Optimization by Pontryagin's Maximum Principle on the Analog Computer

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A computational method has been developed for obtaining the solution to a class of optimization problems by the combined use of the maximum principle and a maximum (or minimum) seeking technique on the analogue computer. Various maximum seeking techniques can be used for this method. However if the random search technique is used, this computational method has the advantage of being able to investigate a large number of operating (or controlling) variables.

The calculation procedure is essentially a trial-and-error procedure which is alternately integration and maximum seeking operations. The variables over which the system is to be optimized are approximated by a finite number of straight line segments n. Thus the maximum (or minimum) of the Hamiltonian function which is obtained by the maximum principle need only be obtained at $n + 1$ points along the optimization path (or trajectory).

To illustrate the use of the method the optimum operating variable profiles (or gradients) in a tubular chemical reactor were computed.

The present method, in addition to making it easier to investigate systems with a moderate number of state variables, can be used to solve problems with almost any kind of constraints and performance index encountered in ordinary optimum design problems. It offers some possibilities for on-line optimizing control of a process. A special purpose analogue computer could be built for this use.

This paper discusses a computational scheme for the solution of a class of optimization problems by the use of the maximum principle on the analogue computer. The maximum principle together with Bellman's dynamic programing are generally regarded as two alternative ways of solving optimization problems of a nonlinear nature. Classical calculus of variations is generally inadequate in solving these problems.

The notion of dynamic programing has been widely used in solving optimization problems because it reduces a complicated problem into a simple algorithm ideally suited for the modern computers. However dynamic programing has its limitations. Instead of treating a single problem, it imbeds the original problem into a family of similar problems. Although this avoids a number of difficulties encountered in the classical method, new difficulties arise. Since both the computer time and the required memory increase rapidly with the number of variables, this technique in general can only be used successfully for problems with one or two variables. Even if it is assumed that the computer time is not a limiting factor, the available memory in the modern computer still limits the use of the simple algorithm of the dynamic programing technique to problems of not more than three state variables (*1*). This computational difficulty is even more pronounced when this technique is used to solve continuous problems where a small step must be used to obtain a reasonably accurate answer. Various methods have been devised to overcome this dimensionality difficulty. A discussion of these however is beyond the scope of this treatment. It is sufficient to say that this difficulty is far from solved at this time.

Another disadvantage of dynamic programing is that it cannot deal with processes in which the optimum conditions at any stage can be disturbed by conditions at a following stage.

A comparison between the notion of dynamic programing and the maximum principle shows some possibility of avoiding the above mentioned difficulties. If the optimization problem is divided into m discrete stages along the optimization path, and there are n state variables in the system, the calculation philosophy by the two methods is essentially reduced to the following. Dynamic programing will start the investigation by searching the entire grid of the n variables at one stage, store this grid of values, and proceed stage by stage; the maximum principle will start the investigation by computing one optimum path along the m stages and then proceed to improve this optimum path based on the values obtained from the preceding computation. This is really an oversimplification of the two methods. However it does give the essence of the methods.

By the use of the maximum principle the optimization problem is essentially reduced to a maximum (or minimum) seeking problem subject to the constraints of a set of ordinary differential equations. If the maximum (or minimum) at each point along the trajectory can be obtained by some maximum seeking method whose computation time does not depend heavily on the number of variables to be investigated, the maximum principle can be used much more readily to investigate systems with many controlling variables. A search among the available maximum seeking methods indicates that the random search technique fulfills these requirements since the computational time involved does not increase as rapidly with the number of variables as does that for sequential search methods (*2, 3*). Thus the random optimization method on the analogue computer, as developed by Favreau and Franks (*4*), was used in the present scheme. Experience indicates that in general the computation time is nearly independent of the number of variables investigated. The computational time is more a function of the magnitude of the random noise and a function of the difference between the starting value and the final optimized value of the variable. As has been pointed out by Satterthwaite (*5*), "with random evolutionary operation, the number of experiments required to find a set of optimum conditions appears, in general, to depend not at all on the number of variables or the complexity of the relationship."

The present method is essentially a trial-and-error procedure with the maximum principle and a maximum (or minimum) seeking method on the analogue computer.

The trajectories of the variables over which the system is to be optimized are approximated by a finite number of straight-line segments. Although the analogue computer was well suited for this work, for more complicated problems combined digital and analogue equipment could be used to overcome certain limitations of the analogue computer.

THE MAXIMUM PRINCIPLE

The principle is briefly outlined. No effort has been made to cover the case in which restrictions are imposed on the final values of the state variables. For more detailed treatment the reader is referred to the series of articles by Rozonoer (*6*) or those by Pontryagin and his associates (*7, 8*).

Let the system be represented by the following set of differential equations:

$$\frac{dx_i}{dt} = f_i(x_1, \ldots, x_n;\ u_1, \ldots, u_r;\ t),\ i = 1, \ldots, n \quad (1)$$

where $x_1, \ldots, x_n$ are the state variables, and $u_1, \ldots, u_r$ are the variables which are to be investigated in order to obtain the optimum of the system. In general $u_1, \ldots, u_r$ are the controllable operating variables. At each moment the optimization variables must satisfy the set of constraints

$$Q_j[u_1(t), \ldots, u_r(t)] \leq 0,\ j = 1, \ldots, m \quad (2)$$

In the future the vector U will be used to represent the set of variables $u_1, \ldots, u_r$ and the vector X to represent $x_1, \ldots, x_n$.

The problem is to optimize a linear combination of the final values of the state variables of the system, that is to optimize the quantity

$$S = \sum_{K=1}^{n} C_k x_k(t_f) \quad (3)$$

In other words one would like to find the values of the optimization variables U from time $t = t_o = 0$ to $t = t_f$, such that the quantity in Equation (3) is maximized (or minimized) subject to the constraints of Equations (1) and (2). Obviously S is the performance index.

The problem formulated above can also be used to optimize other forms of performance indexes and constraints. For example the problem of optimizing an integral expression can be reduced to the optimization of the final value of one state variable whose value equals to this integral expression. This method of formulating one additional state variable can be used to handle a large class of optimization problems such as the optimization of a function of the final values of the state variables and optimization with integral constraints. The series of papers by Rozonoer (*6*) have an excellent discussion on this subject.

To solve this problem one introduces n impulse functions $p_1(t), \ldots, p_n(t)$, whose value at $t = t_f$ are

$$p_i(t_f) = -C_i,\ i = 1, \ldots, n, \quad (4)$$

and are defined by the following set of equations:

$$\frac{dp_i}{dt} = -\sum_{s=1}^{n} p_s \frac{\partial f_s(x_1, \ldots, x_n;\ u_1, \ldots, u_r;\ t)}{\partial x_i}$$
$$i = 1, \ldots, n \quad (5)$$

One further introduces the Hamiltonian function H which is defined by

$$H(X, P, U, t) = \sum_{s=1}^{n} p_s f_s(x_1, \ldots, x_n;\ u_1, \ldots, u_r;\ t) \quad (6)$$

where P is the vector $p_1, \ldots, p_n$. It can easily be shown that

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i},\ \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i} \quad (7)$$

The boundary conditions are

$$x_i(t_o) = x_i^o,\ p_i(t_f) = -C_i,\ i = 1, \ldots, n \quad (8)$$

The maximum principle says that if one wants to maximize (or minimize) S, this maximum (or minimum) is obtained only if the function H is minimized (or maximized) at every moment from $t = 0$ to $t = t_f$ subject to the constraints of the set of Equations (2), (7), and (8).

By the use of the maximum principle an infinite dimensional optimization problem in the independent variable t has been reduced into an r-dimensional optimization problem which must be optimized at every moment $t_o \leq t \leq t_f$ subject to the original constraints and the constraints of a set of ordinary differential equations. In principle this optimization problem is solved. The maximum (or minimum) of H can be found by partial differentiation:

$$\frac{\partial H}{\partial u_i} = \frac{\partial}{\partial u_i} \sum_{1}^{n} p_s f_s(x_1, \ldots, x_n;\ u_1, \ldots, u_r;\ t) = 0$$
$$i = 1, \ldots, r \quad (9)$$

This set of equations can be solved for U, and substituting into Equation (7) one obtains

$$\frac{dx_i}{dt} = f_i(x_1, \ldots, x_n;\ p_1, \ldots, p_n;\ t) \quad (10)$$

and

$$\frac{dp_i}{dt} = g_i(x_1, \ldots, x_n;\ p_1, \ldots, p_n;\ t) \quad (11)$$
$$i = 1, \ldots, n.$$

This can be integrated with the boundary conditions Equation (8), and thus the variables U as a function of t are obtained.

In practice there are several difficulties which prevent the use of this procedure. The variables U may be implicit in the equations and cannot be solved for explicitly; thus Equations (10) and (11) cannot be obtained. Even if U can be solved for explicitly from Equation (9), there is still the problem of proving that Equation (9) gives the real maximum or minimum of H rather than a relative maximum or minimum. It is evident that neither of those two difficulties can be overcome easily by analytical means.

THE COMPUTATIONAL METHOD

In order to avoid the above mentioned difficulties in applying the maximum principle a computational procedure is desirable. First note that Equations (7) and (8) are a two point boundary value problem. Only the final values of the impulse functions P are known. This increases the computation for a solution tremendously. A trial and error, or some kind of a search procedure, has to be used to fit the solution into the final values of P. Another problem involved is the interrelationship between Equations (6) and (7). In order to integrate Equation (7) one must know the values of U as a function of t. But this value is exactly what is hoped to be found from the solution. Thus another trial-and-error procedure is needed.

In order to obtain the values of U as a function of time some approximation is needed. Clearly one cannot make the calculations at every point along the independent variable t coordinate, for then one would need an infinite number of calculations. Thus the author will divide the independent variable t into f intervals as shown in Figure

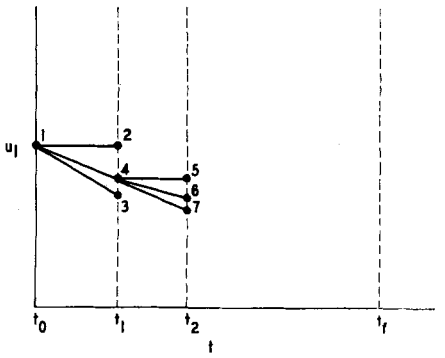

Fig. 1. Optimization procedure.

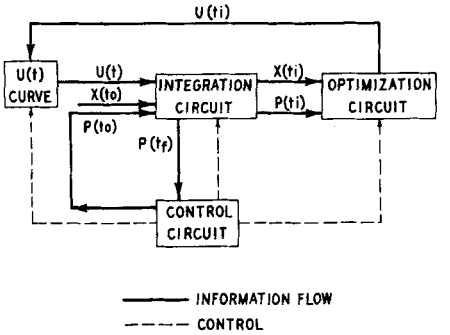

Fig. 2. Block diagram of the numerical optimization method.

1, and the values of U as a function of t will be assumed to be composed of f straight-line segments. Now one only needs to calculate the problem at $f + 1$ points along the t coordinate. The error involved for this approximation is difficult to estimate. It should be noted that this error is accumulative along the independent variable t coordinate.

For simplicity of discussion consider a system which only has one optimization variable u_1, and one would like to find the maximum value of S for this system. Now all that is needed is to find the values of u_1 at $t = t_o, \ldots, t_f$ such that the values of u_1 as a function of t which is formed by straight-line connections between the points $t_o, \ldots, t_f$ will make S a maximum, or the values of u_1; $x_1, \ldots, x_n$; and $p_1, \ldots, p_n$ at $t = t_o, \ldots, t_f$ will always make H a minimum.

The procedure for this computational method is as follows:

1. Assume a set of initial values for the impulse functions, say $P(t_o)$.

2. At $t = t_o = 0$ the value of u_1, which will be called $u_1(t_o)$, is obtained by minimizing H with the known initial conditions for X and the assumed initial conditions for P.

3. At $t = t_1$ assume a value for u_1, say $u_1(t_1)$.

4. Connect $u_1(t_o)$ and $u_1(t_1)$ by a straight line. Integrate Equation (7) along this straight line. A set of values for P and X are thus obtained at time t_1. Call this $P(t_1)$ and $X(t_1)$.

5. Substitute the set of values $P(t_1)$ and $X(t_1)$ into Equation (6), and an improved $u_1(t_1)$ is obtained by minimizing H.

6. When one uses this improved $u_1(t_1)$, steps 4 and 5 are repeated until no further changes occur in the improved $u_1(t_1)$.

7. At $t = t_2$ assume a value for u_1, say $u_1(t_2)$, and steps 4 to 6 are repeated. However now the integration must be performed along the two line segments $u_1(t_o)$ $u_1(t_1)$ and $u_1(t_1)$ $u_1(t_2)$, and the set of values obtained for X and P are $X(t_2)$ and $P(t_2)$, respectively.

8. Similarly one can obtain $u_1(t_3), \ldots, u_1(t_f)$.

9. At $t = t_f$ the calculated values for P are compared with the given final values for P. If they are different, appropriate adjustment is made to obtain a new set of initial values for P, and steps 2 to 8 are repeated until the given final values for P are the same as the calculated final values for P.

For the optimization of systems which have more than one optimization variable u_i the above procedure is essentially the same except that one has to find a set of values for U at each point of the independent variable, t.

In the above discussions a forward integration procedure was assumed. For certain problems it is advantageous to integrate the equations backward. The procedure is the same as the forward procedure listed above except for the boundary conditions. Now the unknown boundary conditions are the final conditions for the state variables. Thus the procedure now is to adjust the assumed final conditions for the state variables until the calculated initial conditions are the same as the given ones. For certain problems the backward integration procedure has been found more stable and less sensitive to errors. Another advantage for this procedure is that for almost any design problems one is not only interested in a specified set of initial conditions but also in the vicinity of these initial conditions. This vicinity is investigated while the final conditions of the state variables are adjusted.

Another procedure which was found to converge faster to the two point boundary values than the above procedure is as follows:

1. Assume a curve for the control variables $U(t)$.
2. Solve Equation (7) by using the above assumed $U(t)$.
3. Obtain an improved curve $U(t)$ by minimizing H with the known values obtained in step 2.
4. Repeat steps 2 and 3 until no further improvement can be made.

This procedure is especially advantageous where a large number of straight-line segments must be used to represent the functions of the control variables $U(t)$.

The computer circuit for the present method consists essentially of three parts as shown in Figure 2. They shall be designated as control circuit, optimization circuit, and integration circuit. The optimization circuit is used to find the values of U such that the function H is a minimum at all times t for $0 \leq t \leq t_f$ with given values for P and X. The details of this circuit will depend upon the optimization method used. A detailed discussion of this circuit and the optimization method will be given in the next section. The integration circuit integrates Equation (7) and obtains numerical values for X and P at specified values of t with the given or assumed initial conditions. The control circuit performs the following functions: it controls the sequence of the alternate integration and optimization processes, it controls and adjusts the curves of U against t, and it adjusts the initial conditions $P(t_o)$ so that the calculated final conditions agree with the given final conditions of P.

If the optimization procedure is done manually on the analogue computer, the control circuit is not needed. The curves of U against t which are composed of straight-line segments can be set up manually on the diode function generators of the computer. The initial conditions $P(t_o)$ can also be adjusted manually by linear interpolation from the given and calculated final conditions of P.

If the optimization calculations are done automatically by the computer, several storage circuits are needed for storing the straight-line segments of the U against t curves. Since these curves have to be changed constantly during the calculation, some easy method must be pro-

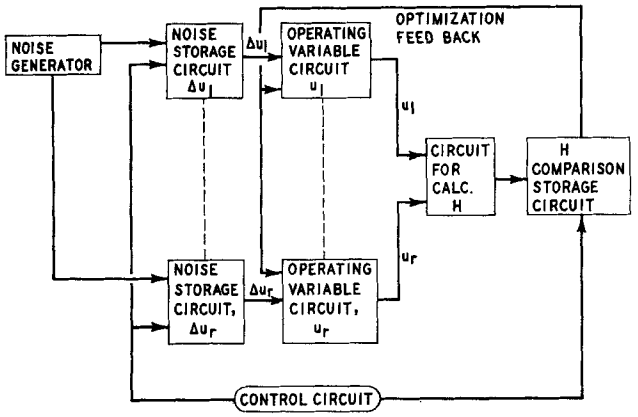

Fig. 3. Block diagram for random search method.

vided to change and adjust these curves automatically. In order to prevent the storage and control circuits from becoming too complicated for a fairly large problem a specially designed storage circuit for the curves of U against t is clearly desirable. Another way to avoid this difficulty is the use of a combined digital-analogue computer. The digital computer would be used mainly for storing the U against t curves and some control functions. The analogue computer would perform the integration and probably the maximum seeking calculations.

The combined digital-analogue computer has another advantage over the analogue computer. It was found that for certain problems the plot of H against the variables to be investigated becomes very flat. In order to locate accurately the maximum (or minimum) of H frequent rescaling of the problem on the analogue computer was necessary. By the use of a combined digital-analogue computer the digital computer could be used for automatic rescaling of the problem as required.

MAXIMUM-SEEKING METHOD

In the above discussions no mention was made concerning the methods which can be used to find the minimum (or maximum) of H at any value of the independent variable t. For systems which have only one or two variables to be investigated there are numerous techniques for determining the system optimum, such as the various versions of the gradient method, factorial design, random search technique, or even just a simple plot of H against the variable to be investigated. However as the number of variables increases, the amount of time required for obtaining the solution becomes prohibitive for any sequential search method. If each possible variable range is to be investigated at m points, and there are n variables, the number of possible combinations is m^n. It can be seen that m^n becomes quite large as $n = 3$ or more. As has been mentioned earlier the computation time does not

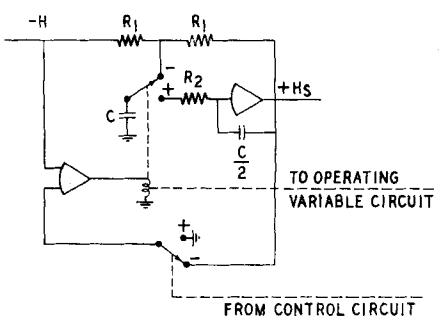

Fig. 4. Comparison-storage circuit.

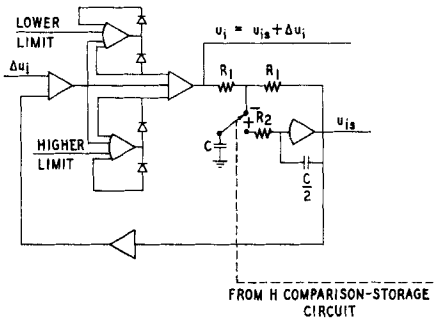

Fig. 5. Operating variable circuit.

increase rapidly for the random search method. This method was used in the present work.

In the following a brief discussion of the random search technique on the analogue computer will be given. More detailed discussion of this technique can be found in the papers by Favreau and Franks (4) and by Munson and Rubin (9).

Random Search Technique

Basically the method is very simple and consists of specifying each of the variables to be investigated in a random manner within the region of interest. Each variable is assumed to be completely independent of all the others.

A block diagram of the components and information flow required for the random search method on the analogue computer is shown in Figure 3. The random noise generated by the noise generator is sampled frequently but at specified intervals and is stored in the noise storage circuit. This noise which is sampled and stored will be called Δu_i. In the operating variable circuit this stored noise Δu_i is added to the stored random variable u_{is} to obtain u_i. The random variable u_i is first passed through a limiting circuit which restricts this variable to the allowed range, and then it is used to calculate H. This calculated H is then compared with the stored H_s. If this H is better than H_s, H is stored and H_s is discarded. At the same time u_i is stored and u_{is} is discarded in the operating variable circuit. This process is repeated until the optimum is obtained.

It should be noted that at the start of the process u_{is} and H_s are the starting values for u_i and H, respectively. As the process proceeds, u_{is} acts as the mean of the random variable u_i. After each successful trial the u_i's which gave that successful trial are stored and made the means of the distributions of future u_i selections. The investigation of the system will proceed with the center of investigation always around the last successful values of the variables. As this procedure continues, the u_{is} values will change always in the direction of the optimum.

The circuit used for the random search method is mainly composed of the comparison storage circuit which is shown in Figure 4 and the operating variable circuit which is shown in Figure 5. Any suitable control method can be used for the control circuit of the random search process.

It should be noted that the standard deviation of the random variables is an extremely important parameter. If it is small, the steps taken will be small and a large number of steps may be required to reach an optimum. On the other hand if one is not far removed from the optimum and the standard deviation is much larger than the distance between the last best value and the true optimum, a considerable time may be required to reach the optimum. A compromise must be taken between these two extremes.

If the system has a local optimum and the standard deviation is fairly small, the search process will stop at this local optimum. In order to obtain the true optimum one of the following two methods may be used. Increase the standard deviation so that a wider search region will be investigated or start from different initial points.

Since the selection of the standard deviation of the random variable is so important and so undefined, it would appear quite reasonable to consider periodically varying this quantity during the process of search for an optimum.

EXAMPLES

Optimum Temperature Gradient in Tubular Reactors

To illustrate the use of the optimization procedure discussed the optimum temperature gradient in a chemical reactor was obtained for a particular set of numerical conditions. The reaction scheme is $A \rightarrow B \rightarrow C$, where B is the desired product. Both reactions are assumed to be first order. This problem has been solved first by Bilous and Amundson (*10*) by functional differentiation and then by Aris (*11*) by the use of dynamic programing.

If x_1 and x_2 are the state variables which represent the concentrations of A and B, the kinetics of the reactions are given by

$$\frac{dx_1}{dt} = -k_1 x_1 \tag{12}$$

$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 \tag{13}$$

where k_1 and k_2 are the rate constants of the reactions, and

$$k_1 = G_1 e^{-\frac{E_1}{RT}}, \quad k_2 = G_2 e^{-\frac{E_2}{RT}} \tag{14}$$

where t is the holding time of the reactor up to a given point and $T(t)$ the temperature there. The yield of B over the total holding time $t = t_f$ of the reactor has to be maximized, and Equation (3) becomes $S = x_2(t_f)$ since $C_1 = 0$ and $C_2 = 1$. From Equation (6)

$$H(x_1, x_2, p_1, p_2, T) = -p_1 k_1 x_1 + p_2 k_1 x_1 - p_2 k_2 x_2 \tag{15}$$

where the temperature T is the variable whose value as a function of t is being sought. The equations for the impulse functions are obtained from the second group of Equation (7):

$$\frac{dp_1}{dt} = p_1 k_1 - p_2 k_1 \tag{16}$$

$$\frac{dp_2}{dt} = p_2 k_2 \tag{17}$$

with the boundary conditions

$$\begin{aligned} x_1(t_o) &= x_1^o, \quad x_2(t_o) = x_2^o \\ p_1(t_f) &= 0, \qquad p_2(t_f) = -1 \end{aligned} \tag{18}$$

It should be noted that this problem cannot be solved analytically by the maximum principle, since the temperature T is implicitly expressed in these equations.

The numerical values chosen were

$G_1 = 0.535 \times 10^{11}$ min.$^{-1}$

$G_2 = 0.461 \times 10^{18}$ min.$^{-1}$

$E_1 = 18{,}000$ cal./mole

$E_2 = 30{,}000$ cal./mole

$R = 2$ cal/mole $-$°K.

$t_f = 8$ min.

$x_1^o = 0.53$ mole/liter

$x_2^o = 0.43$ mole/liter

It should be noted that a fairly large value of x_2^o was chosen to avoid rescaling of the problem on the analogue computer during calculations. The above numerical values are the same as those used by Bilous and Amundson (*10*) in their example A, except for the values of t_f and the initial conditions. The values of x_1^o and x_2^o are approximately equal to their corresponding values at $t = 2$ min.

This problem was solved by minimizing the value of H in Equation (15) by the combined random search and integration procedure as described previously. The results are shown in Figure 6. Since there is only one operating variable to be investigated, a simple plot of H against T at any value of t can also be used to obtain the minimum of H. A set of such plots is shown in Figure 7. This provides a check for the random search technique. The results of Bilous and Amundson which were estimated from their plots compared favorably with the present results.

In actual calculations it was necessary to repeat steps 4 and 5 in section 3 only once to obtain the correct value. For the random search part it was found that the time needed to obtain the minimum depends heavily on the standard deviation of the random noise. If a reasona-

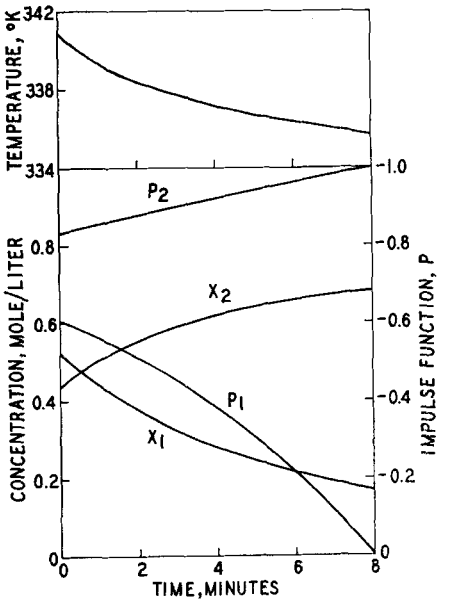

Fig. 6. Temperature and concentration profiles.

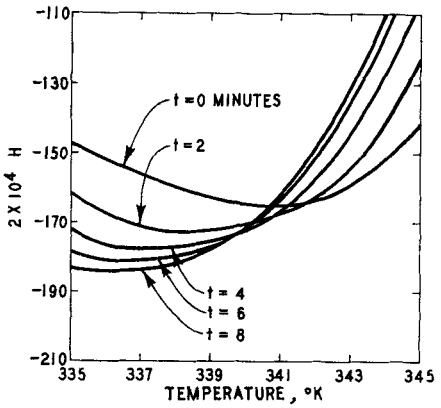

Fig. 7. The Hamiltonian function.

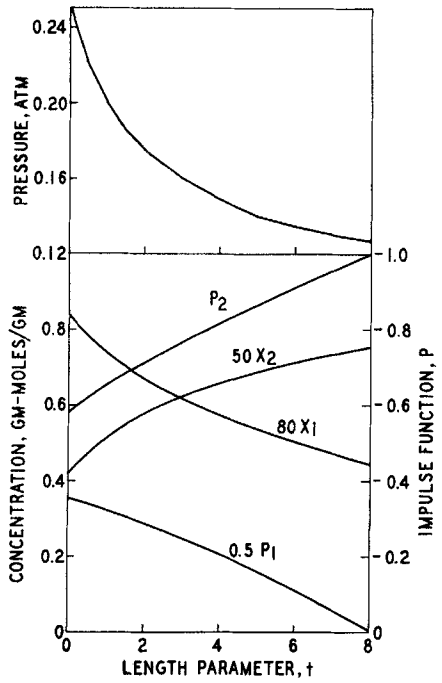

Fig. 8. Pressure and concentration profiles.

ble value for the standard deviation is used, the optimum is obtained in the order of seconds.

This problem can evidently be solved without the use of the maximum principle. Since there are no constraints and only one control variable T to be investigated, several other methods can be used. For example a random search procedure combined with the integration of the original differential equations can be used to obtain the optimum. This example was introduced only to illustrate the procedures of the solution of the computational method.

Optimum Pressure Gradient in Tubular Reactors

As a second example the optimum pressure gradient in a tubular reactor for gaseous reactions was obtained. The reaction scheme discussed is $A \rightarrow 2B \rightarrow C$, where B is the desired product. The first reaction is first order, and the desired product B transforms into C by a second-order reaction. The equations for the reactions are

$$G\frac{dx_1}{dz} = -k_1\pi_1 \qquad (19)$$

$$G\frac{dx_2}{dz} = 2k_1\pi_1 - k_2\pi_2^2$$

For ideal gases where Dalton's law is obeyed

$$\pi_1 = \pi\frac{n_1}{N} = \pi\frac{x_1}{x_1 + x_2 + x_3} \qquad (20)$$

$$\pi_2 = \pi\frac{n_2}{N} = \pi\frac{x_2}{x_1 + x_2 + x_3}$$

Assume only A and B present at the entrance of the reactor; then a material balance at Position z along the reactor gives

$$(x_1^o - x_1) + \frac{1}{2}(x_2^o - x_2) = x3 \qquad (21)$$

By the use of Equations (20) and (21) Equation (19) becomes

$$\frac{dx_1}{dt} = -2k_1\pi\frac{x_1}{A + x_2} \qquad (22)$$

$$\frac{dx_2}{dt} = 4k_1\pi\frac{x_1}{A + x_2} - 4k_2\pi^2\frac{x_2^2}{(A + x_2)^2} \qquad (23)$$

where

$$A = 2x_1^o + x_2^o, \quad t = z/G$$

The Hamiltonian function for the present problem is

$$H(x_1, x_2, p_1, p_2, \pi) = -2p_1k_1\frac{\pi x_1}{A + x_2} + 4p_2k_1\pi\frac{x_1}{A + x_2} - 4p_2k_2\pi^2\frac{x_2^2}{(A + x_2)^2} \qquad (24)$$

where π is the variable whose value as a function of t is being sought such that the yield of B is maximized. The equations for the impulse functions are

$$\frac{dp_1}{dt} = 2p_1k_1\pi\frac{1}{A + x_2} - 4p_2k_1\pi\frac{1}{A + x_2} \qquad (25)$$

$$\frac{dp_2}{dt} = -2p_1k_1\pi\frac{x_1}{(A + x_2)^2} + 4p_2k_1\pi\frac{x_1}{(A + x_2)^2} + 8p_2k_2\pi^2\frac{x_2}{(A + x_2)^2} - 8p_2k_2\pi^2\frac{x_2^2}{(A + x_2)^3} \qquad (26)$$

The boundary conditions are

$$x_1(t_o) = x_1^o, \quad x_2(t_o) = x_2^o \qquad (27)$$

$$p_1(t_f) = 0, \quad p_2(t_f) = -1$$

The numerical values chosen are

$G_1 = 0.2 \times 10^9$ g.-moles/(liter)(min.)(atm.)

$G_2 = 0.63 \times 10^{16}$ g.-moles/(liter)(min.)$(atm.)^2$

$E_1 = 18{,}000$ cal./mole

$E_2 = 30{,}000$ cal./mole

$k_1 = G_1e^{-\frac{E_1}{RT}}$

$k_2 = G_2e^{-\frac{E_2}{RT}}$

$R = 2$ cal./mole-°K.

$t_f = 8$ liter-min/g.

$T = 380$°K.

$x_1^o = 0.0105$ g.-moles/g.

$x_2^o = 0.0085$ g.-moles/g.

$x_3^o = 0$

This problem was solved by this computational scheme, and the results are shown in Figure 8.

This reaction scheme is being investigated further by the use of the combined analogue-digital computer under a variety of different conditions. The results will be discussed in a later paper.

CONCLUSIONS

A computational scheme has been developed for obtaining the solution of a class of optimization problems by the combined use of Pontryagin's maximum principle and a maximum seeking technique on the analogue computer. This technique has the advantage of being able to investigate a large number of operating variables to obtain the optimum of the system. However it is not suited to investigate systems which have a large number of state variables. This restriction arises from the very nature of the maximum principle. Since the initial conditions of the impulse functions P are generally unknown, some kind of search procedure must be used to find these initial condi-

tions from the given final condition. If the number of impulse functions which depend on the number of the state variables is large, this search procedure may become prohibitively tedious.

The present method can be used to handle most of the constraints and performance indexes encountered in ordinary optimum design problems. For a detailed discussion of these problems the reader is referred to the paper by Rozonoer (*6*). The method offers some possibilities for use for on-line optimizing control of a process. A special purpose analogue computer could be built for this use.

The analogue computer is ideally suited for solving two point boundary value problems. However for more complicated problems where frequent rescaling and fairly high accuracy is desired, a combined analogue-digital computer would present many advantages. The optimum gradients of temperature, pressure, and concentrations of certain chemical species in a chemical reactor are being investigated by the use of a combined analogue-digital computer.

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NOTATION

E_1, E_2 = activation energies of the first and second reactions
G = mass flow rate, g./min.
G_1, G_2 = frequency-factor constants in Arrhenius equations
H = Hamiltonian function
k_1, k_2 = reaction rate constants of the first and second reactions
N = total moles
n_1, n_2 = moles of A and B, respectively
$p_1, \ldots, p_n$ = impulse functions
R = gas constant
T = temperature
t = independent variable
$u_1, \ldots u_r$ = control variables
$x_1, \ldots, x_n$ = state variables
z = length parameter of the reactor, liter
π = total pressure, atm.
π_1, π_2 = partial pressures of A and B, respectively, atm.

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A Model Building Technique for Chemical Engineering Kinetics

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The object of much experimentation is to build or discover a suitable model for a given system. Unfortunately very little work has been published on what constitutes good strategies in these situations. This paper is an attempt to formulate an approach to this important problem of iteratively improving models in the area of chemical engineering kinetics. In this technique a statistical analysis is applied to the estimated parameters of a tentatively entertained theoretical model in such a way as to pinpoint its inadequacies, if they exist, so that it is possible to proceed in a logical manner to an appropriate modification of this model. This modified model is then analyzed in a similar way, and further modifications are suggested. In general the cycle is repeated as often as is necessary to reach an adequate model. This sequential method is illustrated by finding an adequate reaction model for the total catalytic oxidation of methane.

A simple method for iterative model building has recently been described (*4*) in which a statistical analysis is applied to the estimated parameters of a theoretical model rather than to the original observations themselves. By adopting this method it should be possible to pinpoint inadequacies of a given model in such a way as to suggest specific ways in which the model can be modified, if necessary, to yield a more useful one. The purpose of this paper is to apply this technique for model building to some kinetics data on the catalytic oxidation of methane