λ = exponent in Equation (12), dimensions meaningless
μ = viscosity, lb.$_m$/(ft.)(sec.)
ρ = density of liquid, lb.$_m$/cu. ft.
ρ_s = true density of solid, lb.$_m$/cu. ft.
ρ_x = $\rho\epsilon_x + \rho_s(1 - \epsilon_x)$, lb.$_m$/cu. ft.
σ_r = stress in radial direction, lb.$_f$/cu. ft.
σ_z = stress in vertical direction, same as p_z, lb.$_f$/sq. ft.
τ_{rz} = frictional shearing force at wall, lb.$_f$/sq. ft.
ψ_x = pressure, lb.$_f$/sq. in.

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Process Optimization by the "Complex" Method

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The "complex" method of M. J. Box has been adapted and used to optimize the design of continuous chemical processes. Such a design involves the extremization of a nonlinear objective function subject to nonlinear equality and inequality constraints. The method consists of finding an original feasible "complex" of solutions, eliminating the worst of these by reflection through the centroid of those remaining, and repeating until an optimum has been reached. An example of significant complexity has been solved and the results are reported. The method looks quite promising for use in the optimization of chemical process designs.

Most problems in chemical engineering design and plant operation have at least several, and possibly an infinite, number of solutions. Selecting the "best" answer to such a problem out of the multiplicity of possible solutions is certainly not a new concept to chemical engineers, but it is rapidly becoming an extremely important part of chemical engineering practice. With the advent of high speed digital computers and sophisticated mathematical techniques for the calculation of optimum conditions, it is now important not only to optimize the objective function, but also to optimize the optimization procedure. In other words, it is desired to find the optimum conditions in the most efficient manner. For this optimization to be done analytically, a mathematical model of the system to be optimized must be known, including the objective function to be extremized plus all of the constraints on the system.

The nonlinear optimization of a complex chemical plant design can be represented mathematically as follows

Maximize

$$F(X_1, X_2, \ldots, X_n) \tag{1}$$

Subject to

$$G_i(X_1, X_2, \ldots, X_k) = 0 \qquad i = 1, 2, \ldots, m \tag{2}$$

$$L_j \leq X_j \leq U_j \qquad j = 1, 2, \ldots, k \tag{3}$$

$F(X_1, X_2, \ldots, X_n)$ is the objective function to be extremized, and is in general a nonlinear function of the n independent variables. $G_i(X_1, X_2, \ldots, X_k)$ are the m equality

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constraints, and are in general nonlinear functions of the independent variables $X_1, X_2, \ldots, X_n$ and the dependent variables $X_{n+1}, X_{n+2}, \ldots, X_k$ (where $X_{n+1}, X_{n+2}, \ldots, X_k$ are functions of the independent variables). The equality sign can also be $\leq$ or $\geq$ for some or all of the m relations. L_j and U_j are the lower and upper limits on the variable X_j, and these limits can be constants or functions of the independent variables.

Although many excellent optimization techniques have been developed and reported in the literature, little has been published on the results of the application of a particular method to a chemical engineering design problem of the size and scope encountered in actual practice. The present paper is an attempt to remedy this defect. A particular optimization method has been selected—the "complex" method of M. J. Box—and the results of its application to chemical process design optimization is summarized and evaluated.

DESCRIPTION OF THE "COMPLEX" METHOD

The "complex" (*constrained simplex*) method was developed by M. J. Box (2) from the simplex method of Spendley, Hext, and Himsworth (5). Essentially, the simplex method is a rudimentary steep ascent procedure, in which a sequence of experimental designs each in the form of a regular simplex is used. (The convex hull of $m + 1$ points is called an m-dimensional simplex.) The direction of steepest ascent is estimated from observations at the vertices of a regular simplex and proceeds from the center of the simplex out through that face which is opposite to (does not contain) the point corresponding to the lowest observation. Thus, the optimization procedure is to continually move into the adjacent regular simplex obtained by discarding the point of the current simplex corresponding to the lowest observation and replacing it by its mirror image in the plane (hyperplane) of the remaining points.

Box used this principle and his desire to solve problems with constraints to devise a new method for finding the maximum of a general nonlinear function of several variables with a constrained region. A constrained optimum is defined as one for which the solution involves certain variables lying at the edges of their permissible ranges, since if this is not so, a method with no provision for bounding the variables will produce the same result.

The "complex" method searches for the maximum (to find a minimum, the negative of the objective function is maximized) value of an objective function

$$f(X_1, \ldots, X_n) \tag{4}$$

where $X_1, \ldots, X_n$ are the independent variables, subject to m constraints of the form

$$g_k \leq X_k \leq h_k \qquad k = 1, \ldots, m \tag{5}$$

where $X_{n+1}, \ldots, X_m$ are functions of the independent variables $X_1, \ldots, X_n$ and the upper and lower constraints h_k and g_k are either constants or functions of the independent variables. It is important to note that in developing his method, Box considered only inequality constraints, as did Umeda (6) in a recent example application.

Box proposed that k points be used to develop the original complex, where $k \geq n + 1$ (n is the number of independent variables). The k points required are obtained one at a time by the use of random numbers and ranges for each of the independent variables, by means of

$$X_i = g_i + r_i\,(h_i - g_i) \tag{6}$$

where r_i is a random number on the interval (0, 1). A point so calculated must satisfy the explicit constraints (constraints on the independent variables), but it need not satisfy all the implicit constraints (constraints on the dependent variables). If an implicit constraint is violated, the trial point is moved half-way toward the centroid of those points already selected, including the point which violated the constraint.

Wilde (7) defines the centroid of a region as

$$\bar{X}_i = \frac{\int_a^b X_i A_i(X_i)\,dX_i}{\int_a^b A(X_i)\,dX_i} \tag{7}$$

where $\bar{X}_i$ is the coordinate of the centroid, a and b are the lower and upper limits of the variable X_i, and $A(X_i)$ is the cross-sectional hyperarea of the intersection of the experimental region with the hyperplane on which X_i is constant. However, for ease of computation, the present authors used a centroid which was defined as the point each of whose coordinates is the numerical average of the corresponding coordinates of the points in the complex, given by

$$\bar{X}_j = (1/k) \left[\sum_{i=1}^{k} \right] X_{ij} \tag{8}$$

where i refers to the point and j refers to the coordinate.

The objective function is evaluated at each point in the complex, and the point of least function value is replaced by a point α (≥ 1) times as far from the centroid of the remaining points as the reflection of the worst point in the complex, the new point being collinear with the rejected point and the centroid of the retained points. This is done by means of the formula

$$X_{kj}\ (\text{new}) = \bar{X}_j + \alpha(\bar{X}_j - X_{kj}\ (\text{old})) \tag{9}$$

where α is the reflection factor (≥ 1), $\bar{X}_j$ is the j^{th} coordinate of the centroid, X_{kj} (old) is the j^{th} coordinate of the worst point in the complex, point k, and X_{kj} (new) is the j^{th} coordinate of the replacement for the worst point in the complex. If this new trial point, replacing the previous worst point, is again the worst (where worst means the point with the smallest objective function value), it is moved half-way toward the centroid of the remaining points to give a new trial value.

If a trial point does not satisfy some constraint on an independent variable, that variable is reset to a value equal to the constraint. If an implicit constraint is violated, the trial point is moved half-way toward the centroid of the remaining points. Ultimately a permissible point is found, and so long as the entire complex has not collapsed into the centroid, progress will continue.

CHEMICAL PROCESS EXAMPLE

The particular process design optimization problem which has been used for testing the actual use of the "complex" method is the one originally proposed by Williams and Otto (8). The process to be optimized includes many of the effects present in chemical manufacturing plants—such as reaction, heat exchange, multiple separations, recycle, etc.—and thus is realistic enough so that steady state optimization has real meaning.

The plant under consideration is to manufacture 40 million lb./yr of a chemical product P. Figure 1 gives a block diagram of the entire plant, consisting of a perfectly

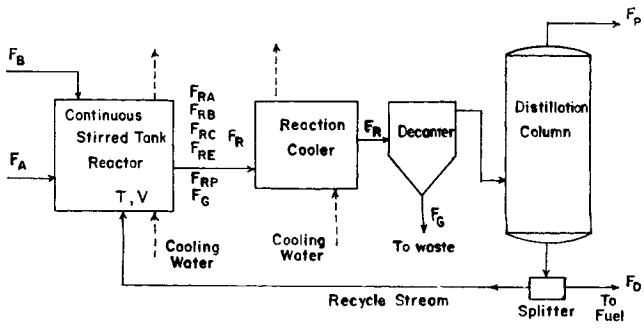

Fig. 1. Block diagram of Williams plant.

stirred reactor, a heat exchanger, a decanter, and a distillation column in series, with recycle from the column reboiler back to the reactor. P is produced by or takes part in the following three second-order irreversible reactions:

$$A + B \rightarrow C \quad \text{reaction coefficient, } k_1 \qquad (10)$$

$$C + B \rightarrow P + E \quad \text{reaction coefficient, } k_2 \qquad (11)$$

$$P + C \rightarrow G \quad \text{reaction coefficient, } k_3 \qquad (12)$$

The initial reactants A and B are fed separately to the reactor in pure form. Components C and E are intermediates and/or by-products of the reaction. They have no sale value but can be disposed of as plant fuel. By-product G is a heavy, oily tar which must be disposed of as a waste material.

The reaction coefficients can be expressed in the Arrhenius form

$$k_i = A_i e^{-B_i/T} \qquad (13)$$

where: $A_1 = 5.9755 \times 10^9$ hr.$^{-1}$, weight fraction
$B_1 = 12{,}000$°R., based on 1 lb. of A or B
$A_2 = 2.5962 \times 10^{12}$ hr.$^{-1}$, weight fraction
$B_2 = 15{,}000$°R., based on 1 lb. of B
$A_3 = 9.6283 \times 10^{15}$ hr.$^{-1}$, weight fraction
$B_3 = 20{,}000$°R., based on 1 lb. of C
T = temperature (variable), °R.

In addition, it has been found that the rate of reaction is negligible below 120°F. and that substantial decomposition occurs above 220°F., so that the reactor temperature T is limited between 120° and 220°F. (580° and 680°R.).

The density of the reaction mixture ρ can be taken as constant at 50 lb./cu.ft., while the molecular weights of the various chemical species are as follows: A, B, P-100; C,E-200; G-300. Following the original analysis of Williams and Otto (8), the mathematical model for the process may be developed, and the objective function defined. The result is the following nonlinear programming problem.

Maximize

$$\% \text{ return} = 100\,[8400\underline{\underline{X}} - 2.22F_R - (0.124)(8400)(0.30F_P + 0.0068F_D) - 60V\rho]/600V\rho \qquad (14)$$

Subject to

$$F_A + F_B - F_G - F_P - F_D = 0 \qquad (15)$$

$$F_{RP} - 0.1F_{RE} - F_P = 0 \qquad (16)$$

$$\left(\frac{M_E}{M_B}\right) k_2 \left(\frac{F_{RB}F_{RC}}{F_R^2}\right) V\rho - F_D\left(\frac{F_{RE}}{F_R - F_G - F_P}\right) = 0 \qquad (17)$$

$$\left[k_2F_{RB}F_{RC} - \frac{M_P}{M_C}k_3F_{RC}F_{RP}\right]\frac{V\rho}{F_R^2} - F_D\left(\frac{F_{RP} - F_P}{F_R - F_G - F_P}\right) - F_P = 0 \qquad (18)$$

$$(-k_1F_{RA}F_{RB})\frac{V\rho}{F_R^2} - F_D\left(\frac{F_{RA}}{F_R - F_P - F_G}\right) + F_A = 0 \qquad (19)$$

$$[-k_1F_{RA}F_{RB} - k_2F_{RB}F_{RC}]\frac{V\rho}{F_R^2} - F_D\left(\frac{F_{RB}}{F_R - F_P - F_G}\right) + F_B = 0 \qquad (20)$$

$$\left[\frac{M_C}{M_B}k_1F_{RA}F_{RB} - \frac{M_E}{M_B}k_2F_{RB}F_{RC} - k_3F_{RP}F_{RC}\right]\frac{V\rho}{F_R^2} - F_D\left(\frac{F_{RC}}{F_R - F_G - F_P}\right) = 0 \qquad (21)$$

$$\left(\frac{M_G}{M_C}\right)k_3F_{RC}F_{RP}\frac{V\rho}{F_R^2} - F_G = 0 \qquad (22)$$

$$F_{RA} + F_{RB} + F_{RC} + F_{RE} + F_G + F_{RP} - F_R = 0 \qquad (23)$$

The overall mass balance Equation (15) may be combined with the original cost function Equation (14) to yield the following modified objective function with the variable F_B eliminated:

$$\% \text{ return} = \left(\frac{1}{6V\rho}\right)(84F_A - 201.96F_D - 336F_G + 1955.52F_P - 2.22F_R - 60V\rho) \qquad (24)$$

The Williams and Otto problem thus fits the general nonlinear optimization problem of Equations (1) to (3). The objective function is Equation (24), the equality constraints are Equations (16) through (23), and one variable is constrained between lower and upper limits. There are twelve variables in all—F_A, F_B, F_D, F_G, F_{RA}, F_{RB}, F_{RC}, F_{RE}, F_{RP}, F_R, V, and T—with eight equality constraints, leaving four independent variables.

METHOD OF SOLUTION

The Williams and Otto plant design has been optimized by means of the "complex" method. As the method was

Table 1. Eight Initial Feasible Points

Point No.	X_1	X_2	X_3	X_4	X_5	% Return
1	656.10	157,390	3,330.83	60,541.7	58.6267	73.28
2	640.00	95,967.4	2,350.60	33,348	90.0674	31.10
3	617.98	130,466	4,790.62	69,967.6	374.062	−1.29
4	590.97	176,681	4,969.15	88,315.7	665.047	8.91
5	609.36	135,819	3,904.80	82,136.6	564.963	1.40
6	615.31	128,028	3,170.47	62,723.3	323.304	16.97
7	615.33	137,843	3,018.38	72,096.9	414.421	13.16
8	622.74	214,063	1,705.51	40,551.8	238.579	−59.97
	(T)	(F_R)	(F_{RC})	(F_{RE})	(V)	

originally developed by Box, there was no provision for handling equality constraints, so the authors had to devise a means to satisfy the eight equality constraints present in this problem. The presence of twelve variables and eight constraints relating these variables means that when values are known for the four independent variables, the system is completely determined. However, the solution of the eight equations for the remaining variables presents a difficult problem, since the equations are highly nonlinear and consist of material balances which should be solved exactly. Two approaches were possible: (1) to solve the eight equations simultaneously by some method, or (2) to combine the equations algebraically. Since the particular equations were tractable enough to be combined algebraically, the second method was chosen. This approach assured that the values for the variables would be exact and more than compensated for the labor involved by the saving in computer time. Human error was possible, but care was taken to eliminate it completely.

The eight constraint equations were combined by eliminating one variable at a time, until only one equation relating five variables was left. Four of these variables were chosen as independent variables—F_{RC}, F_{RE}, F_R, and T—and the resulting equation, which was cubic in V, was solved using a library program based on the method of Muller (*4*). Three values of V were found for each solution, but it was possible to eliminate two of them on physical grounds. It was then possible to calculate the rest of the variables, one at a time, by means of the equations obtained during the previous elimination, and finally, to evaluate the objective function. Adelman (*1*) presents the entire set of equations and summarizes the procedure used for determining the entire set of variables, given a particular choice of independent variables.

As recommended by Box (*2*), a reflection factor α of 1.3 was used, and the value of k, the number of points in the complex, was equal to twice the number of independent variables (eight, in this case). The variables were redefined as X_1 through X_{12} for convenience, with the first four being the independent ones.

The only given constraints were that the temperature X_1 must lie in the range

$$580 \leq X_1 \leq 680°\text{R.} \qquad (25)$$

and of course that all other variables must be greater than, or equal to, zero. However, upper and lower bounds were needed to generate values for the four independent variables at each point of the initial complex. These values were chosen realistically, yet large enough to insure that a significantly large feasible region was explored, as follows:

$$1{,}000 \leq X_2 \leq 500{,}000 \qquad (26)$$

$$0 \leq X_3 \leq 10{,}000 \qquad (27)$$

$$0 \leq X_4 \leq 150{,}000 \qquad (28)$$

Of the eight points used in the original complex, one was the optimal solution vector determined by Williams and Otto (*8*), one was DiBella's optimal solution vector (*3*), and the remaining six were randomly distributed about the feasible region. At each of these eight initial points, with X_1 through X_4 known, X_5 through X_{12} were calculated by means of the combination equations, the constraints were checked, and any point which did not satisfy the constraints was replaced, until eight feasible points, satisfying all constraints, were found. These eight initial feasible points, with their objective function values (percent return on investment), are given in Table 1. Two of these points have negative returns, and they are reasonably well distributed about the feasible region.

A Fortran IV program was written for the CDC 6400 computer, applying the "complex" method to the solution of this problem. The point with the lowest objective function value was replaced, as outlined before, by means of reflection through the centroid, and this procedure was repeated until the complex converged to the optimum. The stopping criterion used was a fairly loose one, calling for the program to stop when three consecutive "worst point" objective function evaluations were within 0.01 of each other. Details of the program can be found in Adelman (*1*).

RESULTS

The optimum percent return in investment for the Williams plant was found to be 121.66%. This represents a very significant improvement over the value of 30.26% reported by Williams and Otto (*8*) and that of 72.75% reached by DiBella (*3*). A summary of the variables involved in each of these three solutions is presented in Table 2. The "complex" method required a total number of 124 iterations to find the optimal solution vector. An iteration is here defined as all the steps and calculations necessary to find a point which satisfies all the constraints (a feasible point), including the determination of the six new initial feasible points. This is many fewer iterations than DiBella required to find his proposed solution.

Figure 2 is a plot of the objective function, percent return on investment, versus a pseudovariable iteration num-

Table 2. "Optimal" and Two Earlier Solutions

Variable	"Optimal" solution	DiBella solution (3)	Williams solution (8)	Units
F_A	13,338.52	13,546.24	14,500.0	lb./hr.
F_B	30,759.72	31,522.56	33,350.0	lb./hr.
F_D	36,159.42	36,696.84	39,369.5	lb./hr.
F_{RA}	45,977.96	18,187.2	11,621.0	lb./hr.
F_{RB}	142,784.52	60,914.68	36,834.0	lb./hr.
F_{RC}	7,725.44	3,330.83	2,350.6	lb./hr.
F_{RE}	141,919.98	60,541.68	33,348.0	lb./hr.
V	32.01	59.56	92.8	cu. ft.
F_R	360,538.72	157,390.53	95,967.4	lb./hr.
F_{RP}	18,955.0	10,817.17	8,099.6	lb./hr.
T	672.61	656.1	640.0	°R
% Return	121.66	72.75	30.26	percent

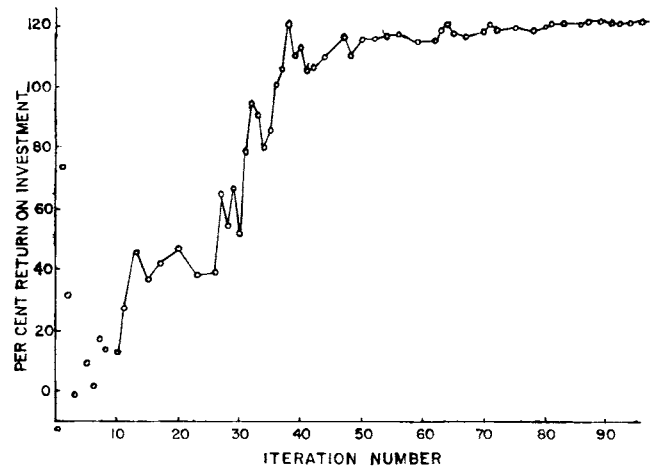

Fig. 2. Williams and Otto design problem: percent return versus iteration number.

ber. Only those points which exhibited an improved percent return have been included; that is, when the point with the least percent return is replaced (by reflection) by a new point that again has the least percent return, that iteration is not counted, and only the final point (which is an improvement) is plotted. It can be seen that at the beginning of the search there are wide fluctuations in the value of the percent return of each new point, but there is continuous improvement in the average percent return for the entire complex, since each iteration has produced a point with a higher objective function value than the point it replaced.

The data of Figure 2 also emphasize the fact that the "complex" method improves the value of the objective function very rapidly. In the case shown, the objective function had converged to within 4% of its final optimum after 37 iterations beyond the initial complex. From here on, the improvement was steady and continuous, but much slower, until the apparent optimum was reached after 124 iterations.

In addition to finding the optimum solution vector giving the "best" set of design variables, the program yields other valuable information about the system under study. For example, the response of the system is well mapped over a wide range of values of the independent variables. Also, the sensitivity of the optimum (that is, the response of the objective function to small changes in the values of the independent variables) is quite apparent, since as the program is converging to the optimum, it is automatically evaluating the response of the objective function to small perturbations in the variables.

CONCLUSIONS

The "complex" method has been shown to be a rapid method for determining the optimal solution vector, by means of an organized search through a series of feasible solutions. Each of the intermediate nonoptimal solution vectors is completely known and has a corresponding value of the objective function associated with it. Such a computational method should be of great value in both the design and the operation of a chemical plant.

It appears that the "complex" method, even though it is another variation of the many organized sequential search techniques proposed recently, may overcome some of the shortcomings of these other methods. In particular, the "complex" method should be able to find the global maximum, rather than the local optimum, nearest the starting point. This is due to the fact that the randomly generated points in the initial complex are scattered throughout the feasible region, with a good chance that at least one will lie in the vicinity of the global maximum. Furthermore, the use of a reflection factor greater than 1.0 causes an initial enlargement of the complex, thus assuring a good initial scan of the entire feasible region.

The real advantage of the method lies in its speed of solution and its relative ease of programming. Simultaneous solution of the constraint equations, as opposed to the method of algebraic combination actually used, will of course increase the computer time required, but a similar rise in time will take place with any method involving a sequential search through a series of feasible solutions (pattern search, parallel tangents, etc.). Thus, it is suggested that the "complex" method be given serious consideration in any optimization of a chemical process design where a good mathematical model of the process exists. Further experience should support this recommendation.

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NOTATION

a = lower limit of variable X_i
A_i = Arrhenius reaction rate pre-exponential factor for i^{th} reaction, (hr.-wt. fraction)$^{-1}$
$A_i(x_i)$ = cross-sectional hyperarea of intersection of experimental region with hyperplane on which X_i is constant
b = upper limit of variable X_i
B_i = Arrhenius reaction rate exponential factor for i^{th} reaction, °R.
e = base of natural logarithms
f = objective function
F = objective function
F_A = flow rate of reactant A to reactor, lb./hr.
F_B = flow rate of reactant B to reactor, lb./hr.
F_D = flow rate from column bottoms to plant fuel, lb./hr.
F_G = flow rate of by-product G from decanter to waste, lb./hr.
F_P = flow rate of product P from column, 40 million lb./yr. = 4,763 lb./hr.
F_{RA} = flow rate of A from reactor, lb./hr.
F_{RB} = flow rate of B from reactor, lb./hr.
F_{RC} = flow rate of C from reactor, lb./hr.
F_{RE} = flow rate of E from reactor, lb./hr.
F_{RP} = flow rate of P from reactor, lb./hr.
F_R = total flow from reactor, lb./hr.
g_k = lower limit on k^{th} variable
G_i = i^{th} equality constraint function
h_k = upper limit on k^{th} variable
i, j, k = subscripts indicating specific variable
k_i = reaction coefficient of i^{th} reaction, (hr.-wt. fraction)$^{-1}$
L_j = lower limit on j^{th} variable
r_i = random number on interval (0, 1)
T = reactor temperature, °R.
U_j = upper limit on j^{th} variable
V = reactor volume, cu.ft.
X_i = value of i^{th} variable
X_{ij} = j^{th} coordinate of i^{th} point in complex
$\overline{X}_i$ = i^{th} coordinate of centroid
$\underline{\overline{X}}$ = grouping of terms = $0.3F_P + 0.0068F_D - 0.02F_A - 0.03F_B - 0.01F_G$
α = reflection factor (≥ 1.0)
ρ = density of reactor solution, lb./cu.ft.

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