A Study of Iterative Optimization

DALE F. RUDD, RUTHERFORD ARIS, and NEAL R. AMUNDSON

University of Minnesota, Minneapolis, Minnesota

A process is considered in which the inputs to the system are stationary random ergodic functions. From the spectral densities of the inputs and cross-spectral densities of inputs and outputs a local linearized model of the process is obtained through the transfer function. There results then a maximum problem involving an objective function and constraints imposed by the model and the physical and arbitrary restraining conditions. Two special cases are solved in detail in which the maximum problem reduces to a linear programing problem. Other methods are needed for the general problem.

The optimum operation of a process has always been a problem of great interest. The introduction of high speed digital computers has brought these problems even more to the forefront allowing the use of methods that were heretofore impossible from a computational standpoint. While the complete operation of a large-scale process by a computer system still lies in the future, partial operation has been achieved.

Computers handle the direct optimization of processes in several ways.

Equation solving: The computer solves a mathematical model of the process to find the set of operating conditions that satisfy certain optimum operating criteria.

Peak searching: The computer seeks the optimum operating conditions by trial and error but does not need to develop a detailed mathematical model of the process.

Equation seeking: The computer correlates process data and develops a mathematical model of the process which is then used to improve the operation of the process.

Equation solving relies heavily on the existence of a detailed mathematical description of the process, and for some processes this description does not exist. For other processes the general model is known, but the parameters involved in the model are unknown and probably will remain so for some time. In many other cases the detailed model is far too complicated for present computers. The peak-searching method is practical for processes with only a few operating variables and does not lead to a useful description of the process. Equation seeking leads to a restricted mathematical model for the process, as in the so-called "evolutionary operation" discussed by Box and Wilson (3).

The present work is concerned with the last category, equation seeking and evolutionary operation. The general aim is the development of a method which will use a computer system to analyze the operating data from a process, gaining enough information to improve the process performance. The method developed here is called *iterative optimization* and is best suited for the optimization of continuous processes. The method obtains information from the normal stationary operation of the process and not primarily from a group of steady state experiments as is the case with most of the evolutionary operation methods now in use.

Two examples are included showing how this method can be applied. In these examples a computer system assumes control of simulated chemical processes with the aim of improving their performance. These examples show how the iterative optimization method can be used in practice as well as some of the difficulties that would be encountered.

Dale F. Rudd is at the University of Wisconsin, Madison, Wisconsin.

THEORY

Consider the optimization of a general process with many inputs and outputs. An input is defined as any quantity of interest that has an effect on the process and is controllable. The inputs are generally the control variables of the process, such as steam pressures, concentrations, etc., while output is defined as any quantity of interest that is completely determined by the values of the input variables and the nature of the process. The outputs are usually associated with the properties of the final products and the general operating level of the process. An output could be for example the yield of a certain product or the operating temperature of a reactor.

It is convenient to think of the process as a mathematical operator M which operates on the set of inputs $\{x_i\}$ to yield the set of outputs $\{y_i\}$. This orientation of thought is in no way limiting, since nothing has been said about the exact nature of the operator. For most problems the operator M cannot be constructed, but its inverse L may be constructed from the material and energy balances, the kinetic relations, and the equilibrium laws related to the physical and chemical transformations occurring in the process. For an even larger class of problems construction of the operator L is not feasible. Note that the operator L is generally multidimensional and highly nonlinear. The equations are usually differential equations, impossible of direct solution, with unknown parameters. It is this latter class of problems that is of interest here.

The process is represented symbolically by Equation (1):

$$M\,[\,\{x_i(t)\}\,] = \{y_i(t)\} \qquad (1)$$

This equation is read. The operator M operates on the set of input variables $\{x_i(t)\}$ to yield the set of output variables $\{y_i(t)\}$. The functional notation (t) indicates time dependence where the time dependence in this paper is caused by random fluctuations in the inputs.

The process has an objective or profit function associated with its operation. This function includes all the important variables related to the operation of the process, such as the costs of the raw materials, processing costs, the value of the products, etc. In its most general form the profit function is

$$P = P\,[\,\{x_i\}, \{y_i\}, R\,] \qquad (2)$$

and depends on the input and output variables as well as the current market conditions designated by R.

In general not all operating levels of the process are allowed, since physical constraints are quite often imposed to eliminate hazards or to conform with certain standards of operation. For example temperatures and pressures must not be so high as to damage the processing equipment. Limits of this type are called *constraints* and are represented by

$$C_j\,(\,\{x_i\}, \{y_i\}\,) < 0 \qquad (3)$$

where C_j is the symbolic notation for the j^{th} kind of constraint.

With the system so defined the general optimization goal can be stated in detail. Locate the set of operating conditions (the set of input variables $\{x_i\}$) which for given market conditions maximizes the profit function and also satisfies the physical constraints. In symbolic form

$$\underset{\{x_i\}}{\text{Max}}\; P\,[\,\{x_i\}, \{y_i\}, R\,] \qquad (4)$$

subject to Equations (1) and (3).

A general solution of Equations (1), (3), and (4) is not possible, so special cases of interest must be considered.

Interest here is limited to the development of methods which extract from

the steady operating data enough information to construct a locally valid estimate of the process operator M, to use this estimate to solve the maximum problem, and to sequence these operations to improve the performance of the process.

THE PROCESS OPERATOR

With the iterative optimization method it is necessary to estimate the process operator by analyzing the process operating data. The method of extracting information from the dynamic operating data is now presented. The term "dynamic" is here used in the sense of random fluctuations on a steady state and does not imply the use of a true transient state.

Considerable work has been done on techniques to obtain from the operating data of a process certain fundamental characteristics of the process. Most of the work has been centered about the problem of obtaining the local dynamic behavior of the process for purposes of control-system design. Homan and Tierney (5) applied these techniques to chemical reactor systems. As will be shown the iterative optimization method uses only information about the local steady states of the process rather than transient information. This is a simpler, but by no means a simple, problem computationally.

One should take advantage of the apparently random changes which occur in the dynamic operation of a chemical process to gain information about the process and to use this information to improve its performance. To achieve this it is necessary to investigate the nature of random disturbances and to study the response of linear systems to such disturbances. From this analysis will come the basic ideas for the development of the iterative optimization method.

It is convenient to consider the input variables as composed of two terms, one time dependent and one constant. The time-dependent term corresponds to the normal random variations of a variable about its mean value. The output variables are a direct result of the response of the process to these time dependent input variables. The outputs then consist of a constant term plus a random time-dependent term.

The nature and the characterization of random time series type of variations is considered in detail by Laning and Battin (6). Consider a typical variable

$$x(t) = x^N + r(t)$$

consisting of a steady state or constant term and a random time-dependent term. Let $r_1(t)$, $r_2(t)$ ... and $r_M(t)$ be measurements of the time-dependent term over a period of time under identical operating conditions. Since $r(t)$ is random in nature, these measurements will not coincide; they may be thought of as samples from an ensemble of variations of $r(t)$.

With each member of that ensemble one may associate a new function $k_{i\tau}(t)$ formed by the time translation of $r_i(t)$:

$$k_{i\tau}(t) = r_i(t-\tau)$$

If the statistical properties of the time-translated functions are identical to those of the original functions, the functions are said to be stationary. It is necessary to assume here that over the period of time the computer is gathering information from the process the time-dependent terms of the input variables are stationary time series. This assumption is valid for a large number of continuous processes.

Statistical properties of random functions are stated in terms of an ensemble of functions. This is inconvenient, and hence the ergodic hypothesis is assumed to be valid. This property allows the equating of the time average of any property of a member of the ensemble to the ensemble average of that property. Precise conditions can be stated for a process to be ergodic; however in practice it is usually impossible to verify that these conditions are satisfied. In order not to be lost in the mire of complete generality the time-dependent terms will henceforth be assumed as stationary, ergodic, random time series with mean zero. While there are no data on chemical processes of the kind desired here in the literature, the ergodic assumption is usually taken as true.

It is now possible to define quantitative measures of the statistical nature of these disturbances. The mean value of a variable is

$$X^N = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} x(t)\, dt = E\,[x(t)] \tag{5}$$

The correlation function between two variables is defined as

$$\phi_{xy}(s) = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \bar{x}(t)\bar{y}(t+s)\, dt = E\,[\bar{x}(t)\,\bar{y}(t+s)] \tag{6}$$

where

$$\bar{x} = x(t) - x^N \text{ and } \bar{y} = y(t) - y^N$$

If $\bar{x}$ and $\bar{y}$ are the same, ϕ_{xx} is called the *autocorrelation function*, otherwise it is called the *cross-correlation function*.

It is also convenient to introduce the spectral densities. A spectral density is the Fourier transform of a correlation function:

$$\theta_{xy}(w) = \int_{-\infty}^{\infty} \phi_{xy}(s)\, e^{-iws}\, ds \tag{7}$$

These functions are sufficient to characterize the nature of the random disturbances and as shall be seen later to describe the response of linear systems to such disturbances.

The dynamic nature of linear systems may be characterized by two alternate methods: the impulse response method and the frequency response method. A stable nonlinear process can be represented in the small by a linear system.

The impulse response method states that the m inputs and n outputs of a physically realizable linear system are related by a convolution integral. That is

$$\bar{Y}(t) = \int_{-\infty}^{\infty} \bar{\bar{w}}(\xi)\, \bar{X}(t-\xi)\, d\xi \tag{8}$$

where

$$\bar{Y} = \begin{bmatrix} \bar{y}_1 \\ \bar{y}_2 \\ \vdots \\ \bar{y}_m \end{bmatrix}, \qquad \bar{X} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_n \end{bmatrix}$$

are output and input vectors, respectively, and $\bar{\bar{w}}(\xi)$ is a matrix of impulse response or weighting functions. The matrix $\bar{\bar{w}}(\xi)$ completely characterizes the dynamic nature of the linear system and has the property

$$w(\xi) = 0, \quad \xi < 0$$

for any stable physically realizable system.

The Fourier transform of the impulse response matrix is called the *transfer function matrix* $\bar{\bar{G}}(w)$:

$$\bar{\bar{G}}(w) = \int_{-\infty}^{\infty} \bar{\bar{w}}(\xi)\, e^{-iw\xi}\, d\xi \tag{9}$$

Suppose in a linear system the inputs are constants, that is steady state values, then $\bar{X} = \bar{X}^N$ and

$$\bar{Y}^N = \int_{-\infty}^{\infty} \bar{\bar{w}}(\xi)\, d\xi \cdot \bar{X}^N$$

On the other hand the integral appearing in this equation is the Fourier transform of $\bar{\bar{w}}(\xi)$ at zero argument, so $\bar{Y}^N = \bar{\bar{G}}(0)\, \bar{X}^N$

For a linear process

$$\bar{Y}^{N+1} - \bar{Y}^N = \bar{\bar{G}}(0)\, [\bar{X}^{N+1} - \bar{X}^N] \tag{10}$$

where N and $N+1$ indicate two steady state values.

Let the vector $\bar{X}$ represent the variations about the steady state $\bar{X}^N$. It will be supposed that these variations are the result of a stationary random ergodic process. Then the outputs from the linear process will have the same properties and be given by

$$\bar{Y}(t) = \int_{-\infty}^{\infty} \bar{\bar{w}}(\xi)\, \bar{X}(t-\xi)\, d\xi$$

Let this equation be post multiplied by the $\bar{X}^T(t-s)$, where the superscript

indicates the taking of the transpose. Then

$$\overline{Y}(t)\,\overline{X}^T(t-s) = \int_{-\infty}^{\infty} \overline{\overline{w}}(\xi)\,\overline{X}(t-\xi)\,\overline{X}^T(t-s)\,d\xi$$

and application of the operator E gives

$$E\,[\overline{Y}(t)\,\overline{X}^T(t-s)] = \overline{\overline{\phi}}_{xy}(s)$$

If the order of integration may be reversed, it follows that

$$\overline{\overline{\phi}}_{xy}(s) = \int_{-\infty}^{\infty} \overline{\overline{w}}(\xi)\,\overline{\overline{\phi}}_{xx}(s-\xi)\,d\xi \quad (11)$$

where $\overline{\overline{\phi}}_{xy}(s)$ is the correlation matrix between inputs and outputs and $\overline{\overline{\phi}}_{xx}(s)$ is the correlation matrix of inputs. The latter is diagonal if there is no input coupling.

The Fourier transform of the correlation matrix is known as the *spectral density matrix*, and since Equation (11) is a convolution integral, it follows that

$$\overline{\overline{\theta}}_{xy}(w) = \overline{\overline{G}}(w)\,\overline{\overline{\theta}}_{xx}(w) \quad (12)$$

giving a relation between the spectral density of the inputs, the cross-spectral densities, and the transfer function of the process. In particular at zero argument

$$\overline{\overline{G}}(0) = \overline{\overline{\theta}}_{xy}(0)\,\overline{\overline{\theta}}_{xx}^{-1}(0) \quad (13)$$

This equation is the key to the analysis in this paper. If one assumes that the random fluctuations are generated by a stationary random ergodic process, the spectral and cross-spectral densities obtained from the process enable one to determine the matrix $\overline{\overline{G}}(0)$ which will give the relationship Equation (10) between neighboring steady states. Thus use is made of the natural noise in the inputs themselves to characterize the system, and the system need not be upset in order to obtain a linear mathematical model of the system.

THE ITERATIVE MAXIMUM PROBLEM

The replacement of the process operator M by a locally valid linear model permitted the estimation of the local process steady state characteristics from an analysis of the operating data. This model is obtained from the analysis of process data for its operation about the N^{th} steady state and hence is valid only in the neighborhood of the N^{th} steady state. This local validity can be expressed by a constraint on $\overline{X}^{N+1}$, where $\overline{X}^{N+1}$ is the input vector of any neighboring steady state condition:

$$\overline{X}^N - \overline{\beta} \leq \overline{X}^{N+1} \leq \overline{X}^N + \overline{\beta} \quad (14)$$

where $\overline{\beta}$ expresses the range of validity of Equation (10) about the operating condition $\overline{X}^N$. The vector $\overline{\beta}$ controls the rate of convergence and the degree of cycling of the iterative optimization method and will actually vary during the optimization as will be shown later.

From the operating data about the N^{th} steady state it is possible to construct a locally valid linear model of the process with Equations (13) and (10). The vector $\overline{X}^{N+1}$ must now be chosen so that the $N+1^{st}$ steady state more nearly optimizes the process. This vector is obtained by solving the maximum problem stated in Equations (1), (3), and (4):

$$\underset{\overline{X}^{N+1}}{\text{Max}}\ P[\overline{X}^{N+1}, \overline{Y}^{N+1}, R]$$

$$\overline{Y}^{N+1} = \overline{Y}^N + G_N(0)\,(\overline{X}^{N+1} - \overline{X}^N) \quad (15)$$

$$\overline{X}^N - \overline{\beta} \leq \overline{X}^{N+1} \leq \overline{X}^N + \overline{\beta}$$

$$C_j(\overline{X}^{N+1}, \overline{Y}^{N+1}) < 0$$

The solution of Equations (15) yields the improved set of operating conditions consistent with the operating criteria.

The general problem given by Equation (15) will not be considered, since the methods of solution are not readily available. It should be recognized that this is a nonlinear programing problem. Problems of this type are receiving attention (7) at the moment, but general methods of broad applicability have not been developed. A special case will be solved in which the physical constraints and the objective function are linear. In this instance the methods of linear programing may be applied.

Consider the case where the profit function and the constraints C_i are linear. That is

$$P = \overline{p}^T\,\overline{Y}^{N+1} - \overline{c}^T\,\overline{X}^{N+1}$$

The physical constraints C_j are of the form

$$\overline{U}_* \leq \overline{X}^{N+1} \leq \overline{U}^* \quad (16)$$

$$\overline{w}_* \leq \overline{Y}^{N+1} \leq \overline{w}^*$$

These constraints limit the operation of the process to a certain region and represent the physical limits imposed on the process. The profit function is, by use of Equation (10)

$$P = \overline{p}^T[\overline{Y}^N + \overline{\overline{G}}_N(0)\,(\overline{X}^{N+1} - \overline{X}^N)] -$$

$$\overline{c}^T\,\overline{X}^{N+1} = [\overline{p}^T\,\overline{\overline{G}}_N(0) - \overline{c}^T]\,\overline{X}^{N+1} + f(X^N)$$

The constraints on the input variables Equations (16) and (14) can be combined into one constraint. The constraints

$$\overline{X}^N - \overline{\beta} \leq \overline{X}^{N+1} \leq \overline{X}^N + \overline{\beta}$$

and

$$\overline{U}_* \leq \overline{X}^{N+1} \leq \overline{U}^*$$

are equivalent to the one constraint

$$\overline{S}_* \leq \overline{X}^{N+1} \leq \overline{S}^*$$

if the vector $\overline{S}_*$ is constructed by selecting for its i^{th} element the greater of the i^{th} elements of the vectors $\overline{U}_*$ and $\overline{X}^N - \overline{\beta}$ and the vector $\overline{S}^*$ is constructed by selecting for its i^{th} element the lesser of the i^{th} elements of the vectors $\overline{U}^*$ and $\overline{X}^N + \overline{\beta}$.

The constraint on the output variable Y^{N+1} is by Equations (16) and (10)

$$\overline{w}_* - Y^N + \overline{\overline{G}}_N(0)\,\overline{X}^N \leq \overline{\overline{G}}_N(0)\,X^{N+1} \leq$$

$$\overline{w}^* - \overline{Y}^N + \overline{\overline{G}}_N(0)\,\overline{X}^N$$

Combining all these into the maximum problem one gets

$$\underset{\overline{X}^{N+1}}{\text{Max}}\ [\overline{p}^T\,\overline{\overline{G}}_N(0) - \overline{c}^T]\,\overline{X}^{N+1} + f(\overline{X}^N) \quad (17)$$

subject to $\overline{S}_* \leq X^{N+1} \leq \overline{S}^*$

$$\overline{w}_* - \overline{Y}^N + \overline{\overline{G}}_N(0)\,\overline{X}^N \leq \overline{\overline{G}}_N(0)\,\overline{X}^{N+1} \leq$$

$$\overline{w}^* - \overline{Y}^N + \overline{\overline{G}}_N(0)\,\overline{X}^N$$

Equation (17) is a linear programing problem, the solution of which can be obtained by any of the standard methods of linear programing. The iterative formulation and solution of Equations (17) comprise the computational sequence of the iterative optimization method. In summary, the computer system must

1. Collect data from the process operating about the N^{th} steady state.
2. Correlate these data [Equation (13)] form the maximum problem [Equation (17)] and solve for the best $N+1^{st}$ steady state.
3. Change the process to this more nearly optimum steady state and return to 1.

There are several points which need clarification before this iterative optimization method can be applied to actual processes. The exact role of the vector $\overline{\beta}$ must be discussed further. $\overline{\beta}$ controls the maximum step that can be made during any given optimization iteration. The most desirable step size depends on the exact nature of the process under consideration and its present operating level. If $\overline{\beta}$ is too large, the true optimum for the process may be bypassed, while if $\overline{\beta}$ is too small, it will take an unduly large number of iterations to achieve the optimum conditions. It seems desirable to choose a relatively large $\overline{\beta}$ until the optimum conditions are approached, then smaller values for fine convergence to the optimum conditions. If a limit cycle is obtained about the optimum conditions (observed by cycling steady state iterations), $\overline{\beta}$ should be reduced.

A question which arises is whether one can determine by a least squares, or regression, technique the relationship between inputs and outputs. That is is it possible to determine the constants in a linear model, like Equation (10), by correlating inputs and outputs for a system with input noise only. The analysis will not be presented here, but it may be shown that this is not the case.

APPLICATIONS

Although the most desirable application would be to an actual chemical processing plant, the iterative optimization method will be applied to simulated chemical processing plants.

The first process has been analyzed in detail by Aris (*1*) in connection with his work on dynamic programing and is the chemical reaction A⇌B occurring in a series of two stirred tank reactors each of unit holding time and will be considered here to show that the same result obtains. The rates of the forward and backward reactions are

$$r_f = A \exp\left[19 - \frac{12{,}000}{T}\right]$$

$$r_b = B \exp\left[41 - \frac{25{,}000}{T}\right]$$

It is desired to locate the temperatures T_1 and T_2 in the first and second reactors such that the production of the valuable product B is a maximum. The temperatures must lie in the range $550° \leq T \leq 650°$R. During the operation of the process random changes occur in the reaction medium temperatures. It is assumed that these changes occur by a combination of phenomena too complicated to resolve, though it is possible to adjust the mean temperatures in any reactor to any desired value by means of a heat exchange system. Temperature measuring instruments are placed in each reactor, and a device is attached to the exit feed stream to measure continuously the concentration of B. These measurements are fed directly to the optimization computer. It is the task of the computer to analyze the random temperature and concentration data, gaining enough information to adjust properly the mean temperature in each reactor to achieve the maximum yield of B from the reactor series.

The second process is far more complicated and more nearly represents the type of problem that is encountered in industry. This process is the reaction system

$$A + B \rightleftharpoons C$$

$$A + C \rightarrow D$$

occurring in a heated stirred tank reactor. These reactions are temperature dependent and have heats of reaction. The reaction rates and heat effects are

1. $A + B \rightarrow C$; $r_1 = A \cdot B \exp\left[32.93 - \frac{25{,}000}{T}\right]$; $\frac{\Delta H_1}{c_f \rho_f} = 320$

2. $C \rightarrow A + B$; $r_2 = C \exp\left[26.4 - \frac{22{,}300}{T}\right]$; $\Delta H_2 = -\Delta H_1$

3. $A + C \rightarrow D$; $r_3 = A \cdot C \exp\left[29.15 - \frac{23{,}000}{T}\right]$; $\frac{\Delta H_3}{c_f \rho_f} = -200$

The heating of the reactor is achieved by a heat exchanger. Random disturbances occur in the feed concentrations A_o and B_o and the flow rate of the heat exchange medium q_c. The reaction products are valuable, and the reactant materials are costly. Their relative worth is given below.

Species	Profit	Species	Cost
$A = y_1$	0.5	$A_o = x_1$	1.0
$B = y_2$	0.5	$B_o = x_2$	1.0
$C = y_3$	10.0	$q_c = x_3$	0.0
$D = y_4$	5.0		

The variables A_o, B_o, and q_c are constrained to the range (0.6, 1.4), and the concentration of product D must always be less than 0.4.

The variations of the input variables and the output variables are measured continually and fed to the optimization computer. The computer correlates these variations and adjusts the operation of the process so that the total profit will be a maximum subject to the constraints. The simulation is achieved by the continuous numerical integration of the ordinary differential equations which describe the dynamic performance of the process. This continuous numerical integration is performed on a high speed digital computer. The stirred tank process was chosen because of the relative simplicity of the differential equations.

The differential equations which describe the dynamic performance of a process are round by use of transient energy and mass conservation laws. Material balances over each of the chemical species on each of the reactors for the first process yield

$$\frac{dA_1}{dt} = \frac{A_o - A_1}{\theta} - A_1 k_f(T_1) + B_1 k_b(T_1)$$

$$\frac{dB_1}{dt} = \frac{B_o - B_1}{\theta} + A_1 k_f(T_1) - B_1 k_b(T_1)$$

$$\frac{dA_2}{dt} = \frac{A_1 - A_2}{\theta} - A_2 k_f(T_2) + B_2 k_b(T_2)$$

$$\frac{dB_2}{dt} = \frac{B_1 - B_2}{\theta} + A_2 k_f(T_2) - B_2 k_b(T_2)$$

where

$$k_f(T_i) = \exp\left[19 - \frac{12{,}000}{T_i}\right]$$

and

$$k_b(T_i) = \exp\left[41 - \frac{25{,}000}{T_i}\right]$$

These equations are subject to the conditions that $A_o = 1$, $B_o = 0$, and the temperatures T_1 and T_2 vary randomly with time.

The second process is more elaborate. The transient mass balances yield

$$\frac{dA}{dt} = \frac{A_o - A}{\theta} - A \cdot B \exp\left[32.93 - \frac{25{,}000}{T}\right] - AC \exp\left[29.15 - \frac{23{,}000}{T}\right] + C \exp\left[26.4 - \frac{22{,}300}{T}\right]$$

$$\frac{dB}{dt} = \frac{B_o - B}{\theta} + C \exp\left[26.4 - \frac{22{,}300}{T}\right] - AB \exp\left[32.93 - \frac{25{,}000}{T}\right]$$

$$\frac{dC}{dt} = \frac{C_o - C}{\theta} + AB \exp\left[32.93 - \frac{25{,}000}{T}\right] - C \exp\left[26.4 - \frac{22{,}300}{T}\right] - AC \exp\left[29.15 - \frac{23{,}000}{T}\right]$$

$$\frac{dD}{dt} = \frac{D_o - D}{\theta} + AC \exp\left[29.15 - \frac{23{,}000}{T}\right]$$

The transient energy balance over the reactor-heat exchanger system yields

$$\frac{dT}{dt} = \frac{T_o - T}{\theta} - \frac{hA}{v\rho_f c_f}[T - T_i]\left[1 - \frac{hA}{2q_c\rho_c c_{pc}}\right] - \frac{1}{c_{pf}\rho_f}\left[AB \exp\left[32.93 - \frac{25{,}000}{T}\right](\Delta H_1) + AC \exp\left[29.15 - \frac{23{,}000}{T}\right](\Delta H_2) + C \exp\left[26.4 - \frac{22{,}300}{T}\right](\Delta H_3)\right]$$

where

$$\frac{hA}{v\rho_f c_f} = 0.223 \text{ sec.}^{-1}$$

$$\frac{hA}{2\rho_c c_c} = 0.1115 \text{ cu. ft. sec.}^{-1}$$

$\theta = 200$ sec.

$T_o = 520°$R.

$T_t = 750°$R.

$C_o = 0$

$D_o = 0$

These equations are subject to the conditions that A_o, B_o, and q_c vary randomly with time. The continuous numerical integration and random modification of these simultaneous equations simulate the second process.

These ordinary simultaneous differential equations which describe both processes are integrated numerically with a four-point Runge-Kutta-Gill subroutine, chosen because it is readily available in coded form. A detailed analytical analysis of the integration error is not practical, so this analysis was performed experimentally. In the first process the integration was performed with ever decreasing integration increment until a steady state was reached in which the sum of the reactant concentration was equal to one to within six significant figures in both reactors. This integration increment, 0.01 θ, was then used in the remaining calculations. In the second process the integration was performed with ever decreasing increment until the solution was invariant to further changes. This increment was 0.01 θ.

The random modification in the input parameters which simulate the disturbances that occur in practice is achieved by a random number generating subroutine. The variations are in the form of random step functions about the mean values. A random number was generated by the subroutine from a population of mean zero, normal distribution, and fixed variance; this number was scaled and added to the mean value of the parameter to form the random step functions. Random modification of the coefficients of the differential equations during the course of the numerical integration are made. In the first process both temperatures were varied every 0.05 θ, with a variance of 1 deg. The second process inputs were varied every 0.05 θ with a variance equal to approximately 10% of the current value of that input.

With the processes so simulated the computer was programed according to the iterative optimization method to take control of the processes in order to improve the performance. The computer was programed to sample the process variables, correlate the data, solve the maxima problem, and modify the processes according to their optimum operating criteria. The stirred tank reactor because of its large capacity serves as an excellent filter for the noise. The output variations due to input noise are almost imperceptible, but the small variations were sufficient for the estimations.

THE OPTIMIZATION OF PROCESS I

The computer in the first example observes the operation of the process and selects the mean values of the temperatures in the first and second vessel so that the production of the reaction product B is a maximum. The theoretical development of the iterative optimization method is now applied to this example.

The data sampled from the process during its operation about the N^{th} steady state must be analyzed to give the information necessary to select the best $N+1^{st}$ steady state. Let the variables $B_2(t)$, $T_1(t)$, and $T_2(t)$ be denoted by $y_1(t)$, $x_1(t)$, and $x_2(t)$. The superscript N or $N+1$ denotes the mean value of a variable.

The steady states of the process are related by the matrix Equation (10) where

$$\overline{Y}^N = [y_1^N]$$

and

$$\overline{X}^N = \begin{bmatrix} x_1^N \\ x_2^N \end{bmatrix}$$

$$\overline{\overline{G}}_N(0) = \overline{\overline{\theta}}_{xy}(0)\ \overline{\overline{\theta}}_{xx}^{-1}(0)$$

where

$$\overline{\overline{\theta}}_{xx}(0) = \begin{bmatrix} \theta_{\bar{x}_1\bar{x}_1} & \theta_{\bar{x}_2\bar{x}_1} \\ \theta_{\bar{x}_1\bar{x}_2} & \theta_{\bar{x}_2\bar{x}_2} \end{bmatrix}$$

and

$$\overline{\overline{\theta}}_{xy}(0) = [\theta_{\bar{x}_1\bar{y}_1}\ \ \theta_{\bar{x}_2\bar{y}_1}]$$

[The functional notation (0) is dropped from here on for simplicity.] Hence

$$\overline{\overline{\theta}}_{xx}^{-1} = \frac{1}{\theta_{\bar{x}_1\bar{x}_1}\theta_{\bar{x}_2\bar{x}_2} - \theta_{\bar{x}_2\bar{x}_1}\theta_{\bar{x}_1\bar{x}_2}} \begin{bmatrix} \theta_{\bar{x}_2\bar{x}_2} & -\theta_{\bar{x}_2\bar{x}_1} \\ -\theta_{\bar{x}_1\bar{x}_2} & \theta_{\bar{x}_1\bar{x}_1} \end{bmatrix}$$

An interesting simplification occurs if the input variables are entirely independent. In that case $\theta_{\bar{x}_1\bar{x}_2} = \theta_{\bar{x}_2\bar{x}_1} = 0$ and

$$\overline{\overline{\theta}}_{xx}^{-1} = \begin{bmatrix} \dfrac{1}{\theta_{\bar{x}_1\bar{x}_1}} & 0 \\ 0 & \dfrac{1}{\theta_{\bar{x}_2\bar{x}_2}} \end{bmatrix}$$

Therefore in this case

$$\overline{\overline{G}}_N(0) = \begin{bmatrix} \dfrac{\theta_{\bar{x}_1\bar{y}_1}}{\theta_{\bar{x}_1\bar{x}_1}} & \dfrac{\theta_{\bar{x}_2\bar{y}_1}}{\theta_{\bar{x}_2\bar{x}_2}} \end{bmatrix}$$

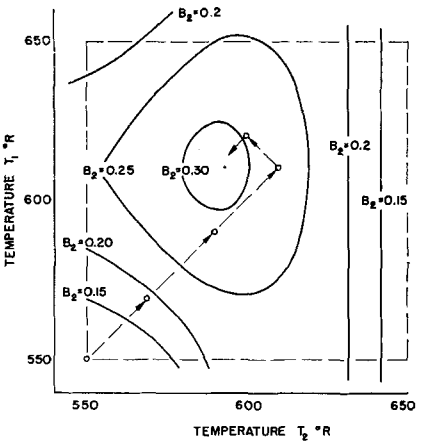

Fig. 1. The response surface for process I and the optimization path.

The input variables in this example are considered as independent.

The physical constraint vectors are [Equation (16)]

$$\overline{U}_* = \begin{bmatrix} 550 \\ 550 \end{bmatrix} \text{ and } \overline{U}^* = \begin{bmatrix} 650 \\ 650 \end{bmatrix}$$

The vectors $\overline{w}^*$ and $\overline{w}_*$ do not enter in this example, since there are no constraints on the outputs.

The vector $\overline{\beta}$ which limits the range of validity of the linear model is

$$\overline{\beta} = \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix}$$

where Δx_1 and Δx_2 are the maximum allowable steps away from the mean values x_1^N and x_2^N during optimization.

Hence the vectors $\overline{S}$ are defined as

$$\overline{S}_* = \begin{bmatrix} \text{Max } (550, x_1^N - \Delta x_1) \\ \text{Max } (550, x_2^N - \Delta x_2) \end{bmatrix}$$

$$\overline{S}^* = \begin{bmatrix} \text{Min } (650, x_2^N + \Delta x_1) \\ \text{Min } (650, x_2^N + \Delta x_2) \end{bmatrix}$$

The maximum problem as given by Equation (17) is

$$\underset{\overline{X}^{N+1}}{\text{Max}}\ [y_1 - \overline{\overline{G}}_N(0)\ \overline{X}^{N+1} + f(\overline{X}^N)]$$

subject to $\overline{S}_* \leqq \overline{X}^{N+1} \leqq \overline{S}^*$.

The solution to this maximum problem is particularly simple. The maximum of the linear objective function lies on an extreme point of the set of constraints. Hence it must be a vector whose elements are composed of elements selected from the vectors $\overline{S}_*$ and $\overline{S}^*$. It must be those elements which make the objective function a maximum. The solution must be

$$x_i^{N+1} = \begin{cases} \text{Max } (550, x_i^N - \Delta x_i), \text{ if } \dfrac{\theta_{x_i y_1}}{\theta_{\bar{x}_i\bar{x}_i}} < 0 \\ \text{Min } (650, x_i^N + \Delta x_i), \text{ if } \dfrac{\theta_{x_i y_1}}{\theta_{\bar{x}_i\bar{x}_i}} > 0 \end{cases}$$

At this stage it has been shown that the computer can select, by a simple choice, the best input variable vector X^{N+1} from information on the signs of the spectral density combinations

$$\frac{\theta_{x_1y_1}}{\theta_{\bar{x}_1\bar{x}_1}} \text{ and } \frac{\theta_{x_2y_1}}{\theta_{\bar{x}_2\bar{x}_2}}$$

The values of these spectral densities are obtained from the statistical analysis of the process operating data about the N^{th} steady state, and the numerical evaluation follows directly from Equation (18). Hence

$$\frac{\theta_{\bar{x}_i\bar{y}_1}}{\theta_{\bar{x}_i\bar{x}_i}} = \frac{\sum_{k=0}^{250}\sum_{l=0}^{1,023-k}\bar{x}_i(l\Delta t)\bar{y}_1((l+k)\Delta t)}{\sum_{k=0}^{32}\sum_{l=0}^{1,023-k}\bar{x}_i(l\Delta t)\bar{x}_i((l+k)\Delta t)}$$

where $\bar{x}_i = x_i(t) - x_i^N$ and $\bar{y}_i = y_i(t) - y_i^N$.

The data used in forming these finite sum approximations to the spectral density ratios were obtained by sampling the process variables every 0.01 θ intervals for a total elapsed time of approximately 10 holding times. The best $N+1^{st}$ steady state conditions were then obtained by the methods described above.

The process was run at the first steady state condition $T_1^1 = T_2^1 = 550$ deg. for approximately 10 holding times with the optimization computer sampling the data. The data were then correlated, and the best second steady state was obtained. The process was then changed to this steady state, and 7.5 holding times were allowed for the transients to die out. The process was then sampled to obtain data for the determination of the best third steady state and so on.

In the first trial run the vector $\bar{\beta}$ was held constant at $\bar{\beta}_1^T = (75°, 75°F.)$. This resulted in a bypassing of the true optimum conditions. In the second trial the vector $\bar{\beta}$ was varied during the optimization. At the beginning of the optimization $\bar{\beta}_2^T = (20°, 20°)$, and whenever a temperature reversal was suggested by the computer the elements of $\bar{\beta}$ were halved. This pattern resulted in the proper convergence of the iterative optimization method to the true optimum. In the third trial the vector $\bar{\beta}_3^T = (1.0, 1.0)$, and this takes an unduly large number of iterations to achieve the optimum conditions.

The results of these optimization runs are shown in Figures 1 and 2. Figure 1 shows the path of optimization on the process response surface for the $\bar{\beta}_2$ pattern; Figure 2 compares the convergence for the various $\bar{\beta}$ patterns.

THE OPTIMIZATION OF PROCESS II

Process II more nearly represents the type of optimization problem that is encountered in industry. As described before the optimization computer must extract enough information from the operation of this process to select the mean values of A_o, B_o, and q_c so that the total profit from the process is a maximum.

The theoretical developments of the iterative optimization method are now applied to this task. Label the variables as follows:

$$y_1 = A \qquad x_1 = A_o$$
$$y_2 = B \qquad x_2 = B_o$$
$$y_3 = C \qquad x_3 = q_c$$
$$y_4 = D$$

The superscripts N and $N+1$ denote the mean values of the variables. The vectors $\bar{X}$ and $\bar{Y}$ are

$$\bar{Y} = \begin{bmatrix}\bar{y}_1\\ \bar{y}_2\\ \bar{y}_3\\ \bar{y}_4\end{bmatrix} \text{ and } \bar{X} = \begin{bmatrix}\bar{x}_1\\ \bar{x}_2\\ \bar{x}_3\end{bmatrix}$$

The steady states for this process are related by Equation (10) where

$$\bar{\bar{G}}_N(0) = \bar{\bar{\theta}}_{xy}(0)\,\bar{\bar{\theta}}_{xx}^{-1}(0)$$

and where

$$\bar{\bar{\theta}}_{xy}(0) = \begin{bmatrix}\theta_{x_1y_1} & \theta_{x_1y_2} & \theta_{x_1y_3}\\ \theta_{x_2y_1} & \theta_{x_2y_2} & \theta_{x_2y_3}\\ \theta_{x_3y_1} & \theta_{x_3y_2} & \theta_{x_3y_3}\\ \theta_{x_4y_1} & \theta_{x_4y_2} & \theta_{x_4y_3}\end{bmatrix}$$

and

$$\bar{\bar{\theta}}_{xx}(0) = \begin{bmatrix}\theta_{x_1x_1} & \theta_{x_1x_2} & \theta_{x_1x_3}\\ \theta_{x_2x_1} & \theta_{x_2x_2} & \theta_{x_2x_3}\\ \theta_{x_3x_1} & \theta_{x_3x_2} & \theta_{x_3x_3}\end{bmatrix}$$

[The functional notation (0) has been dropped for convenience.]

In the case where the input variables are independent, $\theta_{x_ix_j} = 0$ $i \neq j$, the inversion of $\bar{\bar{\theta}}_{xx}$ is particularly simple and

$$\bar{\bar{G}}_N(0) = \begin{bmatrix}\frac{\theta_{x_1y_1}}{\theta_{x_1x_1}} & \frac{\theta_{x_2y_1}}{\theta_{x_2x_2}} & \frac{\theta_{x_3y_1}}{\theta_{x_3x_3}}\\ \frac{\theta_{x_1y_2}}{\theta_{x_1x_1}} & \frac{\theta_{x_2y_2}}{\theta_{x_2x_2}} & \frac{\theta_{x_3y_2}}{\theta_{x_3x_3}}\\ \frac{\theta_{x_1y_3}}{\theta_{x_1x_1}} & \frac{\theta_{x_2y_3}}{\theta_{x_2x_2}} & \frac{\theta_{x_3y_3}}{\theta_{x_3x_3}}\\ \frac{\theta_{x_1y_4}}{\theta_{x_1x_1}} & \frac{\theta_{x_2y_4}}{\theta_{x_2x_2}} & \frac{\theta_{x_3y_4}}{\theta_{x_3x_3}}\end{bmatrix}$$

where all the spectral densities are formed from the data taken from the process during its operation about the N^{th} steady state.

The constraints on the range of validity of this linear model are

$$\bar{X}^N - \bar{\beta} \leq \bar{X}^{N+1} \leq \bar{X}^N + \bar{\beta}$$

where

$$\bar{\beta} = \begin{bmatrix}\Delta x_1\\ \Delta x_2\\ \Delta x_3\end{bmatrix}$$

is the vector whose elements are the maximum allowable steps in the input variables away from the N^{th} steady state conditions.

The physical constraints on the system are

$$\bar{U}_* \leq \bar{X}^{N+1} \leq \bar{U}^*$$

and

$$\bar{Y}^{N+1} \leq \bar{w}^*$$

where

$$\bar{U}_* = \begin{bmatrix}0.6\\ 0.6\\ 0.6\end{bmatrix}, \bar{U}^* = \begin{bmatrix}1.4\\ 1.4\\ 1.4\end{bmatrix},$$

$$\text{, and } \bar{w}^* = \begin{bmatrix}\infty\\ \infty\\ \infty\\ 0.4\end{bmatrix}$$

The vectors $\bar{S}^*$ and $\bar{S}_*$ in the maximum problem are defined as

$$\bar{S}_* = \begin{bmatrix}\text{Max } [x_1^N - \Delta x_1, 0.6]\\ \text{Max } [x_2^N - \Delta x_2, 0.6]\\ \text{Max } [x_3^N - \Delta x_3, 0.6]\end{bmatrix}$$

$$\bar{S}^* = \begin{bmatrix}\text{Min } [x_1^N + \Delta x_1, 1.4]\\ \text{Min } [x_2^N + \Delta x_2, 1.4]\\ \text{Min } [x_3^N + \Delta x_3, 1.4]\end{bmatrix}$$

The profit and cost vectors are

$$\bar{p} = \begin{bmatrix}0.5\\ 0.5\\ 10.0\\ 5.0\end{bmatrix} \qquad \bar{c} = \begin{bmatrix}1.0\\ 1.0\\ 0.0\end{bmatrix}$$

The linear profit function for the process is defined as

$$P = \bar{p}^T\bar{Y}^{N+1} - \bar{c}^T X^{N+1} =$$
$$[\bar{p}^T\bar{\bar{G}}_N(0) - c^T]\bar{X}^{N+1} + f(\bar{X}^N)$$

The maximum problem to be solved in order to select the best $N+1^{st}$ steady state input vector is

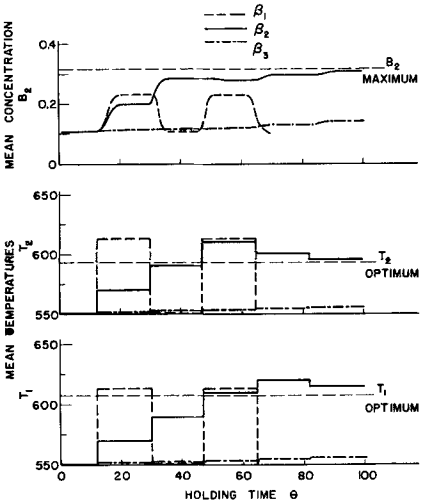

Fig. 2. The optimization of process I showing the effect of the size of the constraint $\bar{\beta}$.

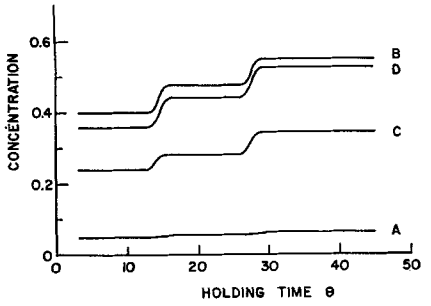

Fig. 3. The optimization of process II, first case, showing the variation of the mean output variables.

$$\underset{\overline{X}^{N+1}}{\text{Max}}\ [(\overline{p}^T\,\overline{\overline{G}}_N - \overline{c}^T)\,X^{N+1} + f(\overline{X}^N)]$$

subject to

$$\overline{S}^* \leq X^{N+1} \leq \overline{S}^*$$

$$\overline{\overline{G}}_N(0)\,\overline{X}^{N+1} \leq \overline{w}^* + \overline{\overline{G}}_N\,\overline{X}^N - \overline{Y}^N$$

This is a problem in three dimensional linear programing. Its solution can be relatively simple. The first set of constraints form a cube in the input variable three space. The last constraint defines a single plane; in reality the vector $\overline{w}^*$ constrains only y_i^{N+1}. The maximum of the linear objective function must necessarily lie at an extreme point of the set of constraints. There are at most twelve extreme points in this case. The optimum X^{N+1} can be determined simply by the direct comparison of the values of the profit function at each of these extreme points. The spectral density ratios are obtained from the data with the following finite sum approximation:

$$\frac{\theta_{x_i y_j}}{\theta_{x_i x_i}} = \frac{\sum_{k=0}^{300}\sum_{l=0}^{1,023-k} \overline{x_i}\,(l\Delta t)\,\overline{y_j}\,((l+k)\Delta t)}{\sum_{k=0}^{s}\sum_{l=0}^{1,023-k} \overline{x_i}\,(l\Delta t)\,\overline{x_i}\,((l+k)\Delta t)}$$

The input and output variables were sampled every 0.01 θ over a period of approximately 10 holding times. The data were then correlated to form the matrix $\overline{\overline{G}}_N(0)$, and the resulting maximum problem was solved. The solution of this maximum problem yielded the improved mean values of $A°$, $B°$, and q_c. The process was then changed to this improved steady state, and approximately 3 holding times were allowed for the transients to die out. This sampling, correlating, and improving sequence was then repeated until the optimum conditions were achieved. Figure 3 shows how the concentrations varied during the course of the optimization.

The second optimization run is similar to the first run except a constraint on the upper value of the output variable y_4 was added. The process must operate at maximum profit subject to constraints on both the input and output variables. Figure 4 shows how the concentration responded to the successive changes. The profit was increased at each step also.

THE CORRELATION FUNCTIONS AND SPECTRAL DENSITIES

Any practical optimization system must obtain the information for optimization in a relatively short time. In the case of a digital system continuous sampling of the process is impossible. The optimization must be made from information gained from a finite amount of discrete data. The analysis of this type of data is considered by Grenander and Rosenblatt (4) and has been applied to a problem similar to the ones presently under consideration by Homan and Tierney (5). These contain methods for approximating the correlation functions and the spectral densities from sets of discrete data.

Let $X_1(t)$ and $X_2(t)$ represent measurements of two given process variables. These measurements are made at discrete intervals of time over a certain period of time. The functions are defined only at integer multiples of the sample period:

$$X_1(t) = \begin{cases} X_1(n\Delta t) & n = 0, 1, 2, \ldots N \\ \text{undefined otherwise} \end{cases}$$

where Δt is the sample period and $N\Delta t$ is the total sample time. The correlation function can be approximated by a finite sum

$$\phi_{x_1 x_2}(k\Delta t) = \frac{\Delta t}{N-k+1}\sum_{l=0}^{l=N-k} \overline{X}_1\,(l\Delta t)\,\overline{X}_2\,((l+k)\Delta t)$$

where

$$\overline{X}(l\Delta t) = X(l\Delta t) - \frac{1}{N+1}\sum_{l=0}^{l=N} X(l\Delta t)$$

The accuracy of this finite sum approximation depends on the amount and nature of the data used. One test of the validity of the finite sum approximation is to compare the correlation function estimate both in the presence and absence of extraneous random disturbances. If the two estimates are approximately the same, the finite sum approximation may be adequate. Figures 5 and 6 show this comparison for the first process. A total of 1,024 pieces of data sampled every 0.01 holding times was used in these estimates. The correlations are made between the reactor temperatures T_1 and T_2 and the concentration of the final product B. Figure 7 compares estimates of the correlation function for the second process. A total of 1,024 pieces of data sampled every 0.01 holding times was used in making these estimates.

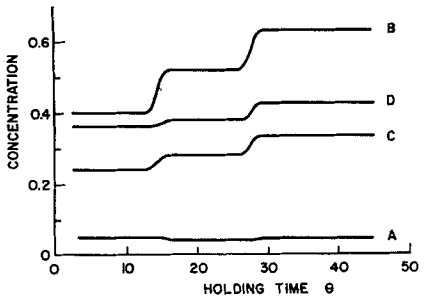

Fig. 4. The optimization of process II, second case, showing the variation of the mean output variables during the course of the run.

Comparison of the correlation functions in the presence and absence of extraneous random disturbances indicates that the finite sum estimates resolve the data up to time displacements of several holding times. After that the estimate became unreliable because less data are used to make the estimates for large time displacements.

It is convenient to compensate for this lack of validity by introducing a weighting function $S(k\Delta t)$ (4, 5).

This weighting function gives more weight in further calculations to the more reliable correlation function estimates. In many cases the validity of the spectral density calculations is quite dependent on the form of the weighting function. A form that has been found to be proper for problems

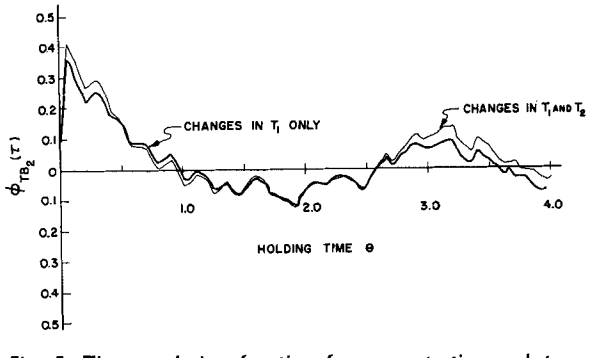

Fig. 5. The correlation function for concentration and temperature for process I.

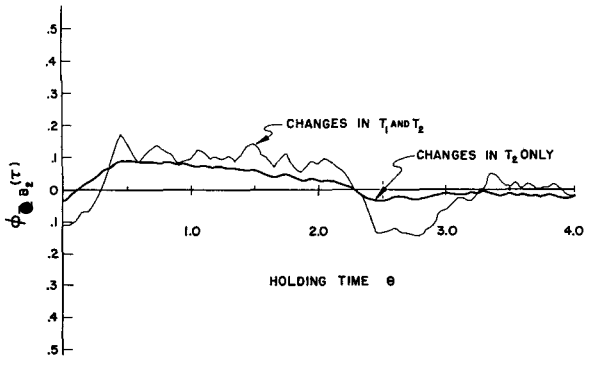

Fig. 6 The correlation function for temperature and concentration for process I.

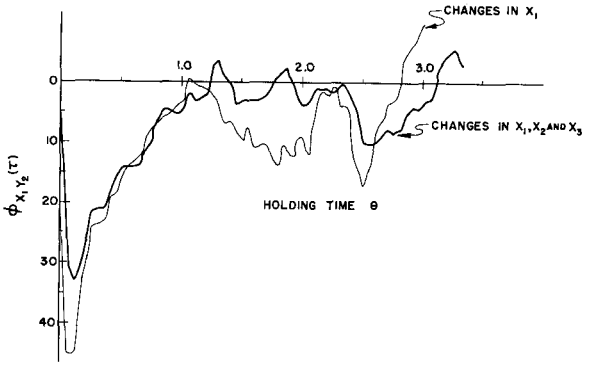

Fig. 7. Correlation function for concentrations in process II.

similar to the ones discussed here is the truncated linear form.

This weighting function weights the correlation estimate linearly up to the point where the data are considered worthless:

$$S(k\Delta t) = \begin{cases} \dfrac{N+1-k}{N+1}, & 0 \leq k < p \\ 0, & p < k < N \end{cases}$$

Beyond the displacement $p\Delta t$ the estimate is considered worthless, and its weight is zero.

The weighted correlation function is then

$$\phi_{x_1x_2}(k\Delta t) = \begin{cases} \dfrac{\Delta t}{N+1} \sum_{l=o}^{N-k} \overline{X}_1(l\Delta t)\, \overline{X}_2((l+k)\Delta t), & 0 \leq k < p \\ 0, & k > p \end{cases}$$

A finite sum approximation to the spectral density function at zero argument is

$$\theta_{x_1x_2} = \frac{\overline{\Delta t}^2}{N+1} \sum_{k=1}^{P} \sum_{l=o}^{N-k} \overline{X}_1(l\Delta t)\, \overline{X}_2((l+k)\Delta t) \quad (18)$$

In process I

$p = 250$ for cross correlations

$p = 32$ for auto correlations

In process II

$p = 200$ for cross correlations

$p = 8$ for auto correlations

In general the sample period should be less than the lowest natural frequency of the process.

The largest time displacement should be at least as large as the time constant of the process.

The total time over which data is gathered must be many times the maximum time displacement.

These generalizations have been obtained through experience and should be considered as rules of thumb for the estimation of the minimum sampling requirements.

DISCUSSION

It is difficult to make general statements about the applicability of the iterative optimization method. Each process presents unique difficulties which may or may not limit the use of the method. Continuous analysis of complex chemical mixtures must be made rapidly. Presently this presents a great limitation in the use of the method for the optimization of chemical reactors. These analytical problems must be solved before the method can be used extensively. The method requires a large scale, high speed, digital computer. The computers now commonly available are capable of optimizing several small processes simultaneously on a time shared basis.

The role of the vector $\overline{\beta}$, which controls the convergence properties of the method, is quite important. The best $\overline{\beta}$ depends heavily on the response surface of the process. More work must be done, both theoretical and experimental, on the characterization of the exact role of $\overline{\beta}$ on many different processes.

In large stage by stage processes, dynamic programing principles reduce the scale of the computations. These methods are particularly well suited to digital computation and hence can be used in conjunction with the iterative optimization method with ease. The developments presented in this work will, it is hoped, provide the stimulus for and the foundation of the work that must follow.

While the method described above may not have general application, it is thought that there will be applications in the future. If a process has no natural noise, then noise of limited variance might be introduced through the inputs. An improvement which might be incorporated into the process is to make use of the values of $\overline{\overline{G}}(0)$ calculated at each step. As the method now stands no use is made of past information on $\overline{\overline{G}}(0)$.

A more serious problem is that of the local representation of a nonlinear process by a linear model and its use in changing the process operation. This problem cannot be discussed here except to say that it is assumed that the random changes involved are small enough that linearity is valid locally. Certainly for large random fluctuations the estimate of the parameters in the linear model may be in considerable error.

NOTATION

A,B,C,D = chemical specie and concentrations of same

A_o,B_o,C_o,D_o = influent concentrations

$\overline{c}$ = cost vector

c_f = specific heat of reactant mixture

E = averaging operator

$\overline{\overline{G}}(0)$ = transfer function matrix at zero argument

$\overline{\overline{G}}(w)$ = transfer function

L = inverse process operator

M = process operator

$\overline{p}$ = profit vector

P = profit or objective function

$r(t)$ = random function

$r_i(t)$ = ith member of an ensemble of random function

T = reactor temperature

T_o = reactor influent temperature

T_i = inlet heating medium temperature

$\overline{U}_*, \overline{U}^*$ = bounds on constraints (inputs)

v = reactor volume

$\overline{\overline{w}}$ = impulse response matrix

w_{ij} = impulse response of jth output to ith input

$\overline{w}^*, \overline{w}_*$ = bounds on constraints (outputs)

x_i = inputs

$\overline{x}$ = average input

$\overline{X}^N$ = Nth steady state input vector

$\overline{\overline{X}}$ = vector of random inputs about steady state

$\overline{Y}$ = vector of random outputs about steady state

y_i = random output

$\overline{y}$ = average random output

$\overline{Y^N}$ = Nth steady state output vector

Greek Letters

$\overline{\beta}$ = vector of linear constraints

$\overline{\overline{\phi}}$ = correlation matrix

ϕ_{xx} = autocorrelation function

ϕ_{xy} = cross-correlation function

θ_{xx} = spectral density

θ_{xy} = cross-spectral density

$\overline{\overline{\theta}}$ = spectral density matrix

θ = nominal reaction holding time

ρ_f = fluid density

Subscript

$*$ = vector of lower bounds of variable

Superscript

$*$ = vector of upper bounds

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Gas Dynamic Processes Involving Suspended Solids

S. L. SOO

University of Illinois, Urbana, Illinois

Basic gas dynamic equations involving suspended solid particles were formulated. Considerations include momentum and heat transfer between the gaseous and solid phases. Significance of these contributions was illustrated with the case of expansion through a de Laval nozzle. Duct flow and normal shock problems were also discussed. The extent of earlier methods of approximation was pointed out.

Many processes and devices involve gas-solid suspension. A few of these are pneumatic conveying, H-iron process (direct reduction of iron ore), nuclear reactor with gas-solid fuel feeding and/or cooling, nuclear propulsion scheme where ablation of reactor is deliberately allowed for the sake of high performance, and rockets having part of the combustion product in the solid phase. A fundamental study on steady turbulent motion of gas-solid suspension was reported earlier (*1*). Where high speed is involved, such as in some of the above examples, gas dynamic aspects of gas-solid suspensions become significant. The general aspects of motion involve acceleration, friction, heat transfer, and flow discontinuity. This study deals with one-dimensional motion for the sake of simplicity and develops some physical understanding of the contribution of interaction between the gas and the solid particles. The effects of turbulence will be accounted for with generalized parameters.

The basic equations of this study will be applicable to the general problem of one dimensional steady motion involving variation in flow area, an insulated wall or a wall with arbitrary distribution of temperature, friction, and motion in supersonic or subsonic range. The latter is particularly interesting in the present case because of the dispersion and absorption of sound by the solid particles. Therefore the speed of sound, usually a thermodynamic property, depends on the transport of momentum and energy between the two phases in the present case. Since the gas dynamic nature of the gas-solid suspension is most easily seen in nozzle flow process, a nozzle is taken as the major example; this is also consistent with its significance in applications. Flow of a gas-solid suspension through a nozzle has been studied by many, with various methods of approximation (*2, 3, 4*). The extent of these approximations will be considered here.

Because of the inertia of solid particles a gas-solid suspension demonstrates an interesting nature of relaxation. The case of the passage of a gas-solid suspension through a shock process is presented in this paper.

All numerical examples are based on a mixture involving 0.3 lb. of magnesia per pound of air, although the methods are applicable to mixtures of any composition.

BASIC EQUATIONS AND SOLUTIONS

To formulate the basic equations the following assumptions are made:

1. There is steady one-dimensional motion, and the effect of turbulence enters only in characteristic parameters.
2. The solid particles are uniformly distributed over each cross section, although it is understood that they are suspended by turbulence and interactions exist between components.
3. The solid particles are uniform in diameter and physical properties. Variations again can be accounted for with characteristic parameters in the following.
4. The drag on the particles is mainly due to differences between the mean velocities of particles and stream. It is expected that the minimum size of solid particles consists of millions of molecules each (even in the submicron range). Hence the velocity of each solid particle due to its thermal state is extremely low. Slip flow, if it occurs, again can be accounted for by an appropriate characteristic parameter.
5. The heat transfer between the gas and the solid is basically due to their mean temperature difference. Effect of fluctuation in temperature will be accounted for by proper characteristic parameters.
6. The volume occupied by the solid particles is neglected; so is the gravity effect.
7. The solid particles, owing to their small size and high thermal conductivity (as compared with those of the gas), are assumed to be at uniform temperatures.