$$z = f(y^1, t)$$
$$y^1 = r$$
$$y^2 = \theta \quad \text{(B1)}$$

These restrictions allow us to say

$$\text{on } C: \quad \mathbf{g}_z \cdot \mathbf{T}^{(\sigma)} \cdot \boldsymbol{\mu} = (\mathbf{g}_z \cdot \mathbf{a}_\alpha) T^{(\sigma)\alpha\beta} (\mathbf{a}_\beta \cdot \boldsymbol{\mu})$$
$$= \frac{\partial f}{\partial y^1} T^{(\sigma)11} \mu_1 \quad \text{(B2)}$$

where from Equation (6)

$$T^{(\sigma)11} = [\gamma + (\kappa - \epsilon) \operatorname{div}_{(\sigma)} \mathbf{v}^{(\sigma)}] a^{11} + 2\epsilon D^{(\sigma)11} \quad \text{(B3)}$$

Using Equation (A9), we can calculate that

$$D^{(\sigma)}_{22} = y^1 \left(v_r{}^{(\sigma)} + \frac{\partial v_\theta{}^{(\sigma)}}{\partial y^2} \right) \quad \text{(B4)}$$

The definition for the surface divergence of a vector given in Equation (A10) may alternatively be written

$$\operatorname{div}_{(\sigma)} \mathbf{v}^{(\sigma)} = tr\, \mathbf{D}^{(\sigma)}$$
$$= a^{11} D^{(\sigma)}_{11} + a^{22} D^{(\sigma)}_{22} \quad \text{(B5)}$$

We can consequently state that, because $\mathbf{v}^{(\sigma)} = 0$ at the pore wall,

$$\text{on } C: \quad \operatorname{div}_{(\sigma)} \mathbf{v}^{(\sigma)} = a^{11} D^{(\sigma)}_{11}$$
$$\operatorname{div}_{(\sigma)} \mathbf{v}^{(\sigma)} a^{11} = D^{(\sigma)11}$$

From Equation (B3), this means

$$\text{on } C: \quad \mathbf{T}^{(\sigma)11} = [\gamma + (\kappa + \epsilon) \operatorname{div}_{(\sigma)} \mathbf{v}^{(\sigma)}] a^{11} \quad \text{(B7)}$$

Let us now observe that

$$\frac{\partial f}{\partial y^1} a^{11} \mu_1 = \mu_z \quad \text{(B8)}$$

Equations (B7) and (B8) permit us to express Equation (B2) in the form of Equation (7).

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Modified One-at-a-Time Optimization

An optimization method has been developed that searches one variable at a time under the conditions that previously searched variables are at their approximate optimum and variables to be searched later are constant. This method provides the optimum and also information on the effects of the variables. The method is based on the Partan and Powell methods and on assuming linear partial derivatives of the objective function with respect to any given variable. The procedure involves searching each variable separately with other variables either constant or varied so that they remain at their estimated optimum for the given conditions. This method provides useful information on the effects of independent variables as well as locating the overall optimum and a number of partial optimums and requires a comparable number of trials.

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SCOPE

This paper reports on a study undertaken to develop and evaluate a search method of optimization that would provide information not only on the location of the optimum, but also on the effects of the individual independent variables on the objective function to be maximized or minimized. The principle of the method is to search one variable $Z_{(J=K)}$ at a time, with previously searched variables $Z_{(J<K)}$ at their estimated partial optimum for any given search point in $Z_{(J=K)}$, while variables to be searched later $Z_{(J>K)}$ are held constant. A partial optimum in this paper is taken to mean the optimum of 1 or more variables at given nonoptimum values of other variables. That is, the best value of $Z_{(1)}$ at given constant nonoptimum values of $Z_{(2)}$, $Z_{(3)}$, $Z_{(4)}$ would be a partial optimum of $Z_{(1)}$. The information obtained in this type search of 4 variables would provide the overall 4-variable optimum plus a number of 3-variable, 2-variable, and 1-variable optimums under various conditions. It would also show the effects of each variable, combined with interaction effects of that

variable, on the objective function as the variable is searched.

The technique used was based on the method of Powell (1962) described by Beveridge and Schechter (1970) and the Partan method described by Buehler et al. (1964). These methods in 2 dimensions involve searching along 2 parallel lines to determine 2 partial optimums, each the optimum along one of the parallel lines. It can be shown that searching a third line connecting the first two local optimums will locate the overall optimum, if the system is second order.

It can also be shown that with a second-order objective function the partial optimum of one or more variables will have a linear relationship with the other variables. While the Powell and Partan methods generally search in a direction related to steepest ascent methods, changing all variables simultaneously, this method attempts to keep changes to one variable at a time, under the conditions that other variables are at estimated partial optimums, or held constant. The estimated optimums are based on assuming a linear relationship between the partial optimum of each variable and the other variables. When changes are sufficiently small that a second-order equation can approximate the objective function, the method will rapidly reach the optimum.

This method was developed in order to obtain the optimum and the effects of independent variables in a single run for preliminary design evaluations and to obtain as much information about a system as possible in a single run.

CONCLUSIONS AND SIGNIFICANCE

An optimization method that searches one variable at a time but uses previous variable searches to maintain previously searched variables at their estimated optimums has been developed and tested. Each independent variable $Z_{(J=K)}$ is searched under the conditions that $Z_{(J<K)}$ are optimum. Thus in one run, the search produces a number of partial optimum points, and as $Z_{(J=K)}$ is searched, the effects of $Z_{(J=K)}$ combined with interaction effects of $Z_{(J=K)}$ and $Z_{(J<K)}$ can be obtained from the search results. In addition, of course, as the final variable is searched, the overall optimum is obtained. With the exception of dynamic programming and one-at-a-time methods, other optimization methods would require one run for each partial optimum desired or additional calculations to determine the effect of each variable.

Some of the advantages of this method are as follows:

1. It is similar to one-at-a-time optimization plus common sense utilization of previous results.
2. It is simple and based on the type of procedures used in design calculations. The principles should be easily understood by design engineers, and any problems in application should be more easily corrected.
3. It is similar to dynamic programming but is not restricted in the way dynamic programming is.
4. It is essentially the Powell or Partan method with movements restricted to one variable at a time so that the effects of each variable combined with some interactions of that variable can be observed.

Disadvantages are as follows:

1. This method has not been tested on more than 4 variables and it could be less favorable with additional variables. The method can be easily reprogrammed and tested if desired and, in any event, can be useful in preliminary design optimizations.
2. At present, the method is not programmed to handle implicit inequality constraints on dependent variables unless they can be related to independent variables. It seems probable that this could be done for most cases by testing for exceeded limits in the object program and reversing the search when limits are exceeded.

In general this method could be useful in design and control studies for finding optimum conditions, finding partial optimums for alternative and contingency conditions, and finding the sensitivity of the objective function to changes in independent variables, all from a single run and printout.

The number of trials required in this study was more than the complex and Rosenbrock methods and less than a gradient method.

SEARCH PROCEDURE

The procedure is based on assuming that a partial optimum value of one variable is a linear function of the other independent variables. If a response surface can be represented by an objective function containing first and second-order terms only in the independent variables, then the partial derivative of the objective function with respect to any given variable is first order. Solving the partial derivative set equal to 0 for the given variable will give a linear relationship with the other variables. This equation will apply whether the other variables are at their optimums or not, and thus 2 partial optimums of one variable at 2 different values of a second variable, with others held constant, will determine the relationship of the partial optimum location of the first to the second variable. In searching for an optimum of a more complicated objective function, application of these principles should lead toward the optimum but require repetition until the optimum is within a small enough region to be represented by a second order function.

This assumption permits the variables to be searched more or less one at a time, except that as the second is searched, the first is also changed to keep it at its estimated partial optimum for the value of the second. As the third variable is searched, the first two are changed to maintain both at their estimated optimums for the value of the third, etc. This allows the procedure to follow a sharp ridge rather than oscillate across it or stop on a false optimum. If it is desired to study the effect of one variable with all other variables constant, that variable should be the first variable. If it is desired to study the effect of one variable with all others at their estimated partial optimums, then that variable should be the last variable.

This method was developed for maximizing the return on investment in a 4-variable plant design problem, and for this reason the objective function is termed *ROI*, and the problem will be considered to be maximization. The independent variables were termed as $Z_{(1)}$ through $Z_{(4)}$

varying from 0 to 1.0. Four independent process variables can be equated to functions of $Z_{(1)}$ through $Z_{(4)}$, according to the expected range of the variables and the inequality constraints. For example, a process variable P_{V1} can be related to $Z_{(1)}$ by $P_{V1} = P_{V\min} + Z_{(1)} (P_{V\max} - P_{V\min})$, where $P_{V\max}$ and $P_{V\min}$ are maximum and minimum expected or allowed values of the process variable and can be a function of other variables previously defined or calculated.

In this method the first variable $Z_{(1)}$ is searched, with the other variables $Z_{(2)}$, $Z_{(3)}$, and $Z_{(4)}$ held constant. If $Z_{(J)I}$ represents the value of the variable $Z_{(J)}$ at the Ith trial level of $Z_{(J)}$, then the starting point is $Z_{(1)1}$, $Z_{(2)1}$, $Z_{(3)1}$, $Z_{(4)1}$. If $Z_{(1)}$ is searched with the other variables constant until *ROI* is a maximum we have the point $Z_{(1)m}$, $Z_{(2)1}$, $Z_{(3)1}$, $Z_{(4)1}$ where m represents the level of $Z_{(1)}$ giving the maximum *ROI* as shown in Figure 1, at point (a).

The second variable is searched with $Z_{(3)}$ and $Z_{(4)}$ constant, but with $Z_{(1)}$ at the optimum or the estimated optimum for each value of $Z_{(2)}$ searched. Thus for each value of $Z_{(2)}$, $Z_{(1)}$ must be searched for the optimum or the optimum must be estimated. In Figure 1, $Z_{(2)}$ is changed to $Z_{(2)2}$ and a second search of $Z_{(1)}$ is made, starting at $Z_{(1)m}$ from point (a), until a new optimum $Z_{(1)}$ is found, $Z_{(1)m(b)}$, $Z_{(2)2}$, $Z_{(3)1}$, and $Z_{(4)1}$. After this search, the optimum $Z_{(1)}$ can be estimated for any value of $Z_{(2)}$ if a linear relationship between $Z_{(1)m}$ and $Z_{(2)}$ is assumed. If

$$R_1 = \frac{Z_{(1)m(b)} - Z_{(1)m(a)}}{Z_{(2)2} - Z_{(2)1}}$$

then

$$Z_{(1)m(n)\text{est.}} = Z_{(1)m(n-1)} + R_1(Z_{(2)(n)} - Z_{(2)(n-1)})$$

After R_1 is determined, $Z_{(2)}$ can be searched further with $Z_{(1)m}$ estimated at each point until a $Z_{(2)}$ is found giving maximum *ROI*, at point (c) in Figure 1, with $Z_{(1)m}$, $Z_{(2)m}$, $Z_{(3)1}$, $Z_{(4)1}$.

The search for optimum $Z_{(2)}$ is not, strictly speaking, one variable at a time since $Z_{(1)}$ may be changing also, possibly by a considerable amount. However, at each value of $Z_{(2)}$, the estimated best value of the objective function (with $Z_{(1)}$ at a partial optimum) is obtained for that $Z_{(2)}$ at constant $Z_{(3)}$ and $Z_{(4)}$. Thus the results would show the effect of changes in $Z_{(2)}$ on the objective function optimized with respect to $Z_{(1)}$, but with $Z_{(3)}$ and $Z_{(4)}$ constant. In some cases these effects might be more important than the effects of $Z_{(2)}$ with $Z_{(1)}$, $Z_{(3)}$, and $Z_{(4)}$ constant as in a true one-at-a-time search.

At this point, $Z_{(3)}$ is changed to $Z_{(3)2}$ and the entire procedure shown in Figure 1 is repeated to obtain point d in Figure 2. Then the following calculations are possible:

$$R_1 = \frac{Z_{(1)m(d)} - Z_{(1)m(c)}}{Z_{(3)2} - Z_{(3)1}}$$

$$R_2 = \frac{Z_{(2)m(d)} - Z_{(2)m(c)}}{Z_{(3)2} - Z_{(3)1}}$$

$$Z_{(1)m(n)} = Z_{(1)m(n-1)} + R_1(Z_{(3)(n)} - Z_{(3)(n-1)})$$

$$Z_{(2)m(n)} = Z_{(2)m(n-1)} + R_2(Z_{(3)(n)} - Z_{(3)(n-1)})$$

$Z_{(3)}$ can then be searched for its optimum, with $Z_{(1)}$ and $Z_{(2)}$ at estimated optimums and $Z_{(4)}$ constant, as shown in Figure 2 as point (e), $Z_{(1)m(e)}$, $Z_{(2)m(e)}$, $Z_{(3)m(e)}$, $Z_{(4)1}$.

After point (e) is found, $Z_{(4)}$ can be changed to $Z_{(4)2}$ and the entire procedure in Figures 1 and 2 can be repeated to find optimum $Z_{(1)}$, $Z_{(2)}$, and $Z_{(3)}$ at $Z_{(4)2}$ which is point (f) in Figure 3. At this point R_1, R_2, and

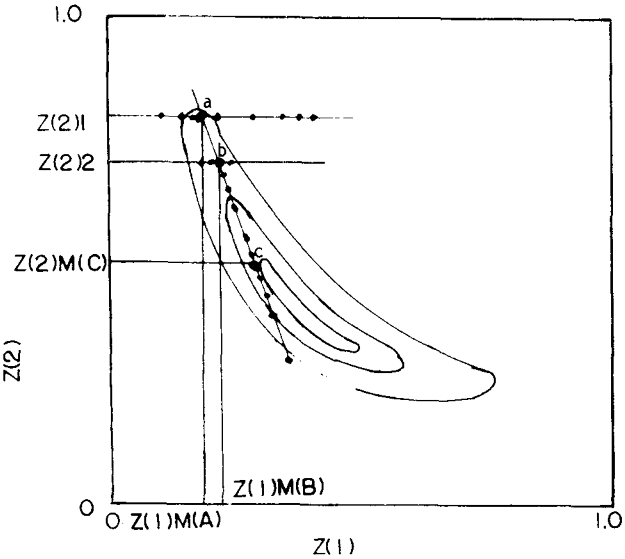

Fig. 1. Search in $Z_{(1)}$ and $Z_{(2)}$ with $Z_{(3)}$ and $Z_{(4)}$ constant.

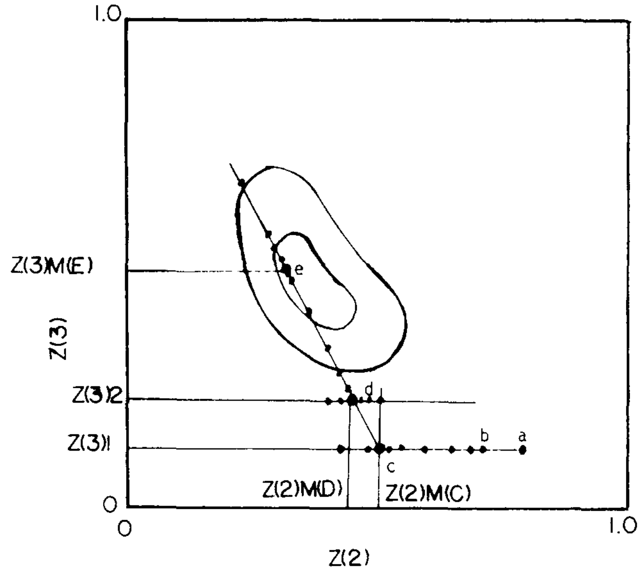

Fig. 2. Search in $Z_{(2)}$ and $Z_{(3)}$ with $Z_{(1)}$ at estimated optimum and $Z_{(4)}$ constant.

R_3 can be calculated as previously, and optimum $Z_{(1)}$, $Z_{(2)}$, and $Z_{(3)}$ can be estimated at any value of $Z_{(4)}$. Searching $Z_{(4)}$ with other variables optimized leads to an approximate overall optimum in four variables, point (g) in Figure 3. Since this point is based on a number of assumptions of linearity, it can be checked by repeating the entire procedure.

The search method used in each direction was first open-ended starting with small steps, with the step length 1.62 times the previous step after each successful step. If the first step produces a decrease in *ROI*, the direction is reversed, but after the first step, a decrease in *ROI* indicates the optimum has been passed and a closed-end search is initiated between the 2 points on each side of the maximum by the Golden Section or Modified Fibonacci technique described by Wilde (1964) and Beveridge and Schechter (1970). When an upper or lower limit is reached, $Z_{(J)} < .001$ or $Z_{(J)} > .999$, a closed-end procedure is also initiated.

On searching the 2d, 3d, and 4th variables, the first change in values of the variables is 10 times the small initial step size so that more accuracy can be obtained in determining the ratios of the optimums of previous variables to the change in the variable searched. The open-end search begins from that one of the first two points which produces the highest *ROI*.

Each search in each direction ends when the range of the optimum is reduced to approximately 2 times the desired accuracy, *ACC*. When each overall optimum is reached, it is compared with the previous overall optimum, and the entire search is repeated if any variable is more than 3 times the desired accuracy from the previous overall optimum.

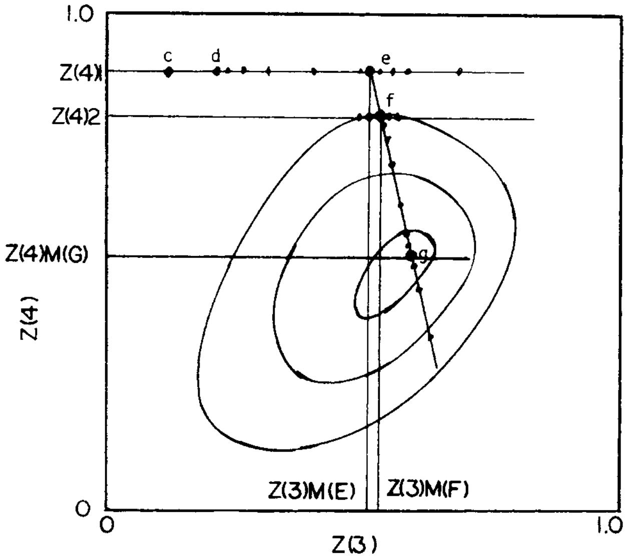

Fig. 3. Search in $Z_{(3)}$ and $Z_{(4)}$ with $Z_{(2)}$ and $Z_{(1)}$ at estimated optimums.

TESTING AND EVALUATION

Williams-Otto Plant Optimization

The procedure was tested primarily by using the Williams-Otto plant problem (Williams and Otto, 1960) with equations as presented by Adelman and Stevens (1972). This problem has four independent variables to optimize, and Christensen (1970) has presented a method of straightforward solution of the 8 basic equations. The solution used in this study is shown in Table 1. The first four equations use the optimization variables $Z_{(1)}$ through $Z_{(4)}$ to establish the four independent process variables T, F_{RE}, F_{RC} and $PHI = F_D/(F_R - F_P - F_G)$. As shown by Mason (1971), the response surface for this system has a sharp curved ridge near the nonfeasible region and is also bimodal in at least the two variables F_{RE} and PHI. Since this search procedure and most others are based on a unimodal surface, some consideration should be given to problems due to bimodality in comparing search techniques.

Runs 1 and 2 in Table 2 give results of optimizing from the best and worst of Adelman and Stevens' starting points in a Complex optimization method.

Runs 3 and 5 combined are a 3-variable optimization at constant $Z_{(4)}$, followed by a 4-variable optimization starting from the 3-variable optimum. The number of trials is less than the equivalent 4-variable optimization, run 4, but due to bimodality which misled both searches, the results only indicate the 2-step procedure is comparable in number of trails to the 4-variable search.

Adelman and Stevens used F_R as an independent variable which requires much more complicated calculation of the objective function than using PHI as in the program in Table 1. For this reason the comparison of trials with their Complex optimization is not appropriate for runs 1 through 5. Equation (3) in Table 1 was changed as shown in Table 1 for runs 6 through 13. This change makes $Z_{(3)}$ approximately proportional to F_R even though it de-

TABLE 1. EQUATIONS USED FOR WILLIAMS-OTTO PLANT SOLUTION

Runs 1-5

1. T=Z(4)*100.+580.
2. FRC=Z(2)*20000.
3. PHI=Z(3)
4. FRE=(Z(1)*2.+1.)*11910./PHI
5. X2=PHI*FRE*.5
6. FRP=.1*FRE+4763.
7. X3=(X2−PHI*(FRP−4763.)−4763.)*2.
8. X1=(PHI*FRC+X3)/2.+X2
9. ZK1=.59755E10*EXP(−12000./T)
10. ZK2=.25962E13*EXP(−15000./T)
11. ZK3=.96283E16*EXP(−20000./T)
12. VF=X3/(ZK3*FRP*FRC*50.)
13. FRB=X2/(ZK2*FRC*VF*50.)
14. FRA=X1/(ZK1*FRB*VF*50.)
15. FG=300.*X3/200.
16. FR=FRA+FRB+FRC+FRE+FG+FRP
17. FB=X1+PHI*FRB+X2
18. FA=X1+PHI*FRA
19. V=VF*FR**2.
20. FD=PHI*(FR-4763.−FG)
21. SALE=1955.52*4763.

Other runs if different

1. Run 14 T=Z(3)*100.+580.
3. Run 6-13 PHI=25000/(475000*Z(3)+25000)
3. Run 14 PHI=25000./(475000.*Z(4)+25000.)

Return on investment equations

Adelman and Stevens (A&S)
ROI=(84.*FA-201.96*FD−336.*FG+SALE−2.22*FR−V*3000.)/300./V
Sriram and Stevens (S&S)
DIV=150.*V+.13*FR
ROI=(84.*FA−201.9629*FD−336.*FG+SALE−3.52*FR−1500.*V)/DIV

fines *PHI* and makes the search more comparable to Adelman and Stevens' search.

In runs 6 and 7 the number of iterations required is considerably less than runs 1 and 2 and these runs require only about twice the number of iterations required by Adelman and Stevens and have the advantage of more usable information on the effects of variables.

In run 8, the effect of requiring higher accuracy (*ACC* = 0.005) decreased the number of trials compared to run 7. This was probably due to better accuracy in locating partial maximums and the following better estimated maximums in succeeding trials. Normally this would be true only for fairly sharp ridges, and higher accuracy would require more trials.

Runs 9, 10, and 11 compare results with those of Sriram and Stevens' (1972) who used a gradient search method and a different *ROI*. In all three runs fewer iterations were required by this method, but more importantly, the nonoptimum information is more usable with this method than with a gradient method.

In order to show what type of information can be obtained in addition to the optimum, runs 12, 13, and 14 were made, again using the same equations as runs 6 through 8. Run 12 was used to plot 7 points in Figure 4 from the printout of the optimization, with points given in Table 3. Four of these points allow a line to be plotted which locates the optimum $Z_{(3)}$ for a given $Z_{(4)}$ when $Z_{(1)}$ and $Z_{(2)}$ are at estimated optimums for the given $Z_{(3)}$ and $Z_{(4)}$. From the printout, optimums for $Z_{(2)}$ and $Z_{(1)}$ would also be available at these values of $Z_{(4)}$. To determine

TABLE 2. OPTIMIZATION OF WILLIAMS-OTTO PLANT

Run No.	Remarks	ROI	Starting point	Optimum ROI	Optimum Z(1)	Optimum Z(2)	Optimum Z(3)	Optimum Z(4)	Optimum PHI	Optimum $F_R/10^5$	No. trials	Comparison trials
1	PHI = Z(3)	A&S	A&S #1	120.9	0.108	0.434	0.093	0.942	0.093	0.398	343	A&S = 124
2	PHI = Z(3)	A&S	A&S #2	121.4	0.114	0.374	0.104	0.953	0.104	0.358	326	A&S = 124
3	PHI = Z(3) OPT. 3 VAR., Z(4) = CONSTANT	A&S	ALL Z = 0.5	68.5	0.075	0.617	0.112	0.5	0.112	0.314	218*	—
4	PHI = Z(3)	A&S	ALL Z = 0.5	121.2	0.115	0.373	0.105	0.95	0.105	0.353	474*	—
5	PHI = Z(3)	A&S	OPT. RUN 3	121.5	0.111	0.388	0.099	0.956	0.099	0.373	159	
3 + 5	PHI = Z(3)	A&S	ALL Z = 0.5	121.5	0.111	0.388	0.099	0.956	0.099	0.373	377*	Run 4 = 474
6	$PHI = \frac{25000}{475000Z(3) + 25000}$	A&S	A&S #1	121.4	0.115	0.385	0.473	0.957	0.103	0.369	188	A&S = 124
7	$PHI = \frac{25000}{475000Z(3) + 25000}$	A&S	A&S #2	121.2	0.108	0.395	0.477	0.952	0.099	0.376	246	A&S = 124
8	$PHI = \frac{25000}{475000Z(3) + 25000}$ ACC = .005	A&S	A&S #2	121.5	0.113	0.392	0.472	0.953	0.100	0.370	204	A&S = 124
9	$PHI = \frac{25000}{475000Z(3) + 25000}$	S&S	S&S #1	50.8	0.105	0.175	0.161	0.546	0.246	0.145	269	S&S = 313
10	$PHI = \frac{25000}{475000Z(3) + 25000}$	S&S	S&S #2	50.8	0.108	0.177	0.166	0.545	0.241	0.146	206	S&S = 332
11	$PHI = \frac{25000}{475000Z(3) + 25000}$	S&S	S&S #3	50.8	0.105	0.171	0.163	0.547	0.244	0.145	139	S&S = 236
12	$PHI = \frac{25000}{475000Z(3) + 25000}$	A&S	ALL Z = 0.75	121.3	0.109	0.409	0.481	0.946	0.099	0.378	199	—
13	$PHI = \frac{25000}{475000Z(3) + 25000}$	A&S	ALL Z = 0.25	121.5	0.111	0.398	0.474	0.951	0.100	0.372	204	—
14	$PHI = \frac{25000}{475000Z(3) + 25000}$ Z(3), Z(4) reversed	A&S	ALL Z = 0.75	121.4	0.109	0.394	0.951	0.477	0.099	0.375	203	—

ACC = 0.01 in all runs except run 8.

Starting points	Z(1)	Z(2)	Z(3)	Z(4)
Run 6-14 A&S #1	0.01	0.16	0.27	0.76
Run 6-14 A&S #2	0.01	0.1	0.38	0.42
Run 6-14 S&S #1	0.01	0.9	0.66	0.08
Run 6-14 S&S #2	0.1	0.75	0.99	0.95
Run 6-14 S&S #3	0.01	0.34	0.33	0.46
Run 1-5 A&S #1	0.01	0.16	0.07	0.76
Run 1-5 A&S #2	0.01	0.1	0.05	0.42

* Number of trials increased significantly due to bimodality.

TABLE 3A. DATA USED TO PLOT CONTOURS FROM RUN 12 IN FIGURE 4

$Z_{(1)}$ and $Z_{(2)}$ at Estimated Partial Optimums
$T = f_1(Z_{(4)}), PHI = f_2(Z_{(3)})$

Point no.	Description	Z(3)	Z(4)	ROI	Symbol Figure 5
1	Overall Opt.	0.481	0.946	121.34	○
2	Opt. Z(3) for Z(4) = 0.864	0.467	0.864	117.99	○
3	Opt. Z(3) for Z(4) = 0.939	0.480	0.939	121.30	○
4	Opt. Z(3) for Z(4) = 0.856	0.464	0.856	117.50	○
5	Opt. Z(3) for Z(4) = 0.570	0.424	0.570	79.58	○
6	Other conditions	0.562	0.939	119.52	○
7	Other conditions	0.530	0.864	117.04	○
8	Calc. Z(3) at Z(4) = 0.939 at ROI = 120	0.550	0.939	120	•
8A	Calc. Z(3) at Z(4) = 0.939 at ROI = 120	0.410	0.939	120	•*
9	Calc. Z(3) at Z(4) = 0.939 at ROI = 118	0.591	0.939	118	•
9A	Calc. Z(3) at Z(4) = 0.939 at ROI = 118	0.369	0.939	118	•*
10	Calc. Z(4) along Opt. Z(3) at ROI = 120	see figure	0.894	120	•

Table 3b. Data Used to Check Contours in Figure 4 from Run 14

$Z_{(1)}$ and $Z_{(2)}$ at Estimated Partial Optimums
$T = f_1(Z_{(3)})$, $PHI = f_2(Z_{(4)})$

Point no.	Description	Z(4)	Z(3)	ROI	Symbol Figure 5
11	Overall Opt.	0.477	0.951	121.37	▽
12	Opt. Z(3) for Z(4) = 0.540	0.540	0.955	120.40	▽
13	Opt. Z(3) for Z(4) = 0.465	0.465	0.950	121.31	▽
14	Opt. Z(3) for Z(4) = 0.448	0.448	0.948	121.31	▽
15	Opt. Z(3) for Z(4) = 0.523	0.523	0.957	120.59	▽
16	Other conditions	0.540	0.900	119.06	▽
17	Other conditions	0.448	0.907	120.41	▽
18	Calc. Z(3) at Z(4) = 0.540 at ROI = 120	0.540	0.925	120	▼
19	Calc. Z(3) at Z(4) = 0.448 at ROI = 120	0.448	0.898	120	▼
20	Calc. Z(3) at Z(4) = 0.540 at ROI = 118	0.540	0.881	118	▼
21	Calc. Z(3) at Z(4) = 0.448 at ROI = 118	0.448	0.870	118	▼
22	Calc. Z(4) along Opt. Z(3) + direction at ROI = 120	0.552	See fig.	120	▼
23	Calc. Z(4) along Opt. Z(3) + direction at ROI = 118	0.594	See fig.	118	▼
24	Calc. Z(4) along Opt. Z(3) − direction at ROI = 120	0.339	See fig.	120	▼*
25	Calc. Z(4) along Opt. Z(3) − direction at ROI = 118	0.260	See fig.	118	▼*

partial optimums such as given in points 2, 3, 4, and 5 at four different values of $Z_{(4)}$ as well as the overall optimum would require 5 different runs using optimization techniques that do not move one variable at a time. Points 1, 2, 3, 4, and 5 permit determination of the effect of $Z_{(4)}$ with $Z_{(1)}$ through $Z_{(3)}$ optimized for the given $Z_{(4)}$. Part of these effects may be due to changes in $Z_{(1)}$ through $Z_{(3)}$, but the changes will be either effects of $Z_{(4)}$ or interaction effects of $Z_{(4)}$ with other independent variables. The points do represent the best values that can be obtained at the various values of $Z_{(4)}$. Such data will permit the rapid estimation of optimums of $Z_{(1)}$ through $Z_{(3)}$ if for some reason (process troubles, material changes, other contingencies) $Z_{(4)}$ must be at a nonoptimum value.

Inherent in the procedure and printout* are points such as 1 through 7 in Table 3 and Figure 4, and these can be used to estimate points on an *ROI* contour line, at least in one quadrant. However, a linear extrapolation is not appropriate since the partial of *ROI* with respect to $Z_{(3)}$ must change. A second-order extrapolation or interpolation, $\Delta ROI = K\Delta[Z_{(3)} - Z_{(3)M}]^2$ is more appropriate and points 8 and 9 were calculated this way at $ROI = 120$ and $ROI = 118$.

A similar relationship applies to $Z_{(4)}$ along the optimum $Z_{(3)}$ line, and $Z_{(4)}$ corresponding to $ROI = 120$ was calculated as point 10. Point 2 is close enough to 118 to be used directly for a 118 contour. From points 2, 8, 9, and 10, plus the fact that the contour at points 2 and 10 will be parallel to the $Z_{(3)}$ axis, the contour lines can be estimated reasonably well for approximately ¼ of their circumference. If it is assumed that the slopes are similar on both sides of the optimum, a complete contour could be drawn, but this is very questionable in a complicated system. In Figure 4, this assumption is applied and points 8A, and 9A are used to estimate the contours on the left side of the graph.

In run 14, $Z_{(3)}$ and $Z_{(4)}$ were exchanged in the objective function system so that a different approach would occur, and points 11 through 25 were obtained and plotted

* Supplementary material may be obtained by writing to the author.

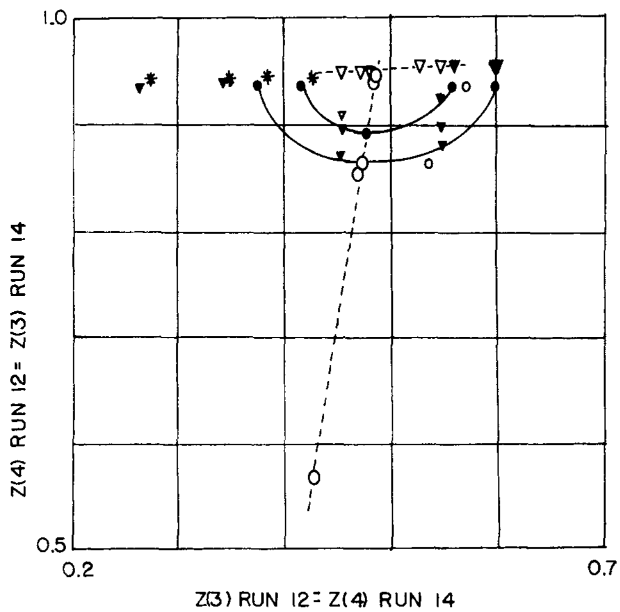

Fig. 4. Response surface from Run 12 in $Z_{(3)}$ and $Z_{(4)}$ with $Z_{(1)}$ and $Z_{(2)}$ at estimated partial optimums, and similar points from Run 14: ——— contour lines; ------ optimum $Z_{(3)}$ at given $Z_{(4)}$;* extensive extrapolation.

in the same way as in run 12 except that the directions are at right angles. Contour lines were not plotted from run 14, but comparing values in Table 3 with the locations in Figure 4 it can be seen that all the points correspond reasonably well with the estimated contours, except points 24 and 25 and 8A and 9A, all of which involved extensive extrapolation. Similar plots could be made of $Z_{(3)}$ vs. $Z_{(2)}$ and $Z_{(2)}$ vs. $Z_{(1)}$.

Optimization of Other Functions

This method was applied to two other functions for testing and evaluation, a 2-variable function used by Rosenbrock (1960), and a 4-variable function similar to the Rosenbrock function. The Rosenbrock function is a

TABLE 4. OPTIMIZATION OF ROSENBROCK FUNCTION AND 4-VARIABLE ROSENBROCK TYPE FUNCTION

Rosenbrock function $ROI = -Y = -100(X_1^2 - X_2^2)^2 - (X_1 - 1)^2$

4-Variable Rosenbrock-Type function $ROI = -Y = -100(X_1^2 = X_2^2)^2 - (X_1 - 1)^2 - 20(X_3^2 - X_1^2)^2 - (X_4 - 1)^2$

Run	Object func.	Start point	ROI	Z(1)	Optimum Z(2)	Z(3)	Z(4)	No. trials	Comparison
15	Rosenbrock $X_1 = -2 + 4Z(1)$	$Z(1) = 0.2, X_1 = -1.2$							Rosenbrock 200
	ACC = 0.001 $X_2 = -2 + 4Z(2)$	$Z(2) = 0.75, X_2 = 1$	−0.001	0.744	0.256	—	—	127	more accurate
	Exact solution		0	0.75	0.25 or 0.75				
16	Rosenbrock $X_1 = -2 + 4Z(1)$	$Z(1) = 0.2, X_1 = -1.2$							Rosenbrock 200
	ACC = 0.001 $X_2 = 4Z(2)$	$Z(2) = 0.25, X_2 = 1$	0.000	0.755	0.255	—	—	243	more accurate
	Exact solution		0	0.75	0.25				
17	Same as 16								Rosenbrock 200
	ACC = 0.0005		0.000	0.751	0.252	—	—	260	same accuracy
18	4-Var. Rosenbrock	$Z(1) = Z(3) = 0.25$	0.000	0.508	0.507	0.508	0.498	290	
	$X_1 = 2Z(1)$ $X_2 = 2Z(2)$	$Z(2) = Z(4) = 0.75$							
	$X_3 = 2Z(3)$ $X_4 = 2Z(4)$	Exact solution	0	0.5	0.5	0.5	0.5		
19	4-Var. Rosenbrock								
	$X_1 = 2Z(4)$ $X_2 = 2Z(2)$	$Z(1) = Z(2) = 0.75$	−0.001	0.501	0.493	0.494	0.494	261	
	$X_3 = 2Z(3)$ $X_4 = 2Z(1)$	$Z(3) = Z(4) = 0.25$							
20	4-Var. Rosenbrock								
	$X_1 = 2Z(4)$ $X_2 = 2Z(3)$	$Z(1) = Z(3) = 0.75$	0.000	0.495	0.495	0.495	0.501	258	
	$X_3 = 2Z(2)$ $X_4 = 2Z(1)$	$Z(2) = Z(4) = 0.25$							

sharp ridge following two parabolas symmetrical about the x_1 axis, through the 0,0 point with a minimum of 0 at $x_1 = 1$, $x_2 = 1$ or $x_1 = 1$, $x_2 = -1$. The ridge is very sharp and it was found that accuracy limits had to be small to locate the ridge sufficiently for this method to be consistent. The Rosenbrock function and the 4-variable Rosenbrock type function are given in Table 4.

The starting point used by Rosenbrock is the $x_1 = -1.2$, $x_2 = 1$ point. To follow the ridge to the optimum, the search must proceed down the parabola approximately to $x_1 = x_2 = 0$, then up the parabola to $x_1 = x_2 = 1.0$, or down the mirror image parabola to $x_1 = 1$, $x_2 = -1$.

Run number 15 shows that if x_2 can be negative, the search using this method, with $ROI = -y$, proceeds to the 1, −1 point in 127 iterations. However, Rosenbrock's method located the optimum at 1,1 so the relation of x_2 to $Z_{(2)}$ was changed to eliminate negative x_2 values in run number 16. In this run the search proceeded to near 0,0 and then up to 1,1 in 243 iterations. Rosenbrock's method located the optimum more accurately in 200 iterations. Thus this function can be adequately optimized without an excessive number of iterations. If desired, it could provide additional information on the effect of the variables.

Table 4 shows that the actual accuracy of this method is not equal to the desired accuracy *ACC* used in the program. Thus *ACC* should only be considered as approximately the desired accuracy and should be programmed somewhat smaller than desired.

A 4-variable function similar to Rosenbrock's was used to test the effect of interaction among variables. As can be seen by inspection x_1 and x_2 are highly interacting, while x_1 and x_3 moderately interact, and there is no interaction between x_4 and other variables.

Runs number 18, 19, and 20 show the effects of changing the order in which the variables are optimized. By inspection, there appears to be a slight benefit in associating the initially optimized variables with the least interactive process variables. It should be noted that although this 4-variable optimization required only a few more iterations than the 2-variable optimization, the difference in starting points makes comparison invalid.

This program has been used successfully by senior classes for optimizing a 3-variable vapor recompression evaporator and a 2-variable recovery heat exchanger, and 4 variables of the 1967 AIChE contest problem.

NOTATION

ACC = accuracy limits for partial optimum location

$F_A, F_B, F_D, F_G, F_R, F_{RA}, F_{RB}, F_{RC}, F_{RE}, F_{RP}, PHI, SALE, T, V, V_F, Z_{K1}, Z_{K2}, Z_{K3}$ = variables in Williams-Otto plant calculation, four of which are independent

K = constant

P_V = independent process variable

R_J = ratio of a change in $Z_{(J)m}$ to the change in another variable

ROI = return on investment, objective function to be maximized, or -objective function to be minimized

x_1, x_2 = dependent variables in Williams-Otto plant and independent variables in Rosenbrock function

x_3 = dependent variable in Williams-Otto plant and independent variable in 4-variable Rosenbrock type function

x_4 = independent variable in 4-variable Rosenbrock type function

$Z_{(J)}$ = independent variable number j, limited to a range of 0 to 1.0, used to define independent process or objective function variables

$Z_{(J)m}$ = optimum value of $Z(j)$ under certain conditions

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