Therefore the starting simplex (in this case a triangle) will have the following combination of levels, if we let the present dosage be the origin.

$$S_o = \begin{array}{c} \begin{matrix} x_1 & x_2 \end{matrix} \\ \begin{bmatrix} o & o \\ p & q \\ q & p \end{bmatrix} \end{array}$$

Where p = 0.966

And q = 0.260

Mention should be made at this time of a possible second situation in which an investigator might find himself. The situation is one where no starting point is known from which to form the starting simplex. The first step in the procedure given above is not altered in any way except a starting point (origin) must be chosen. The starting point can be picked completely at random within the response surface. An example of this situation might occur at a design office where no previous knowledge of the raw water was at hand. The designer could make a rough estimation of the optimum dosage and conditions, and start his system of simplexes from this point.

The next step in the procedure is to choose the scales of each variable so as to make the simplex "regular." If we let a unit change in one variable be of the same interest as a unit change in the other variable and plot these on graph paper, the triangle formed will be an equilateral triangle with unit sides. To make this so requires a suitable linear scale transformation. Each investigator will have to decide what transformations are best suited for his particular problem.

For example, if it were decided that an increase of 0.5 ppm of coagulant aid was of the same interest as 5 ppm of ferric sulfate, the scale transformation would be 5 for the ferric sulfate and 0.5 for the coagulant aid. The coordinates of the triangle would be represented by:

$$
\begin{array}{cc}
5 & 0.5 \text{ (scale factor)} \\
x_1 & x_2
\end{array}
$$

$$
S_o = \begin{bmatrix}
20 & 0.2 \\
20 + 5(0.966) & 0.2 + 0.5(0.260) \\
20 + 5(0.260) & 0.2 + 0.5(0.966)
\end{bmatrix}
$$

Two other comments should be made at this time. They are:

1. The simplex should not be too large; that is, it should not cover the entire response range.

2. The simplex should not be too small; that is, it should not cover too small a response region.

However, if the experimenter does choose too large or too small a range, it will be detected in due course, usually after the first run of experiments.

Fig. 10 shows a plot of the points representing three possible starting simplexes. Points 1, 2 and 3 represent a simplex which is too large. Points 1, 4 and 5 represent a simplex which is about right. Points 1, 6 and 7 represent a simplex which is too small. If the experimenter chooses a simplex represented by points 1, 2 and 3 he would find after the new point for the second simplex was calculated it would fall outside the response region; therefore it would be concluded that the starting simplex covered too much of the response surface. If the experimenter chose the simplex represented by points 1, 6 and 7, then after the first runs were made it would be impossible to detect the differences between the samples. Therefore it becomes apparent imme-

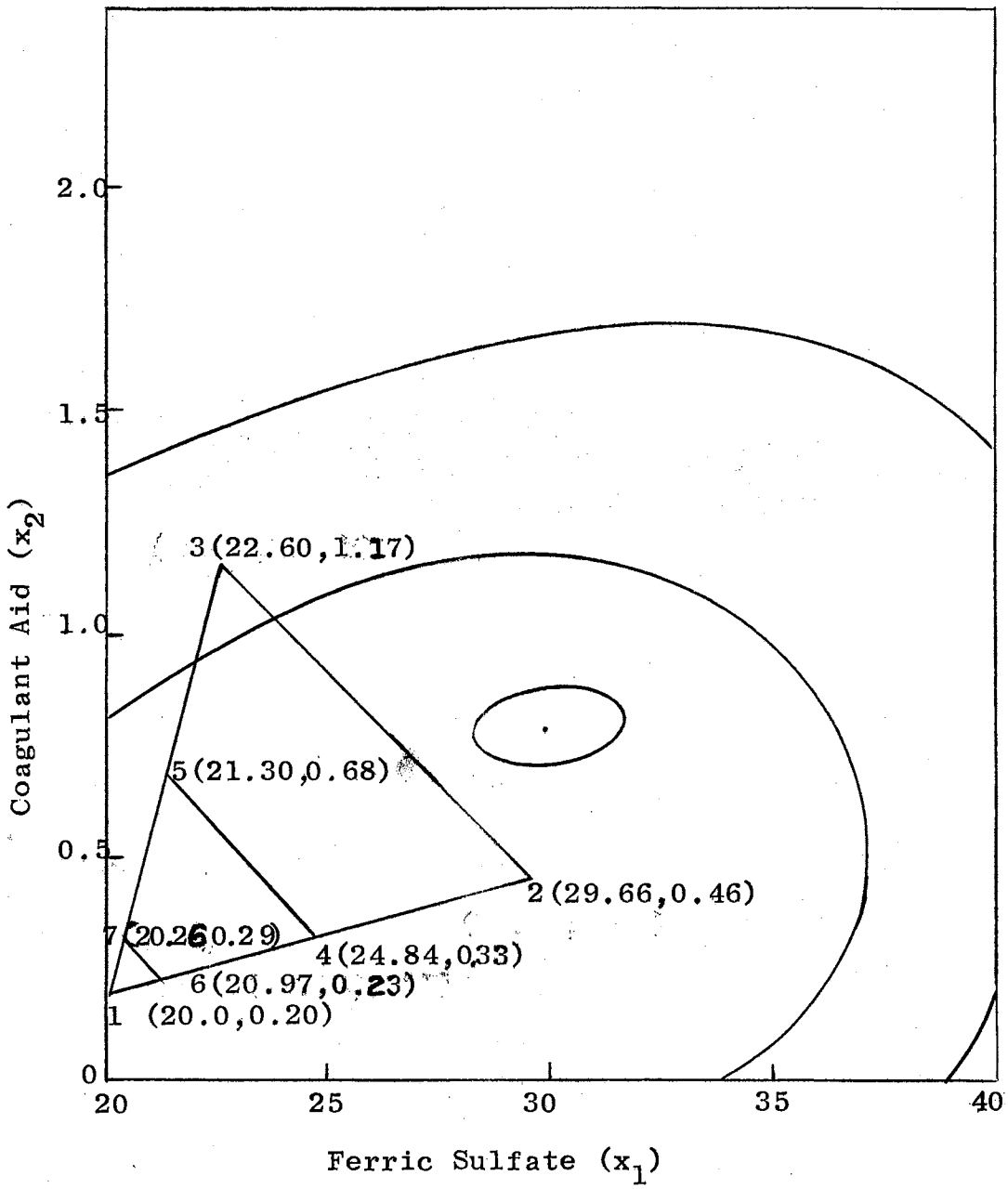

Fig. 10 - THREE POSSIBLE STARTING SIMPLEXES FOR EXAMPLE PROBLEM

diately that the levels of the factors will have to be increased in order to be able to discriminate between the samples.

The next step after obtaining the starting simplex is to test the various combinations by the standard jar test procedure. Once this is done, the calculations needed to obtain the combination of levels for Run No. 4 are straight forward and are shown in Fig. 11. Note that Run No. 1 was discarded in accordance with Rule No. 1 (Chapter III). Rule No. 1 states that the combination of levels which gives the lowest ranking response be discarded.

In Fig. 12 the starting simplex is represented by the vertices of the triangle labeled "1". The triangle labeled "2" represents Simplex No. 2, which is the retained points of Simplex No. 1 and the calculated new point of Simplex No. 1.

After ranking Run No. 4 along with the other retained runs of Simplex No. 1, the same calculations are carried out to obtain the combination of levels for the fifth run. The procedure does not require that a repeat test of the retained points of the previous simplex be made, but if a check is desired on these combinations a repeat test could be made at the time the new combination is run.

Calculations for Simplex Nos. 2, 3, 4, 5, and 6 are given below. It should be noted that the lowest rank in Simplex No. 5 was not rejected, but the second lowest response was rejected. This is due to the application of Rule No. 3 (Chapter III). Rule No. 3 states that if a cal-

Simplex No. 1

Line No.			Run No.	Rank	x_1 Fe_2SO_4	x_2 Coag. Aid	
(1)	Co-ordinates of Points		1	3	20.00	0.20	*
(2)			2	1	24.80	0.33	
(3)			3	2	21.30	0.68	
(4)	Sum of Retained Co-ordinates	Sum of 2 Numbers			46.10	1.01	
(5)	2x(Average of Retained Points)	Line(2) x $\frac{2}{2}$			46.10	1.01	
(6)	Co-ordinate of Discarded Point				20.00	0.20	
(7)	Co-ordinate of New Point	Line(5) - Line(6)			26.10	0.81	

Remarks: *Discarded Point

Fig. 11 - CALCULATION SHEET FOR SIMPLEX NO. 1

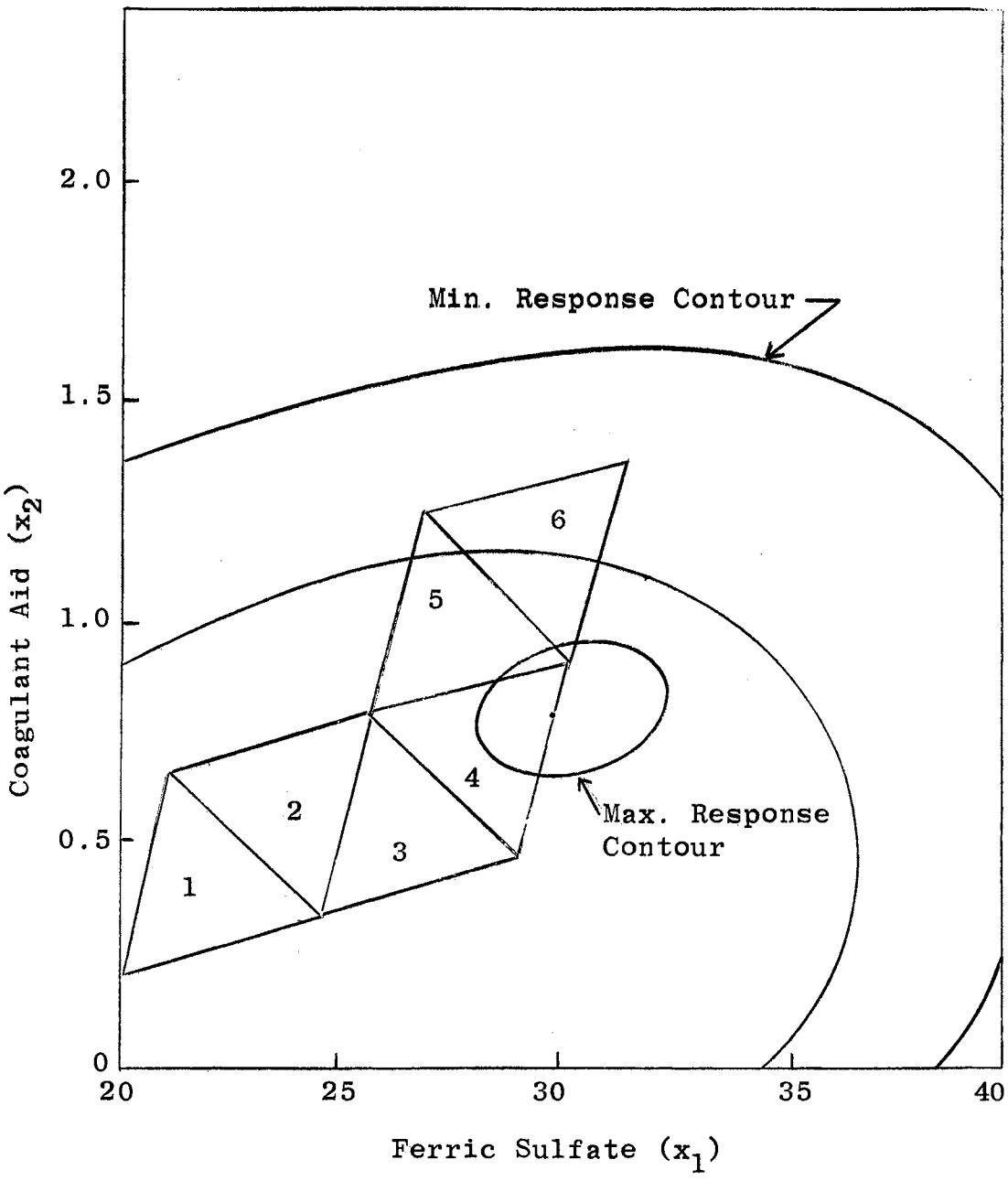

Fig. 12 - RESPONSE CONTOUR MAP AND SYSTEM OF SIMPLEXES LEADING TO SUMMIT

culated new point in a simplex returned to the previous simplex, the lowest rank in the present simplex should not be discarded, but the second lowest reading should be discarded. This will reduce wandering caused by returning to a previous simplex. Therefore, the second lowest ranking response was discarded and the new point calculated from the first and third responses.

Simplex No. 2

Line No.	Run No.	Rank	x_1	x_2
(1)	2	2	24.8	0.33
(2)	3	3	*21.3	0.68
(3)	4	1	26.1	0.81
(4)			50.9	1.14
(5)			50.9	1.14
(6)			21.3	0.68
(7)			29.6	0.46

* Discarded Point

Simplex No. 3

Line No.	Run No.	Rank	x_1	x_2
(1)	2	3	*24.8	0.33
(2)	4	2	26.1	0.81
(3)	5	1	29.6	0.46
(4)			55.7	1.27
(5)			55.7	1.27
(6)			24.8	0.33
(7)			30.9	0.94

*Discarded Point

Simplex No. 4

Line No.	Run No.	Rank	x_1	x_2
(1)	4	2	26.1	0.81
(2)	5	3	*29.6	0.46
(3)	6	1	30.9	0.94
(4)			57.0	1.75
(5)			57.0	1.75
(6)			29.6	0.46
(7)			27.4	1.29

*Discarded Point

Simplex No. 5

Line No.	Run No.	Rank	x_1	x_2
(1)	4	2	*26.1	0.81
(2)	6	1	30.9	0.94
(3)	7	3	27.4	1.29
(4)			58.3	2.23
(5)			58.3	2.23
(6)			26.1	0.81
(7)			32.2	1.42

*Discarded Point

Simplex No. 6

Line No.	Run No.	Rank	x_1	x_2
(1)	6	1	*30.9	0.94
(2)	7	2	27.4	1.29
(3)	8	3	32.2	1.42
(4)				
(5)				
(6)				
(7)				

*Optimum Combination

After obtaining the response from the jar test on Run No. 8 and ranking the results, it is seen that the same response has occurred in (k + 1) simplexes for Run No. 6. Therefore Rule 2 (Chapter III) is applied. Rule 2 states that if the same response has occurred in (k + 1) successive simplexes, and is not then eliminated by application of Rule 1, do not move in the direction indicated by Rule 1 but discard the result (Run 6 in this case) and replace it by a new observation at the same point. If the point is a genuine optimum, the repeat observation will also tend to be high. If, however, the result was high only by reason of errors of observation, it is unlikely that the repeat observation will also give so high a result, and the point will be eliminated in due course.

Fig. 12 represents the response contours and the system of simplexes leading to the summit for the example problem.

Although the example problem involved only two variables, any number of variables could have been used. In fact the use of this technique with only two variables will prove to be inefficient as compared with the Univariate Method. Therefore the use of this technique will prove to be of most value when three or more variables are under study.

SUMMARY OF THE PROCEDURE

The procedure can be summarized as follows:

1. Determine the scales of measurement of each variable in such a manner so that a unit change in one variable is of equal interest as a unit change in the other variables.

2. Select a starting point (origin) in factor space - either a present point or a point selected completely at random.

3. Calculate the vertices of the starting simplex and make the suitable scale transformation if necessary.

4. Test the combinations $(k + 1)$ of the levels of the k variables.

5. Rank the responses.

6. Calculate the co-ordinate of the new point in accordance with Rules 1 and 3 given in Chapter II.

7. Test the new combination and rank the response along with the retained responses of the previous simplex.

8. Continue the process until the optimum is reached, which is given by Rule 2 of Chapter II.

CHAPTER V

SUMMARY AND CONCLUSIONS

The purpose of this study was to select a method of empirical optimization and apply it to the jar test procedure.

The Sequential Simplex Method appears to be the method best suited for use as an optimization technique in the jar test procedure when three or more variables are under study.

Even though the main purpose of the study was to select a method of empirical optimization for use as an aid in the jar test procedure, the Sequential Simplex Method is equally suited for use as an aid in any continuous optimization problem.

The main disadvantages of the technique are:

1. The method is intended as a permanent mode of operation, and not as a short-term investigational technique.

2. It is more efficient than other methods only when the number of variables is equal to or greater than three.

The main advantages of the techniques are:

1. The calculations involved are trivial, calling for no mathematical or statistical knowledge.

2. Each move is determined completely by a previous result.

3. It is easy to add an extra variable at any time.

4. It is not necessary to have a numerical measure of the response, since the technique is also valid for only ranking the responses.

5. The problem of restraints is easily dealth with.

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