Evaluation of Optimal Control Strategies

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In a recent article* in this journal, a computational method for minimal time control of nonlinear systems was presented. The generality of the method was based on the claim that Silva and LaSalle had shown that optimum control is on the boundaries of its limits except possibly for the very end of the transient response. This is not a correct interpretation. Silva required this to be the control action and demonstrated that the response was close to optimal for high-order linear systems. LaSalle also treated linear systems. Therefore, no general conclusions may be drawn for nonlinear systems. As a matter of fact, time-optimal control of a particular nonlinear process may never be on the boundaries. A good example may be found in reference *10* of the article by Grethlein and Lapidus.

One useful method for examining optimal strategies is the maximum principle of Pontriagin (*1*). If one is given a system described by n equations in the state variables (x_i) and control variables (u_j)

$$\frac{dx_i}{dt} = f_i(x_i, u_j, t)$$

and a performance function to be minimized

$$\int_o^\tau f_o\,(x_i, u_j, t)\; dt$$

then the maximum principle states that the Hamiltonian function

$$H\;(x_i, \chi_i, u_j, t) = \sum_{i=0}^{i} \chi_i f_i$$

must necessarily be a maximum along the trajectory for $0 \leqq t \leqq \tau$. The adjoint variables, χ_i, are defined as

$$\frac{d\chi_i}{dt} = -\frac{\partial H}{\partial x_i} \quad i = 1 \ldots n$$

χ_o is constant
and $(\chi_1, \chi_2 \ldots \chi_n) \neq 0$

An interesting comparison may be seen in the minimum time operation of a batch reactor with a single exothermic reaction controlled by a cooling coil. The reaction is pseudo-first order.

Irreversible reaction: rate $= -x\, k_1(T)$ where x = reactant mole fraction, T = reaction temperature, $k_1(T)$ = specific reaction velocity.

The system equations are then

$$\frac{dx}{dt} = -\frac{x\,V\,k_1(T)}{W_x}$$

$$\frac{dT}{dt} = \frac{VH_r x\, k_1\,(T)}{W_T} - [T - T_o]\frac{\varphi}{W_T}$$

Now $f_o = 1$ for minimum time control, so that

$$H = \chi_o - \chi_1\, x \frac{V}{W_x} k_1(T) + \frac{\chi_2}{W_T} \{VH_r x\, k_1(T) - [T - T_o]\varphi\}$$

The control strategy is determined by the coefficient of φ, $\frac{-\chi_2}{W_T}[T - T_o]$.

In order to maximize H

$$\varphi = \min \varphi \text{ if } \chi_2 > 0$$
$$\varphi = \max \varphi \text{ if } \chi_2 < 0$$

This is bang-bang control; but if χ_2 goes to zero for any finite time, more investigation is required. This implies that χ_2 and $\frac{d\chi_2}{dt}$ must go to zero together. But

$$\frac{d\chi_2}{dt} = -\frac{\partial H}{\partial T} = \chi_1\, x \frac{V}{W_x}\frac{dk_1}{dT} - \frac{\chi_2}{W_T}\left[VH_r x \frac{dk_1}{dT} - \varphi\right]$$

so χ_1 would have to go to zero with χ_2; but this is impossible, since the vector

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* Grethlein, H. E., and Leon Lapidus, *A.I.Ch.E. Journal*, **9**, No. 2, p. 230 (1963).

Comments on the Above Communication to the Editor

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The basic premise of the paper by Grethlein and Lapidus is to ascertain an optimal control sequence for a nonlinear process subject to the constraints of physical reality. In many physical systems the input is automatically of the bang-bang type; this paper then illustrates the implications and results for one approach to handling this problem. It may be that in certain cases the controlled results are not truly optimal but the approach to optimality is probably quite close and within the limits imposed by a partial knowledge of the process model.

The minor amount of discussion in the paper dealing with the theoretical justification for bang-bang minimum time control was, of course, only to provide a broad-gauged foundation for its use. Unfortunately this discussion should have specified that only normal-type systems were under consideration. Thus if the system model is given by the linear equations (all in vector-matrix form)

$$\dot{x}(t) = A\,x(t) + B\,m(t)$$

where A and B are constant matrices then the solution is given by

$$x(t) = X(t)\,x(0) + X(t) \int_0^t X^{-1}(\lambda)\; B\,m(\lambda)\; d\lambda$$

where $X(t)$ satisfies

$$\dot{X}(t) = A\,X(t) \quad X(0) = I$$

For every fixed $t \geqq 0$ there is a subset $C(t)$ of n-dimensional space which represents the set of all initial conditions from which the origin may be reached in t time units. If the actual initial condition x_0 is given then LaSalle has shown that there is at least one new vector η such that

$$-\eta \cdot x_0 \geqq \eta \cdot w \text{ for all } w \in C(t_o)$$

This means that the function $\eta \cdot w$ takes on its maximum in $C(t_o)$ when $w = -x_0$.

The system under consideration is said to be normal if no component of $[\eta \cdot X^{-1}(t)\, B]$ vanishes on any interval, no matter what the vector $\eta \neq 0$. In this case the optimal control is bang-bang, and unique, and is given by

$$m(t) = \text{sgn}\,[\eta \cdot X^{-1}(t) B]$$

Obviously this analysis applies only to linear systems and merely indicates a direction in the case of nonlinear systems. In the latter case, as Dr. Cotter has pointed out, the maximum principle may be used to define the type of optimal control. However, when there are more than a few state variables it is almost impossible to use this method to evaluate the explicit control strategy. Thus considerable research work must be done before a truly optimal control sequence for nonlinear systems may be always defined. The purpose of the paper under discussion was to illustrate one method of handling this problem.

INFORMATION RETRIEVAL

(*Continued from page 588*)

Solution of the linearized equations of multicomponent mass transfer: II matrix methods, Toor, H. L., **A.I.Ch.E. Journal, 10,** No. 4, p. 460 (July, 1964).

Key Words: Multicomponent Mass Transfer-8, Multicomponent Diffusion-8, Convective Diffusion-8, Unsteady Diffusion-8, Interphase Transfer-8, Coupled Differential Equations-1, Uncoupled Differential Equations-2, Matrix Methods-10, Cross Diffusion Coefficients-6, Mass Transfer Rates-2, 7, Concentration Profiles-2, 7, Gases-9, Liquids-9, Solids-9.

Abstract: Solutions of the equations of multicomponent mass transfer are matrix generalizations of binary solutions when initial and boundary concentrations are constant and concentration differences are small. The analogue of the binary mass transfer coefficient is a multicomponent mass transfer coefficient matrix. When interphase transfer takes place, the inverse mass transfer coefficient matrices of each phase sum to the inverse of the overall multicomponent mass transfer coefficient matrix.

Heat transfer for turbulent flow in rectangular ducts with two heated and two unheated walls, Novotny, J. L., S. T. McComas, E. M. Sparrow, and E. R. G. Eckert, **A.I.Ch.E. Journal, 10,** No. 4, p. 466 (July, 1964).

Key Words: Heat Transfer-8, Heat Transfer Coefficient-7, Nusselt Number-7, Wall Temperature Distribution-7, Reynolds Number-6, Rectangular Duct-5, Aspect Ratio-6, Turbulent Flow-5, Air-5, Experiment-10.

Abstract: The fully developed heat transfer characteristics for air flowing turbulently in rectangular ducts of aspect ratio 1:1, 5:1, and 10:1 have been determined experimentally. The heating condition is such that the two longer walls of the rectangle are uniformly heated, while the two shorter walls are unheated. The results cover the Reynolds number range from 10,000 to 140,000. An anlysis, based on the Deissler-Taylor model, of the heat transfer in finite aspect ratio rectangular ducts with uniform peripheral wall temperature is also described.

Correlation of thermodynamic properties of amine-water solutions with molecular structure, Davison, R. R., D. W. Hood, and W. D. Harris, **A.I.Ch.E. Journal, 10,** No. 4, p. 471 (July, 1964).

Key Words: Equilibria (VLE)-, Activities-, Correlation-, Molecular Structure-, Solutions-, Amines-, Water-, Enthalpy-, Thermodynamics-, Tchebycheff Polynomials-, Regression Analysis-.

Abstract: Enthalpy of solution of amines in water at infinite dilution and activities of amine-water solutions are correlated by steric and inductive constants which are functions only of the molecular structure of amines. The activities for five 6-carbon atom amine-water solutions at 10°C. are fitted with Tchebycheff polynomials, and the polynomial constants are correlated with the structural parameters.

Fluctuations in the local rate of turbulent mass transfer to a pipe wall, Van Shaw, Paul, and Thomas J. Hanratty, **A.I.Ch.E. Journal, 10,** No. 4, p. 475 (July, 1964).

Key Words: Mass Transfer-8, 7, Wall Turbulence-8, 6, Turbulent Transport-8, Pipe Flow-10, Electrochemical-10, Mass Transfer Fluctuations-9, 7, Mechanism of Turbulent Exchange-9, Diffusion Controlled Reaction-10, Finite Probe Correction-9, Diffusion Layer-9, Viscous Layer-9.

Abstract: The fluctuations in the local rate of turbulent mass transfer to a point on a large mass transfer surface on a pipe wall were measured with an electrochemical technique. The results are the antithesis of the laminar film model and demonstrate that the process of turbulent mass transfer is chaotic. The intensity of the mass transfer fluctuations is estimated to be 0.47. The mass transfer fluctuation field is greatly elongated in the direction of flow, and the characteristic frequency of the fluctuations is low.

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χ is non zero. Therefore, bang-bang control is the only possibility.

Reversible reaction:

$$\text{rate} = -\{x\,k_1(T) - [1-x]\,k_2(T)\}$$
$$= k_2(T) - x\,[k_1(T) + k_2(T)]$$

$$\frac{dx}{dt} = \frac{V}{W_x}\{x[k_1(\mathrm{T}) + k_2(T)] - k_2(T)\}$$

$$\frac{dT}{dt} = \frac{VH_r}{W_T}\{k_2(T) - x[k_1(T) + k_2(T)]\} - [T - T_o]\frac{\varphi}{W_T}$$

Now

$$\frac{d\chi_2}{dt} = -\chi_1\frac{V}{W_x}\left\{x\left[\frac{dk_1}{dT} - \frac{dk_2}{dT}\right] - \frac{dk_2}{dT}\right\} + \chi_2\frac{\varphi}{W_T} + \left(\chi_2\frac{VH_r}{W_T}\right)\left\{\frac{dk_2}{dT} - x\left[\frac{dk_1}{dT} + \frac{dk_2}{dT}\right]\right\}$$

Therefore, it is feasible for χ_2 and $\frac{d\chi_2}{dt}$ to go to zero independently of χ_1, because the coefficient of χ_1 may be zero. During these periods, the control will not be on the boundaries and the feedback control law applies:

$$x = \frac{dk_2/dT}{dk_1/dT + dk_2/dT}$$

This regime of control is fully discussed in reference 2.

NOTATION

f_i = any function, $i = 0, 1, \ldots n$, which is continuous in all x_i and u_j and continuously differentiable with respect to all x_i
H_r = heat of reaction
i = index of the state and adjoint variables
$k_1(T)$ = specific reaction velocity
$k_2(T)$ = specific reverse reaction velocity
T = reaction temperature
T_o = cooling water temperature at coil inlet
u_j = control variables
V = reactor contents volume
W_T = molar heat capacitance of reactor contents
W_x = moles in reactor
x = reactant mole fraction
x_i = state variables
φ = nonlinear function of cooling water flow rate; may be used as the control variable
τ = final time
χ_i = adjoint variables

LITERATURE CITED

1. Pontriagin, L. S., V. G. Boltyanskii, R. V. Gamkrelidze, and E. F. Mishchenko, "The Mathematical Theory of Optimal Processes," Interscience, New York (1962).
2. Johnson, C. D., and J. E. Gibson, Institute of Electrical and Electronics Engineers Transactions on Automatic Control, AC-8, 4-15 (January, 1963).