Dynamic Optimization of a Two-Stage Reactor System

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With the development of relatively inexpensive control computers and on-stream analyzers, on-line dynamic optimization of nonlinear, multistage systems has become more feasible. Investigators have been concerned with the static optimization and control of single-stage and multistage systems, but few have considered the optimization of a multistage system whose behavior is nonstatic owing to stochastic changes in its input and environment, and whose optimal control policy is time varying.

This paper looks at the problem of dynamic optimization as it applies to the analysis of a multistage continuous stirred-tank reactor system. A variational approach, in which the physical restraints on the manipulatable variables are included by a parametric representation, led to a bang-bang, sampled-data, optimal control law, or an equivalent analytical expression for continuous optimal control. Inclusion of the inequality relationships, specifying amplitude constraints on the manipulatable variables by a penalty function, resulted in a set of nonlinear Euler-Lagrange equations specifying the control law.

Dynamic optimization involves the evaluation of an optimal dynamic control strategy, which specifies the manner in which the manipulatable variables of a system should be controlled so as to extremize some criterion of system performance over some future interval of time. This paper discusses the dynamic optimization of a two-stage, continuous, stirred-tank reactor system. The objective is to determine a control law specifying how the coolant flow rate to each reactor should be controlled to maximize the time average conversion of the reactants to a particular product over a specified control time interval.

THEORY OF DYNAMIC OPTIMIZATION

In the subsequent general discussion, the term "system" will refer to controllable units of a chemical plant whose purpose is to transform the state of its inputs to more valuable output states. The system and associated subsystems are assumed to be in situ, and optimization pertains only to the mode in which the system is controlled. Dynamic optimal control, as discussed in this paper, refers to the strategy by which the controllable parameters of the system are manipulated so as to extremize (maximize or minimize) some criterion of the system performance over some future interval of time. The performance criterion is assumed to be an analytical function of the state of the system, its inputs and surroundings, and represents a measure of the effectiveness of the control strategy. The future behavior of the system is predictable via the system equations, or mathematical model, which may be represented by a set of first-order, nonlinear, differential equations relating the dependent output state variables to the independent variable, time, the stochastic input variables, and the independently controllable, manipulatable variables. Physical limitations on the system, as imposed by safety considerations, subsystem dynamics, limiting, etc., representing constraints on the state variables, manipulatable variables, and time rates of change of manipulatable variables, are formulated in terms of inequality relationships.

The following discussion reiterates the basic problem in mathematical terms. In subsequent mathematical formulas, lower case letters such as x will denote a vector notation for a class of variables with components x_1, $x_2, \ldots x_n$. Manipulatable variables are independent, external variables subject to direct control and providing the means by which the system performance is altered. Uncontrollable variables are independent input variables changing in a random manner and representing load changes and external disturbances. State variables are dependent variables characterizing the output of the system. In all subsequent discussions, unless otherwise noted, the variables m, u, and x are functions of time.

The initial step involves the definition of an objective whose satisfaction justifies the expenditure of time, effort, and resources to accomplish it. In problems of dynamic optimization, this object normally involves the extremization of a performance criterion, an analytical function of the state of the system and its environment defined over some future interval of time and giving some measure of the quality of performance.

Dynamic optimal control problems have been classified into three basic problems resulting in three fundamental dynamic performance criteria. The basic optimal control problems of universal importance have been referred to as the *minimum time control problem,* the *terminal control problem,* and the *minimum-integral control problem.*

The minimum-time control problem involves an admissible control strategy which will take the system from its present state $x(0)$ to a final state $x(f)$ in the shortest possible time. Such a problem is discussed in the paper by Eckman and Lefkowitz (6), wherein the objective is the minimization of the total processing time in a batch reactor.

A terminal control problem may be stated as the determination of an admissible control vector $m(t)$, such that, in a given time interval, the system will be taken from an initial state $x(0)$ into a state in which one or a combination of the state variables will be a minimum or maximum, and the remaining state variables will have fixed values within physical limits. Terminal control problems thus involve the achievement of a desired system response at one time only, since the response at earlier times is arbitrary within limits.

Minimum (or maximum) integral control problems involve an admissible control law $m(t)$ which extremizes an integral performance criterion. Such a problem might be stated as

$$\text{extremize} \qquad P = \int_0^{T_R} F(x; m; u; t)\, dt$$

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Subsequent analyses will be concerned with extremizing integrals of this type, as most problems in chemical process dynamic optimization involve, or can be reduced to, the extremization of an integral performance criterion.

The input variables are independent, fluctuating in an uncontrolled, random fashion with time. The state variables, on the other hand, are dependent and constrained with regard to their time rates of change and also with regard to their allowable magnitudes by physical limitations, safety considerations, etc. The dynamic constraints on the state variables may be represented by a set of first-order, differential equations, which define the time rate of change of each state variable and constitute the system equations which may be presented in the form

$$\frac{dx}{dt} = \dot{x} = G(x; m; u; t)$$

The constraints on the magnitude of the state variables may be represented by the following inequality relationships:

$$x \min \leq x \leq x \max$$

Physical limitations on the controlling elements of the system impose constraints on the rate of change and the amplitude of the manipulatable variables. These constraints may be represented by the inequalities

$$m \min \leq m \leq m \max$$

and

$$\dot{m} \min \leq \dot{m} \leq \dot{m} \max$$

Any control law $m(t)$ which satisfies these constraints may be regarded as an admissible control law.

Mathematically the basic problem is dynamic optimization can be stated in general terms as

find $\quad m(t) = C(x; u; t, \tau_R)$

so as to maximize

$$P = \int_0^{\tau_R} F(x; m; u; t)\, dt$$

subject to the equality constraints

$$\dot{x} = G(x; m; u; t)$$

and the inequality constraints

$$x \min \leq x \leq x \max$$
$$m \min \leq m \leq m \max$$
$$\dot{m} \min \leq \dot{m} \leq \dot{m} \max$$

Problems involving the extremization of an integral, the variables of whose integrand are constrained by equality and inequality relationships, are best solved by one of three basic techniques, the application of Pontryagin's maximum principle, Bellman's principle of optimality, or the theories of variational calculus. Pontryagin's maximum principle is well presented in his text (*10*) with applications in articles by Rozonoer (*11*) and Desoer (*5*). Bellman's principle of optimality, as applied to constrained integral extremizing, is defined in general terms in his texts (*2*), (*3*), and (*4*), with applications in Aris (*1*). Fox (*7*) discusses the classical variational theory, while Kipiniak (*8*) considers in some detail the variational approach to dynamic optimization problems. A somewhat tutorial presentation of these three methods, as applied to a simple problem, is offered in a companion paper (*12*). A more detailed discussion may be found in reference *13*.

DEFINITION OF SYSTEM AND APPROACH TO OBJECTIVE

The objective is to establish a dynamic optimal control strategy for a multistage system consisting of two identical, continuous, stirred-tank reactors, separated by an inter-

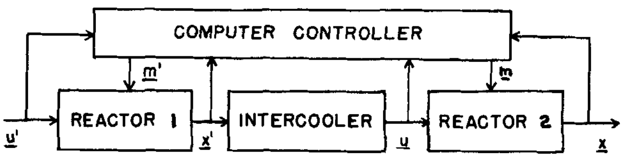

Fig. 1. Information flow block diagram.

cooler. Each externally cooled chemical reactor is fed with a single stream, five-component (A, B, C, D, and diluent), incompressible solution, and in each reactor the homogeneous, liquid-phase, exothermic, reversible reaction $A + B \rightleftarrows C + D$ is occurring. The capacity of each well-lagged, perfectly mixed reactor is sufficiently large, in comparison with that of the cooling facilities, to justify neglecting the dynamic aspects of the reactor cooling coils and intercooler.

The information flow block diagram presented in Figure 1 describes the orientation of the system with respect to a computer controller.

Dynamic control in the form of a sampled data control system is assumed to exist, since the control strategy depends upon data derived at some discrete instant of time, and the subsequent evaluation of the optimal control law takes a finite length of time. The sampling and control interval is short, compared with the mean period of fluctuation of the inputs, justifying the assumption that the inputs are constant at their sampled values during the subsequent control interval.

At the sampling instant, information regarding the state of the inputs and environment associated with the two reactors is fed forward to the control computer and is combined with information fed back from the outputs of each reactor. The initial step in the development of the subsequent control policy is to use this information to evaluate the terminal, or boundary, values for the appropriate variables associated with the dynamic control policy. This steady state optimization inherently involves a trial-and-error application of the principle of optimality, wherein arbitrary values for the steady state control effort for the first reactor of the sequence are combined with the corresponding optimal control values for the second reactor. The values of m', together with the corresponding values of m lead to a maximum value for the steady state performance criterion, serve to establish the terminal control policy. The next step is the specification of the path by which m and m' change from initial values $m(0)$ and $m'(0)$ toward these optimal steady state values.

It can be postulated from physical intuition or by the principle of optimality that, no matter what control strategy is selected for the first reactor of the sequence, the entire system will not be dynamically optimized unless the control strategy for the second reactor is dynamically optimal. This implies that, for any control interval, the optimal control vector $m(t)$ associated with reactor 2 extremizes the constrained performance criterion associated with reactor 2. The control strategy for any control interval for the first reactor of the sequence, on the other hand, has no effect on the control of the second reactor until the subsequent control interval. Then it affects the control policy for the second reactor only as it affects the values of the input variables to reactor 2 at the subsequent sampling instant.

Thus, the control policy for reactor 1 is a terminal control policy specifying that the admissible control vector $m'(t)$ should be such as to take the system from its initial sampled state $x'(0)$ toward a final state $x'(f)$ in a control interval. The final state $x'(f)$ is that state which results in inputs to the second reactor $u(0)$ which would lead to an overall global optimal policy for the subsequent control interval. If during each control interval one attains the state $x'(f)$ in the first reactor, the dynamic optimal policy is analogous to the steady state optimal policy involving the selection by trial-and-error of a control policy for reactor 1 which, when combined with the dynamic optimal control policy for reactor 2, results in an overall extremum for the performance criterion. The basic difference from the steady state optimization by dynamic programing involves the dynamic nature of the control policy and the fact that the control policy for the first reactor of the sequence affects the second reactor's policy only in the subsequent control interval.

If the mean period of fluctuation of the inputs is much larger than the time constant of the system, a suitable control policy might involve changing m' to that value which would result in an optimal steady state, and then changing m from $m(0)$ toward its corresponding optimal value along a trajectory which extremizes the performance criterion.

The subsequent section deals with the application of these principles to the analysis of the predescribed system.

SYSTEM EQUATIONS, CONSTRAINTS, AND PERFORMANCE CRITERION

The dynamic material balance around either reactor yields

$$V\frac{dC_C}{d\theta} = qC_{Ci} - qC_C + r\,(C_C, T)\,V \tag{1}$$

where

$$r(C_C, T) = k_1^* \exp\,(-E_1/RT)\,(C_{Ai} + C_{Ci} - C_C)\,(C_{Bi} + C_{Ci} - C_C) - k_2^* \exp\,(-E_2/RT)C_C\,(C_{Di} - C_{Ci} + C_C) \tag{2}$$

Multiplying (1) through by τ_R/VC_R one obtains

$$\frac{dC_C/C_R}{d\theta/\tau_R} = \frac{q\tau_R}{V}\left(\frac{C_{Ci}}{C_R} - \frac{C_C}{C_R}\right) + \frac{\tau_R}{C_R}r(C_C, T) \tag{3}$$

The energy balance for either reactor may be represented by

$$\rho C_p V\frac{dT}{d\theta} = q\rho C_p T_i - q\rho C_p T - \Delta H r(C_C, T)V - UA_C\Delta T_m \tag{4}$$

where

$$UA_C\Delta T_m = \frac{UA_C(T - t_i)}{1 + UA_C/2wC_{pc}} \tag{5}$$

Substituting (5) into (4) and multiplying through by $\tau_R/VT_R\rho C_p$ one gets

$$\frac{dT/T_R}{d\theta/\tau_R} = \frac{q\tau_R}{V}\left(\frac{T_i}{T_R} - \frac{T}{T_R}\right) - \left(\frac{\Delta H\tau_R}{\rho C_p T_R}\right)r(C_C, T) - \frac{UA_C\tau_R}{V\rho C_p}\left(\frac{1}{1 + UA_C/2wC_{pc}}\right)\left(\frac{T}{T_R} - \frac{t_i}{T_R}\right) \tag{6}$$

The energy balance for the intercooler may be represented by the expression

$$U_iA_i\Delta T_{mi} = U_iA_i\left[\frac{(T_i - t_o) + (T - t_i)}{2}\right] \tag{7}$$

$$= w_iC_{pc}\,(t_o - t_i) \tag{8}$$

$$= q\rho C_p\,(T_i - T) \tag{9}$$

Combining (7), (8), and (9) one gets

$$T = \left[\frac{q(2/U_iA_i + 1/w_iC_{pc})\rho C_p - 1}{q(2/U_iA_i + 1/w_iC_{pc})\rho C_p + 1}\right]T_i + \left[\frac{2}{q(2/U_iA_i + 1/w_iC_{pc} + 1}\right]t_i \tag{10}$$

Multiplying (10) thorugh by $1/T_R$ and then multiplying the numerator and demoninator by τ_R/V one obtains

$$\frac{T}{T_R} = \left\{\frac{\frac{q\tau_R}{V}\left(\frac{2\rho C_p}{U_iA_i} + \frac{\rho C_p}{w_iC_{pc}}\right) - \frac{\tau_R}{V}}{\frac{q\tau_R}{V}\left(\frac{2\rho C_p}{U_iA_i} + \frac{\rho C_p}{w_iC_{pc}}\right) + \frac{\tau_R}{V}}\right\}\frac{T_i}{T_R} + \left\{\frac{2\frac{\tau_R}{V}}{\frac{q\tau_R}{V}\left(\frac{2\rho C_p}{U_iA_i} + \frac{\rho C_p}{w_iC_{pc}}\right) + \frac{\tau_R}{V}}\right\}\frac{t_i}{T_R} \tag{11}$$

The system variables may be redefined according to the following dimensionless classes.

Uncontrollable input variables

$$\frac{q\tau_R}{V} = u_1 \quad \frac{C_{Ai}}{C_R} = u_2 \quad \frac{C_{Bi}}{C_R} = u_3 \quad \frac{C_{Ci}}{C_R} = u_4$$

$$\frac{C_{Di}}{T_R} = u_5 \quad \frac{T_i}{T_R} = u_6 \quad \frac{t_i}{T_R} = u_7$$

State variables

$$\frac{C_C}{C_R} = x_1 \quad \frac{T}{T_R} = x_2$$

Manipulatable variable

$$\frac{1}{1 + UA_C/2wC_{pc}} = m_1$$

Time

$$\frac{\theta}{\tau_R} = t$$

Constants

$$-\frac{\Delta HC_R}{\rho C_p T_R} = a \quad \frac{UA_C\tau_R}{V\rho C_p} = b$$

$$\frac{2\rho C_p}{U_iA_i} + \frac{\rho C_p}{w_iC_{pc}} = c \quad \frac{\tau_R}{V} = d$$

$$k_1^* C_R\tau_R = A_1 \quad k_2^* C_R\tau_R = A_2$$

$$-E_1/RT_R = B_1 \quad -E_2/RT_R = B_2$$

In terms of these dimensionless variables, the system equations are written as follows (primed variables relate to reactor 1):

Reactor 1

$$\frac{dx_1'}{dt} = u_1'(u_4' - x_1') + r(x_1', x_2') \tag{12}$$

$$\frac{dx_2'}{dt} = u_1'(u_6' - x_2') + ar(x_1', x_2') - bm_1'(x_2' - u_7') \tag{13}$$

where

$$r(x_1', x_2') = A_1 \exp\,(B_1/x_2')\,(u_2' + u_4' - x_1')\,(u_3' + u_4' - x_1') - A_2 \exp\,(B_2/x_2')x_1'\,(u_5' - u_4' + x_1') \tag{14}$$

Reactor 2

$$\frac{dx_1}{dt} = u_1(u_4 - x_1) + r(x_1, x_2) \tag{15}$$

$$\frac{dx_2}{dt} = u_1(u_6 - x_2) + ar(x_1, x_2) - bm_1(x_2 - u_7) \qquad (16)$$

where

$$r(x_1, x_2) = A_1 \exp(B_1/x_2)(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) - A_2 \exp(B_2/x_2)x_1(u_5 - u_4 + x_1) \qquad (17)$$

Intercooler

$$u_6 = \left(\frac{CU_i - d}{CU_i + d}\right) x_2' + \left(\frac{2d}{CU_i + d}\right) u_2' \qquad (18)$$

To obtain an admissible control law, it is necessary to take into account the physical limitations on the amount of available coolant. This entails satisfying the following inequalities:

$$0 \leq m_1' \leq m_1'\max$$

and

$$0 \leq m_1 \leq m_1 \max \qquad (19)$$

The objective is to vary m_1 and m_1' such that the conversion of component C, $q(C_c - C_{ci})$, over the subsequent control interval is as large as possible. The time average value of conversion to be maximized over the interval of time from the present time $\theta = 0$ to the future time $\theta = \tau_R$ becomes

$$\frac{1}{\tau_R} \int_0^{\tau_R} q(C_c - C_{ci})\, d\theta \qquad (20)$$

Maximizing this integral is equivalent to maximizing the integral P, where

$$P = \int_0^1 \frac{q\tau_R}{V}\left(\frac{C_c}{C_R} - \frac{C_{ci}}{C_R}\right) d\left(\frac{\theta}{\tau_R}\right) \qquad (21)$$

DEVELOPMENT OF OPTIMAL CONTROL STRATEGY

The initial step in the formulation of the control law is the evaluation of an optimal, steady state, control policy based on the sampled values for the system inputs. This involves the determination of that value of m_1', restricted only by the relationship $0 \leq m_1' \leq m_1'$ max together with m_1, which maximizes the conversion in the second reactor such that the overall conversion $u_1(x_1' - u_4)$ is maximized. The constraints on the value of m_1 involve the satisfaction of the steady state equations

$$0 = u_1(u_4 - x_1) + r(x_1, x_2)$$
$$0 = u_1(u_6 - x_2) + ar(x_1, x_2) - bm_1(x_2 - u_7) \qquad (22)$$

and the constraints on the magnitude of m_1 represented by

$$0 \leq m_1 \leq m_1 \max$$

This is equivalent to minimizing L', where

$$L' = u_1(x_1 - u_4) - \mu_1[u_1(u_4 - x_1) + r(x_1, x_2)] - \mu_2[u_1(u_6 - x_2) + ar(x_1, x_2) - bm_1(x_2 - u_7)]$$

subject to the constraint on the manipulatable variable, which can be rewritten equivalently in terms of the equality

$$m_1 = 0.5\, m_1 \max(1 + \sin\theta_1)$$

Since $0 \leq 1 + \sin\theta_1 \leq 2$, m_1 is forced to satisfy its constraint. If one includes this equality constraint, one may define the following objective criterion, whose maximization specifies the optimal steady state control policy for reactor 2:

$$L' = [u_1(x_1 - u_4)] - \mu_1[u_1(u_4 - x_1) + r(x_1, x_2)] - \mu_2[u_1(u_6 - x_2) + ar(x_1, x_2) - bm_1(x_2 - u_2)] - \mu_3[0.5\, m_1 \max(1 + \sin\theta_1) - m_1] \qquad (23)$$

The maximum of L is defined by the following relationships:

$$\frac{\partial L}{\partial x_1} = 0 = u_1(1 + \mu_1) - (\mu_1 + a\mu_2)\frac{\partial r}{\partial x_1} \qquad (24)$$

$$\frac{\partial L}{\partial x_2} = 0 = \mu_2(u_1 + bm_1) - (\mu_1 + a\mu_2)\frac{\partial r}{\partial x_2} \qquad (25)$$

$$\frac{\partial L}{\partial \mu_1} = 0 = u_1(u_4 - x_1) + r(x_1, x_2) \qquad (26)$$

$$\frac{\partial L}{\partial \mu_2} = 0 = u_1(u_6 - x_2) + ar(x_1, x_2) - bm_1(x_2 - u_7) \qquad (27)$$

$$\frac{\partial L}{\partial \mu_3} = 0 = 0.5\, m_1 \max(1 + \sin\theta_1) - m_1 \qquad (28)$$

$$\frac{\partial L}{\partial m_1} = 0 = b\mu_2(x_2 - u_7) + \mu_3 \qquad (29)$$

$$\frac{\partial L}{\partial \theta_1} = 0 = -0.5\, m_1 \max \mu_3 \cos\theta_1 \qquad (30)$$

From (27) either $\mu_3 = 0$ or $\cos\theta_1 = 0$. If $\cos\theta_1 = 0$, $\sin\theta_1 = +1$ or -1, and from (25) $m_1 = m_i$ max or 0, respectively. If $\mu_3 = 0$ from (26), $\mu_2 = 0$. If $\mu_2 = 0$ from (22), $\mu_1 = 0$ or $\partial r/\partial x_2 = 0$. Since $\mu_2 \neq 0$ from (21), then $\partial r/\partial x_2 = 0$. Therefore, the optimal, steady state, control policy implies m_1 is either at one of its boundary values or is defined by the equations

$$u_1(1 + \mu_1) - \mu_1\, \partial r/\partial x_1 = 0 \qquad (31)$$

$$\partial r/\partial x_2 = 0 \qquad (32)$$

$$u_1(u_4 - x_1) + r(x_1, x_2) = 0 \qquad (33)$$

and

$$u_1(u_6 - x_2) + ar(x_1, x_2) - bm_1(x_2 - u_7) = 0 \qquad (34)$$

Having defined the boundary values for the state and manipulatable variables, it is next necessary to determine the path by which the manipulatable variable associated with reactor 2 should change from an initial value $m_1(0)$ toward this calculated final optimal steady state value.

Mathematically, the problem involves the determination of

$$m_1(t) = C(x_1, x_2; u_1, u_2, \ldots u_7)$$

where

$$0 \leq m_1 \leq m_1 \max$$

so as to maximize

$$P = \int_0^1 u_1(x_1 - u_4)\, dt$$

where the variables of the integrand are subject to constraints represented by Equations (12), (13), and (14).

Of the variety of methods for including inequality constraints on integrals to be maximized by variational techniques, consider initially the technique described by Kipiniak (8) involving a penalty function. Rather than maximizing P, a modified performance criterion P' to be maximized is defined as

$$P' = \int_0^1 \{u_1(x_1 - u_4) - f(m_1)\}\, dt$$

where $f(m_1)$ is a penalty function defined as

$$f(m_1) = K[(2m_1 - m_1 \max)/m_1 \max]^{2N}$$

where K is a sufficiently small constant such that $f(m_1) << u_1(x_1 - u_4)$ when $0 \leq m_1 \leq m_1$ max, and N is sufficiently large to effect as sharp a constraint as desired. By inspection it can be seen that if m_1 becomes $>$ m_1 max or < 0, the positive quantity defined by $f(m_1)$ becomes large, tending to penalize P'. In terms of Lagrange multipliers, the problem may be reformulated as follows. find $m_1(t)$ so as to maximize the integal:

$$P' = \int_0^1 \left\{ u_1(x_1 - u_4) - K\left[\frac{2m_1 - m_1 \max}{m_1 \max}\right]^{2N} + \lambda_1[\dot{x}_1 - u_1(u_4 - x_1) - r(x_1, x_2)] + \lambda_2[\dot{x}_2 - u_1(u_6 - x_2) - ar(x_1, x_2) + bm_1(x_2 - u_7)] \right\} dt$$

Taking the variation of P' and equating the coefficients of δx_1, δx_2, $\delta\lambda_1$, $\delta\lambda_2$, and δm_1 to zero one gets the following Euler-Lagrange equations, respectively:

$$u_1(1 + \lambda_1) - (\lambda_1 + a\lambda_2)\,\partial r/\partial x_1 - \dot{\lambda}_1 = 0 \qquad (35)$$

$$\lambda_2(u_1 + bm_1) - (\lambda_1 + a\lambda_2)\,\partial r/\partial x_2 - \dot{\lambda}_2 = 0 \qquad (36)$$

$$-u_1(u_4 - x_1) - r(x_1, x_2) + \dot{x}_1 = 0 \qquad (37)$$

$$-u_1(u_6 - x_2) - ar(x_1, x_2) + bm_1(x_2 - u_7) + \dot{x}_2 = 0 \qquad (38)$$

$$\frac{-4\,KN}{m_1 \max^{2N}}(2m_1 - m_1 \max)^{2N-1} + b\lambda_2(x_2 - u_7) = 0 \qquad (39)$$

where

$$r(x_1, x_2) = A_1 e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) - A_2 e^{(B_2/x_2)} x_1(u_5 - u_4 + x_1) \qquad (40)$$

$$\frac{\partial r}{\partial x_1} = -A_1 e^{(B_1/x_2)}(u_2 + u_3 + 2u_4 - 2x_1) - A_2 e^{(B_2/x_2)}(u_5 - u_4 + 2x_1) \qquad (41)$$

and

$$\frac{\partial r}{\partial x_2} = -\frac{A_1 B_1}{x_2^2} e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) + \frac{A_2 B_2}{x_2^2} e^{(B_2/x_2)} x_1(u_5 - u_4 - x_1) \qquad (42)$$

Combination of Equations (35) through (42) leads to the following set of equations:

$$\dot{\lambda}_1 = u_1(1 + \lambda_1) + [\lambda_1 + a\lambda_2][A_1 e^{(B_1/x_2)}(u_2 + u_3 + 2u_4 - 2x_1) + A_2 e^{(B_2/x_2)}(u_5 - u_4 + 2x_1)] \qquad (43)$$

$$\dot{\lambda}_2 = \lambda_2(u_1 + bm_1) + [\lambda_1 + a\lambda_2)/x_2^2][A_1 B_1 e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) - A_2 B_2 e^{(B_2/x_2)} x_1(u_5 - u_4 + x_1)] \qquad (44)$$

$$\dot{x}_1 = u_1(u_4 - x_1) + A_1 e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) - A_2 e^{(B_2/x_2)} x_1(u_5 - u_4 + x_1) \qquad (45)$$

$$\dot{x}_2 = u_1(u_6 - x_2) + a\,A_1 e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) - a\,A_2 e^{(B_2/x_2)} x_1(u_5 - u_4 + x_1) - bm_1(x_2 - u_7) \qquad (46)$$

$$m_1 = 0.5\left[\frac{bm_1 \max^{2N} \lambda_2\,(x_2 - u_7)}{4\,KN}\right]^{\frac{1}{2N-1}} + 0.5\,m_1 \max \qquad (47)$$

The solution of Equations (43) through (47) defines necessary conditions for an optimal control policy $m_1(t)$ for reactor 2. To facilitate a solution to this set of nonlinear, first-order equations, the following simplifying assumptions are made.

1. A sampled data sensing system with a short sampling interval with respect to the system time constant and the period of input variable fluctuation is assumed to exist. Hence, over the control interval, the input variables are assumed to be constant at their sampled values $u(0)$.

2. The terminal time is assumed to be that time at which the system would effectively reach equilibrium following any step change in its input variables, thus permitting the specification of a boundary condition as a solution to the steady-state Euler-Lagrange equations.

Propagation of a solution to the Euler-Lagrange equations by numerical or electronic analogue integration constitutes the evaluation of the control law for reactor 2. The initial values for the state variables $x_1(0)$ and $x_2(0)$ are known from sampling. However, the required initial values for the Lagrange multipliers $\lambda_1(0)$ and $\lambda_2(0)$ cannot be sampled nor evaluated analytically. One must resort, therefore, to a repetitive trial-and-error procedure, wherein a convenient set of values for the initial conditions for the Lagrange multipliers is estimated and a solution is propagated toward the steady state. At some appropriate time, a comparison is made between the values of the variables and the precalculated, steady state values. Based on the variance from the steady state boundary conditions, new initial values for the Lagrange multipliers may be assumed in accordance with some gradient technique until trajectories satisfy the boundary conditions within suitable limits.

Having solved the integral control problem associated with the dynamic optimization of reactor 2, one concerns himself with the terminal control problem specifying the control policy for reactor 1. However, before attempting this analysis, consider the results obtained by re-examining the dynamic optimization of reactor 2 by a different method.

Consider the redefinition of the constrained manipulatable variable in terms of the parameter θ_1, in accordance with $m_1 = 0.5 \max\,(1 + \sin\theta_1)$. The modified performance criterion may be rewritten to include this new equality constraint to result in a problem involving the maximization of the integral:

$$\int_0^1 \{u_1(x_1 - u_4) + \lambda_1[\dot{x}_1 - u_1(u_4 - x_1) - r(x_1, x_2)] + \lambda_2[\dot{x}_2 - u_1(u_6 - u_2) - ar(x_1, x_2) + bm_1(x_2 - u_7)] + \lambda_3[0.5\,m_1 \max\,(1 + \sin\theta_1) - m_1]\}\,dt$$

Taking variations of the integral and equating the coefficient of δx_1, δx_2, $\delta\lambda_1$, and $\delta\lambda_2$ to zero one gets a set of equations identical to Equations (35) through (38). Also, equating the coefficients of ∂x_3, ∂m_1, and $\partial\theta_1$ to zero one obtains

$$0.5\,m_1 \max\,(1 + \sin\theta_1) - m_1 = 0 \qquad (48)$$

$$b\lambda_2(x_2 - u_7) - \lambda_3 = 0 \qquad (49)$$

$$0.5\,m_1 \max \lambda_3 \cos\theta_1 = 0 \qquad (50)$$

From (50), either $\lambda_3 = 0$ or $\cos\theta_1 = 0$. If $\cos\theta_1 = 0$, $\sin\theta_1 = +1$ or -1, and from (48), $m_1 = m_1 \max$ or 0. If $\lambda_3 = 0$ from (49), $\lambda_2 = 0$. If $\lambda_2 = 0$ from (36), $\lambda_1 = 0$ or $\partial r/\partial x_2 = 0$. Since $\lambda_1 \neq 0$ from (35), then $\partial r/\partial x_2 = 0$. Therefore, the control law is defined as

$$m_1 = \begin{cases} m_1 \max \\ C(x_1, x_2; u) \\ 0 \end{cases} \qquad (51)$$

That is, the control law consists of a series of subarcs over which the manipulatable variable is either at one of its boundary values or is defined by the following solution of the Euler-Lagrange equations:

$$\dot{\lambda}_1 = u_1(1 + \lambda_1) + \lambda_1 A_1 e^{(B_1/x_2)}(u_2 + u_3 + 2u_4 - 2x_1) + \lambda_1 A_2 e^{(B_2/x_2)}(u_5 - u_4 + 2x_1) \qquad (52)$$

$$\dot{x}_1 = u_1(u_4 - x_1) + A_1 e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - u_1) - A_2 e^{(B_2/x_2)} x_1(u_5 - u_4 + x_1) \qquad (53)$$

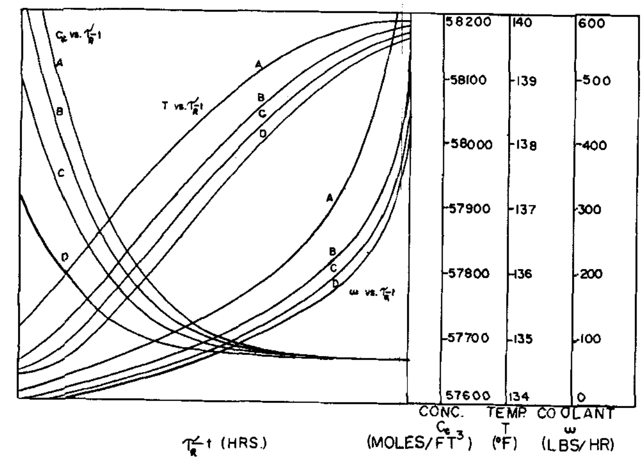

Fig. 2. Backward propagation of extremals.

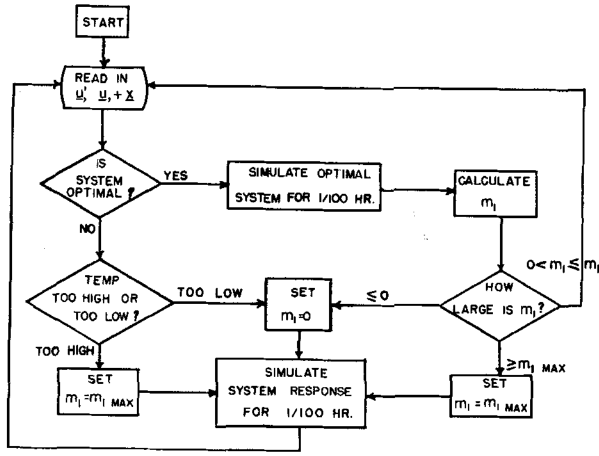

Fig. 3. Block diagram for simulation of optimal control.

$$\dot{x}_2 = u_1(u_6 - x_2) + a\,A_1e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) - a\,A_2e^{(B_2/x_2)}x_1(u_5 - u_4 + x_1) - bm_1(x_2 - u_7) \quad (54)$$

$$0 = -A_1B_1e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) + A_2B_2e^{(B_2/x_2)}x_1(u_5 - u_4 + x_1) \quad (55)$$

Solving Equation (55) for x_2 one gets

$$x_2 = (B_1 - B_2)/\ln\{[A_2B_2\,x_1(u_5 - u_4 + x_1)]/[A_1B_1(u_2 + u_4 - x_1)(u_3 + u_4 - x_1]\} = f(x_1) \quad (56)$$

Hence, $\dot{x}_2 = f^1(x_1)$.

Solving Equation (54) for m_1 one obtains

$$\begin{aligned} m_1 &= \{u_1(u_6 - x_2) + a\,A_1e^{(B_1/x_2)}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) - a\,A_2e^{(B_2/x_2)}x_1(u_5 - u_4 + x_1) - \dot{x}_2\}/b(x_2 - u_7) \\ &= \{u_1[u_6 - f(x_1)] + a\,A_1e^{(B_1/f(x_1))}(u_2 + u_4 - x_1)(u_3 + u_4 - x_1) - a\,A_2e^{(B_2/f(x_1))}x_1(u_5 - u_4 + x_1) - f^1(x_1)\}/b[f(x_1) - u_7] \\ &= C(x_1; u) \end{aligned} \quad (57)$$

Although an analytical expression has been obtained for the control law, in general the analysis of a nonlinear system will not lead to one.

An examination of the results obtained for the dynamic optimal control policy for reactor 2 shows that it specifies that the temperature should be controlled in a time-varying manner, which will maximize the reaction rate at all times.

For any control interval, the magnitude of the optimal reaction rate for reactor 2 depends upon the input concentration of component C. This implies that the control strategy for reactor 1 for the preceding control interval is such as to maximize the output concentration of component C for all sampling frequencies, that is at all times. As might be expected from the optimization of a multistage reactor system with a single reaction and a stoichiometric performance criterion, the control strategy is disjoint, and each reactor is individually controlled in a dynamically optimal fashion. Thus, the control law for reactor 1 is specified by Equation (57).

STEADY STATE OPTIMIZATION RESULTS

Although the steady state, optimal control policy is also disjoint, use was not made of this fact other than to verify the results of the optimization via dynamic programing. Numerical results indicated that the conversion of reactants into product C was a unimodal function of the magnitude of the manipulatable variable associated with reactor 1.

CONTROL LAW VIA POINT TECHNIQUE

To explore the feasibility of this technique, a single factorial program was designed very close to previously calculated initial conditions for the Lagrange multipliers. Solutions were propagated for 0.5 hr. of real time and required approximately 1 min. IBM-709 computer time. Since the time constant for the system was only 3 min., this method was deemed unfeasible for the on-line digital computer control. The instability of the highly nonlinear Euler-Lagrange equations, coupled with the necessity for high accuracy, tends to invalidate the high-speed, rep-op, analogue computer solution by the point technique.

CONTROL LAW VIA FLOODING TECHNIQUE

Since the singularities of the Euler-Lagrange equations are unstable saddle points, the control law may be precalculated by propagating trajectories backwards in time from the vicinity of the steady state points. By judiciously choosing the magnitude and nature of the initial perturbations from the steady state values, the state space can often be flooded adequately with a number of trajectories. Since the independent variable time is neither explicitly defined in the performance criterion nor in the constraints, very efficient use of this flooding technique can be made.

The set of trajectories resulting from flooding is reduced to an equivalent analytical expression for the control law.

To evaluate the facility with which the $x_1 - x_2$ state plane could be flooded, an arbitrary steady state point defined by T = 139.879°F., C = 0.57666 lb. moles/cu.ft., $\lambda_1 = 0.5025$, and $\lambda_2 = 0.6840 \times 10^{-5}$ was selected. Before propagating trajectories, the temperature was perturbed to the values of 139.87, 139.80, 139.70, and 139.60, resulting in trajectories A, B, C, and D, respectively, as indicated in Figure 2.

As the results indicate, very small perturbations from the singularity result in substantially different trajectories, implying that adequate flooding is feasible.

In order to utilize the set of trajectories defining the control law, it must be reduced to a more tractable form, such as polynomial.

IMPLEMENTATION OF ANALYTICAL CONTROL LAW FOR BOTH REACTORS

By including the constraint on the amplitude of the manipulatable variable by a parametric representation, an analytical expression for the control law of the form

$$m_1 = \begin{cases} 0 \\ C(x_1; u) \\ m_1 \max \end{cases} \quad (58)$$

was obtained for both reactors, where $C(x_1; u)$ is defined by Equation (57). At the sampling instant, the feedforward and feedback information is sufficient to determine whether the reactor is presently in an optimal state or not, that is whether the temperature is defined by the dimensionless relationship $\partial r/\partial x_2 = 0$ as represented by Equation (56). In general, the temperature is nonoptimal, resulting in an initial control strategy involving the manipulatable variable m_1, its upper boundary $m_1 \max$ if the temperature is higher than the optimal, or at its lower value 0 if the temperature is lower than optimal. This initial control strategy is maintained until the temperature changes to the optimal value, at which time the manipulatable variable on the reactor is changed according to the relationship defined by Equation (57).

A program was written for the digital (IBM-709) simulation of the response of the system subject to step changes in various input variables under this control law. The block diagram represented by Figure 3 indicates the steps involved in simulating dynamic optimal control for a single control interval, for either reactor.

The initial control effort involving m_1 and m_1' at their appropriate boundary values caused each reactor to approach an optimal state at as fast a rate as possible. The interval of time that m_1 or m_1' remained at a boundary value depended upon the magnitude of the perturbation of the initial state of the system from the optimal steady state. Recorded values for the accumulated conversion during optimally controlled and fixed controlled intervals indicated an augmentation of system performance due to the control effort. With short sampling intervals, the control law for each reactor may be specified by a bang-bang control law with the switching function defined by expression (56) or a proportional control law with the difference between x_1 and x_2 optimal providing the signal effecting the control action.

CONCLUSIONS

The nature of the mathematical model for this particular system led to an analytical expression for the control law which, in general, would not be obtained. However, from the analysis of this system, it may be postulated that the initial step in the dynamic optimization of a multistage system via variational techniques initially involves the establishment of the final steady state optimal control policy. Associated with this problem is the so-called *dimensionality curse* defined by Bellman (4). Following this, the optimal control strategy is evaluated by propagating trajectories in accordance with that solution of the Euler-Lagrange equation which satisfies the precalculated boundary conditions. The trial-and-error point technique for the solution of the boundary value problem associated with the Euler-Lagrange equations solution was deemed unfeasible by a digital or analogue computer technique. This implies that the control law might best be implemented by precalculating the control strategy and representing it by a flexible analytical expression.

NOTATION

A_C = heat transfer area of internal heating coils = 100 (sq. ft.)
A_i = heat transfer area for intercooler = 100 (sq. ft.)
$C_{Ai}, C_{Bi}, C_{Ci}, C_{Di}$ = inlet concentrations of components A, B, C, D, respectively (lb. moles/cu. ft.)
C_A, C_B, C_C, C_D = outlet concentrations of components A, B, C, D, respectively (lb. moles/cu. ft.)
C_p — heat capacity of inlet and outlet reactor streams = 0.5 (B.t.u./lb. °R.)
C_{pc} = heat capacity of coolant = 1.0 (B.t.u./lb. °R.)
C_R = reference concentration = 1.0 (lb. moles/cu. ft.)
E_1 = activation energy for forward reaction = 25,000 (B.t.u./lb. mole C produced)
E_2 = activation energy for reverse reaction = 50,000 (B.t.u./lb. mole C reacted)
$-\Delta H$ = heat of reaction = 25,000 (B.t.u./lb. mole C produced)
K = coefficient of penalty function = 0.001
k_1° = frequency factor for forward reaction = 2×10^{10}
k_2° = frequency factor for reverse reaction = 7×10^{18}
k_1 = forward reaction rate constant (lb. moles C/lb. mole A · lb. mole B · hr.)
k_2 = reverse reaction rate constant (lb. moles C/lb. mole C · lb. mole D · hr.)
m = manipulatable variables
N = penalty function power
q = volumetric flow rate of inlet and outlet streams (cu. ft./hr.)
$r(C_C,T)$ = reaction rate (lb. moles C produced/cu. ft. hr.)
R = gas constant = 1.986 (B.t.u./lb. mole · °R.)
t_i = inlet temperature of coolant (°R.)
t_o = outlet temperature of coolant (°R.)
T_i = inlet temperature of reactor feed solution (°R.)
T = outlet temperature of reactor solution (°R.)
ΔT_m = arithmetic average temperature difference (°R.)
T_R = reference temperature = 1,000 (°R.)
t = time
U = overall heat transfer coefficient for reactor coolant coils = 50 (B.t.u./hr. · sq. ft. °R.)
U_i = overall heat transfer coefficient for intercooler = 50 (B.t.u./hr. · sq. ft. °R.)
u = uncontrollable variables
V = volume of reactor contents = 100 (cu. ft.)
w = mass flow rate of coolant to reactor cooling coils (lb./hr.)
w_i = mass flow rate of coolant to intercoolers = 150,000 (lb./hr.)
w_{max} = maximum allowable coolant flow rate to reactors = 10,000 (lb./hr.)
x = state variables

Greek Letters

λ_j = Lagrange multipliers
μ_j = Lagrange multipliers
μ_1, μ_2, μ_3 = Langrange multipliers
ρ = density of feed and reactant solutions = 50 (lb./cu. ft.)
τ = sampling intervals (hr.)
τ_R = reference time = 1 (hr.)
θ = time (hr.)

LITERATURE CITED

1. Aris, Rutherford, 'The Optimal Design of Chemical Reactors: A Study in Dynamic Programming," Academic Press, New York (1961).
2. Bellman, R. E., "Dynamic Programming," Princeton University Press, Princeton, New Jersey (1957).
3. ———, "Adaptive Control Process: A Guided Tour," Princeton University Press, Princeton, New Jersey (1961).
4. ———, and S. E. Dreyfus, "Applied Dynamic Programming," Princeton University Press, Princeton, New Jersey (1962).
5. Desoer, C. A., *J. Franklin Inst.*, 271, 5 (1961).
6. Eckman, D. P., and I. Lefkowitz, *Control Eng.*, 4, 9 (1957).
7. Fox, Charles, "An Introduction to the Calculus of Variations," Oxford University Press, London, England (1954).

8. Kipiniak, Waleriau, "Dynamic Optimization and Control," The M.I.T. Press and Wiley, New York (1961).
9. Lapidus, Leon, et al., *A.I.Ch.E. Journal*, 7, 288 (1961).
10. Pontryagin, L. S., "The Mathematical Theory of Optimal Processes," Interscience, New York (1962).
11. Rozonoer, L. E., *Automation and Remote Control*, 20 (1959).
12. Thibodeau, R. D., and W. F. Stevens, "Dynamic Optimization," paper accepted for publication in *Chemical and Process Engineering*.
13. ———, Ph.D. thesis, Northwestern University, Evanston, Illinois (1963).

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Fluid-Flow Characteristics of Concurrent Gas-Liquid Flow in Packed Beds

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Reactions involving the concurrent flow of liquids and gases through packed beds are becoming increasingly common in both the petroleum and chemical industries. For proper design of these packed reactors, knowledge of the heat transfer and fluid-flow characteristics of the two-phase flow is required. Only one paper (*1*) has been published, dealing with pressure drop and liquid holdup, which covers a fairly wide range of two-phase flow conditions in packed beds. No studies that discuss the problem of heat transfer in packed beds operating with gas-liquid flow have come to the authors' attention.

The present paper deals only with the fluid-flow characteristics; a subsequent paper (*11*) is concerned with the heat transfer studies. An early paper by Piret, Mann, and Wall (*2*) reported a small scattering of pressure-drop data for concurrent gas-liquid flow through packed beds. More

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