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OPTIMAL CONTROL OF DIFFUSION-REACTION SYSTEMS.(U)
MAY 78 H T BANKS, M C DUBAN, J P KERNEVEZ AFOSR-76-3092
AFOSR-TR-78-1023 NL

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18 REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM	
1. REPORT NUMBER AFOSR-TR-78-1023	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER	
6 TITLE (and Subtitle) OPTIMAL CONTROL OF DIFFUSION-REACTION SYSTEMS		9 TYPE OF REPORT & PERIOD COVERED Interim Repts	
10 AUTHOR H.T. Banks M.C. Duban J.P. Kernevez		8. CONTRACT OR GRANT NUMBER(s) 15 AFOSR-76-30923 NSF-GP 28932	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Lefschetz Center for Dynamical Systems Division of Applied Mathematics Brown University, Providence, R.I. 02912		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102F 2304YA1	
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Office of Scientific Research/NM Bolling AFB, Washington, DC 20332		12. REPORT DATE May 3, 1978	
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) 11 3 May 78		13. NUMBER OF PAGES 19	
16. DISTRIBUTION STATEMENT (of this Report) 12 22 p		15. SECURITY CLASS (of this report) UNCLASSIFIED	
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report) Approved for public release; distribution unlimited.		15a. DECLASSIFICATION DOWNGRADING SCHEDULE	
18. SUPPLEMENTARY NOTES			
19. KEY WORDS (Continue on reverse side if necessary and identify by block number)			
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) We discuss several formulations of optimization problems which arise in a natural way in the investigation of transport properties of artificial membranes and general diffusion-reaction media. Nonlinear reaction velocity approximations dictated by reactions of interest to biochemists place the problems in a class to which one cannot apply the usual computational techniques (e.g. gradient, conjugate-gradient) in a straightforward manner. The inherent difficulties, how one might			

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OPTIMAL CONTROL OF DIFFUSION-REACTION SYSTEMS*

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* This research supported in part by the National Science Foundation under grant NSF-GP-28931x3, in part by the U.S. Air Force under contract AF-AFOSR-76-3092, in part by Centre National de la Recherche Scientifique under grant 38097, and in part by the Université de Technologie de Compiègne.

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OPTIMAL CONTROL OF DIRECT REACTION SYSTEMS

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Abstract: We discuss several formulations of optimization problems which arise in a natural way in the investigation of transport properties of artificial membranes and general diffusion-reaction media. Nonlinear reaction velocity approximations dictated by reactions of interest to biochemists place the problems in a class to which one cannot apply the usual computational techniques (e.g. gradient, conjugate-gradient) in a straightforward manner. The inherent difficulties, how one might circumvent them, and some of our initial efforts towards development of feasible computational schemes are discussed.

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We consider control problems governed by the following nonlinear diffusion-reaction systems:

$$\frac{\partial s}{\partial t} = \frac{\partial^2 s}{\partial x^2} - \sigma \frac{a}{1+a} \frac{s}{1+s+ks^2} \quad (1)$$

$$\frac{\partial a}{\partial t} = \alpha \frac{\partial^2 a}{\partial x^2} \quad 0 < \underline{x} < 1, \quad 0 < \underline{t} < T,$$

$$s(0, t) = s_0(t) \quad \frac{\partial s}{\partial x}(1, t) = 0 \quad (2)$$

$$a(0, t) = a_0(t) \quad \frac{\partial a}{\partial x}(1, t) = 0$$

$$s(x, 0) = f_0(x) \quad s(x, T) = f_1(x) \quad (3)$$

$$a(x, 0) = g_0(x) \quad a(x, T) = g_1(x).$$

The control of systems such as (1)-(3) is of importance in the investigation of enzymatically active artificial membranes similar to those employed by D. Thomas and his coworkers in experiments at Université de Technologie de Compiègne (see [2] for more details). In such systems the variables s and a represent respectively normalized variables for substrate and activator concentrations. The nonlinear reaction term in (1) is a Michaelis-Menten-Briggs-Haldane type (see Chap. 1 of [1]) velocity

approximation term for a reaction in which one has inhibition by excessive substrate. The boundary conditions are those appropriate for a one dimensional diffusion-reaction medium in contact with a reservoir (at $x = 0$) and an electrode or impermeable wall (at $x = 1$) as depicted in Figure 1.

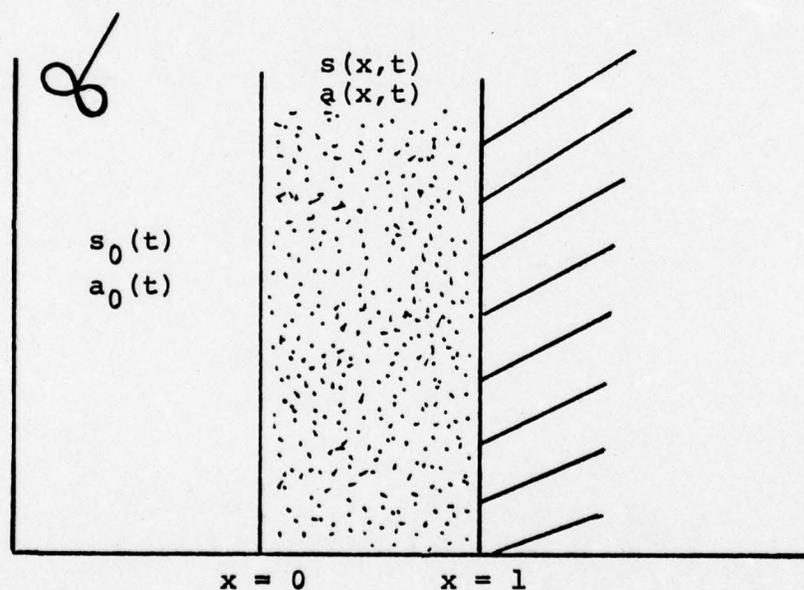


Figure 1

For the nonlinear system (1)-(2) it can be argued that multiple steady-state solutions exist and the initial and terminal

functions in (3) are taken to be distinct such steady-states.

That is, f_i, g_i , $i = 0, 1$ are solutions of

$$0 = f_{xx} - \sigma \frac{g}{1+g} \frac{f}{1+f+kf^2}$$

$$0 = g_{xx}$$

(4)

$$f(0) = \beta_i \quad f_x(1) = 0$$

$$g(0) = \gamma_i \quad g_x(1) = 0.$$

The basic question we address here is: Given the system in an initial steady-state configuration (f_0, g_0) at time $t = 0$, how does one use boundary controls s_0, a_0 to transfer the system in time $0 \leq t \leq T$ to a second steady-state configuration (f_1, g_1) and do this in an efficient manner. That is, there is some cost associated with adding (or deleting) substrate and/or activator to the system via the boundary controls and one should try to minimize some measure of this cost as the transfer from one steady-state to another is made. We take as cost functional a measure of the total flux (in the L_2 sense) of s and a into the system at the boundary $x = 0$. Thus, we desire to choose control functions s_0, a_0 in some control space \mathcal{U} (e.g. $L_2(0, T)$) so as to minimize

$$J = \int_0^T \left\{ \left| \frac{\partial s}{\partial x}(0, t) \right|^2 + \left| \frac{\partial a}{\partial x}(0, t) \right|^2 \right\} dt \quad (5)$$

subject to (1)-(3). (In general the system (1)-(3) need not be exactly solvable for a given $f_i, g_i, i = 0, 1$ (i.e., controllability questions arise) and one must replace the above posed problem by one of transferring f_0, g_0 to a terminal state close to f_1, g_1 . One thus actually considers for both theoretical and computational purposes the modified problem of minimizing $J_\epsilon \equiv J + \frac{1}{\epsilon} \int_0^1 \{ |s(x, T) - f_1(x)|^2 + |a(x, T) - g_1(x)|^2 \} dx$ subject to (1), (2) and $s(x, 0) = f_0(x), a(x, 0) = g_0(x)$.)

The above might appropriately be called a "1-dimensional medium" reaction-diffusion problem. An analogous "0-dimensional medium" problem is of interest in the event that one has (i) reaction and diffusion separated within the medium or (ii) very rapid diffusion (i.e., a well-mixed medium for reaction-diffusion). The latter assumption is valid in general models for continuously stirred tank reactors. In the "0-dimensional medium" problem the spatial variable is ignored and one has as control system (for $s = s(t), a = a(t)$)

$$\begin{aligned} \frac{ds}{dt} &= s_0 - s - \sigma \frac{a}{1+a} \frac{s}{1+s+ks^2} \\ \frac{da}{dt} &= \alpha \{ a_0 - a \} \quad 0 \leq t \leq T, \end{aligned} \quad (6)$$

$$\begin{aligned} s(0) &= f_0 & s(T) &= f_1 \\ a(0) &= g_0 & a(T) &= g_1, \end{aligned} \quad (7)$$

where one still chooses the controls s_0, a_0 from some space \mathcal{Q} of admissible policies. However, now the initial and terminal states $(f_0, g_0), (f_1, g_1)$ are constants which satisfy

$$\begin{aligned} 0 &= s_0^i - f_i - \sigma \frac{g_i}{1+g_i} F(f_i) \\ 0 &= a_0^i - g_i, \quad i = 0, 1, \end{aligned} \quad (8)$$

where $(s_0^0, a_0^0) = (s_0(0), a_0(0))$, $(s_0^1, a_0^1) = (s_0(T), a_0(T))$ and $F(s) \equiv s/(1+s+ks^2)$. The cost functional is taken as

$$J = \int_0^T \{ |s_0(t) - s(t)|^2 + |a_0(t) - a(t)|^2 \} dt. \quad (9)$$

Just as in the case of the "1-dimensional" problem, one can show that multiple steady-states (i.e., solutions of (8)) are possible for the system (6). Also, one usually must consider a modification of the minimization problem since (6), (7) may not be exactly solvable (i.e., again controllability questions arise).

There are a number of interesting nontrivial theoretical questions (controllability, existence, uniqueness, etc.) associated with the control problems formulated above but we shall not discuss those questions directly here. Our initial interest in these problems arose from an attempt to use computational schemes (i.e., software packages) in connection with experimental efforts. From the descriptions above one might anticipate this to be a rather routine task since the problems would appear tractable using standard ideas from the theory of boundary control of partial differential equations in the case of the "1-dimensional" problems (see [2]) or those from the theory of nonlinear ordinary differential equation control problems in the case of the "0-dimensional" problem (see [3]) along with gradient, conjugate-gradient type numerical techniques. Initial numerical experiments revealed that this is not the case and our efforts here will be limited to an explanation of the difficulties along with suggestions as to possible alternative formulations which might lead to problems amenable to solution on the computer.

To facilitate discussions of the above-mentioned difficulties it is helpful to consider the quasi-steady-state approximation to the "0-dimensional medium" problem (a similar approximation reveals the inherent difficulties in the "1-dimensional medium" problem). In light of the small transient times found in experimental realizations of these models, one can make a plausible argument that the quasi-steady-state approximations are reasonable approximations to the problems formulated above. We shall not do that here but turn instead to the problem of minimizing J given in (9) subject to the constraint equations (steady-state approximations to (6))

$$s_0(t) - s(t) - \sigma \frac{a(t)}{1+a(t)} F(s(t)) = 0 \quad (10)$$

$$a_0(t) - a(t) = 0.$$

Since in this case $a_0 \equiv a$, we define for convenience the variable $\rho \equiv \sigma a / (1+a)$ and consider the problem of minimizing J while transferring a "state" $X^0 = (s_0(0), \rho(0), s(0))$ to a state $X^1 = (s_0(T), \rho(T), s(T))$ subject to the constraint

$$s_0(t) - s(t) - \rho(t)F(s(t)) = 0, \quad 0 \leq t \leq T. \quad (11)$$

A sketch of the surface in (s_0, ρ, s) space described by (11) is given in Figure 2, where one recognizes the well-known "cusp" (catastrophe) surface of Whitney [5] and Thom [4]. In Figure 2

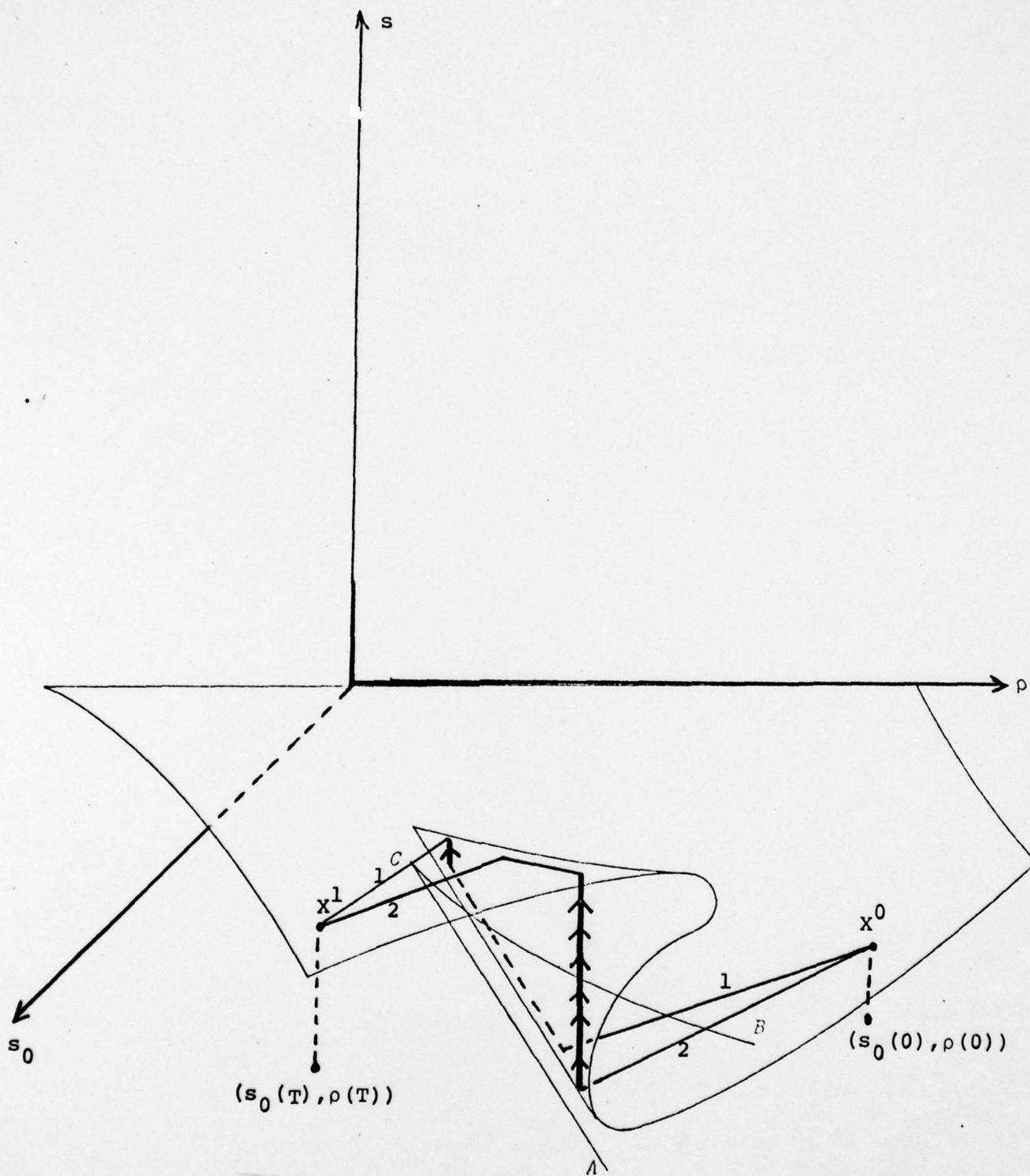


Figure 2

the folds in the cusp surface are projected down into the (s_0, ρ) plane as the (infinite) arcs containing CA and CB. We are thus choosing control strategies (paths in the (s_0, ρ) plane) which yield corresponding "trajectories" that move on this (multi-valued in some regions) surface.

Consider a problem which requires transfer of an initial configuration x^0 to a terminal configuration x^1 as depicted in Figure 2. Two possible distinct control strategies $\{(s_0(t), \rho(t))\}$, $0 \leq t \leq T$, are depicted in Figure 3.

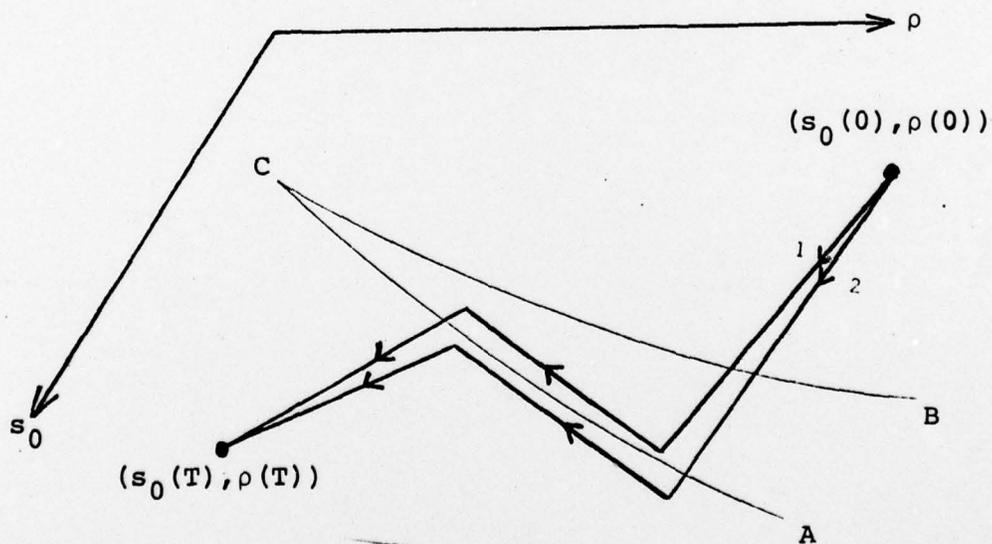


Figure 3

It is clear that two such strategies can be made arbitrarily close (using any reasonable measure of closeness) in the (s_0, ρ) plane while the corresponding "trajectories" $(s_0(t), \rho(t), s(t))$, $0 \leq t \leq T$, lying on the constraint surface will not be close. The trajectory corresponding to strategy 1 (see Fig. 3) "travels" along the lower fold (see Fig. 2) while strategy 2 yields a trajectory which during the corresponding time "travels" along the upper fold of the surface defined by (11). (The heavy lines with arrows in Fig. 2 represent jump discontinuities in s for the quasi-steady-state model. For the original problems, i.e., the non-quasi-steady-state models, these correspond to extremely rapid "motion" from trajectories near the lower surface to trajectories near the upper surface.)

From these considerations it is clear that the trajectories for the quasi-steady model are not even continuous as a function of the control strategies and hence it is not surprising that methods (e.g. gradient, conjugate-gradient) involving derivatives (with respect to controls) of the cost function are troublesome when applied to the problems governed by (1)-(3) or (6)-(7).

Once one has visualized the problems in this heuristic but informative way, it is apparent that the difficulties are a result of the particular nonlinear reaction velocity approximation found in (1) and subsequent associated versions of this system equation employed above. The models entail a region Γ (for (6) and (11) with transfer from x^0 to x^1 as shown in Figs. 2,3 this region is depicted in Fig. 4) in "control" space in which one must choose control strategies with extreme care.

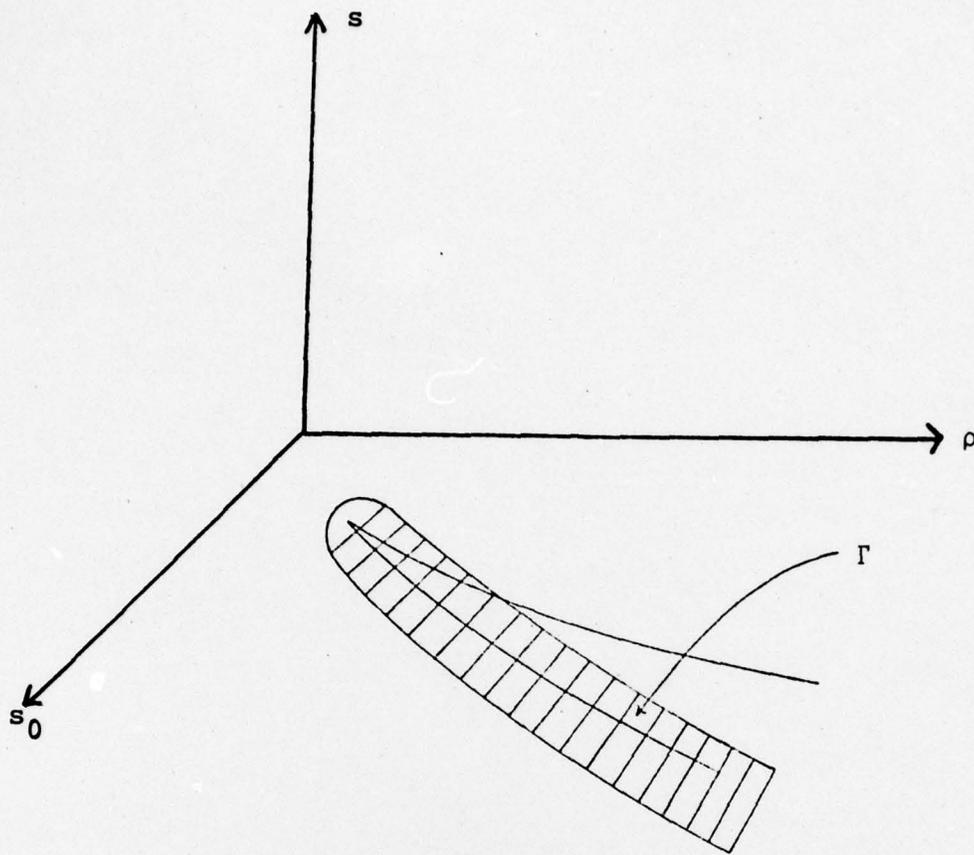


Figure 4

In carrying out laboratory experiments, this region is observed to be one in which the system is highly unstable. Thus from both a theoretical and practical viewpoint, additional constraints on operation of the system in this region are desirable. Careful formulation with additional constraints can lead to tractable problems. We illustrate this first with a sketch of how one might formulate such a control problem for a discretized version of the quasi-steady approximation to the "0-dimensional medium" problem.

Considering the controls s_0, a_0 to be piecewise constant on $[0, T]$, one can reformulate the quasi-steady problem as a multi-stage discrete control problem with "controls" $\{s_0(t_i), a_0(t_i)\}$, $i = 1, \dots, k$, constrained to lie outside Γ (see Fig. 4) with "states" $\{s(t_i)\}$ given implicitly by

$$s_0(t_i) - s(t_i) - \sigma \frac{a_0(t_i)}{1+a_0(t_i)} F(s(t_i)) = 0.$$

The payoff is then taken as

$$J = \sum_{i=1}^k \{s_0(t_0) - s(t_i)\}^2 \Delta t_i.$$

The most natural formulation along these lines leads to immediate difficulties with regard to necessary conditions (multiplier rules or maximum principles are not readily available for discrete control problems with implicit state equations). However, one can reformulate this slightly as a constrained "state" and "control" problem so that necessary conditions are easily obtained. If one identifies s_0, a_0 as "states" and defines a mapping $\Lambda: \mathbb{R}^2 \rightarrow \mathbb{R}^1$ by $x_3 = \Lambda(x_1, x_2)$ where x_3 is a solution (appropriately chosen when multiple solutions exist) to

$$x_1 - x_3 - \sigma \frac{x_2}{1+x_2} F(x_3) = 0$$

and introduces "controls" v_i, w_i (with suitable constraints), the problem becomes one of minimizing

$$J = \sum_{i=1}^k \{s_0(t_i) - \Lambda(s_0(t_i), a_0(t_i))\}^2 \Delta t_i$$

subject to state equations

$$s_0(t_i) = s_0(t_{i-1}) + v_i$$

$$a_0(t_i) = a_0(t_{i-1}) + w_i$$

and constraints

$$\phi_j(s_0(t_i), a_0(t_i)) \leq 0$$

defined to prohibit values of s_0, a_0 in the region Γ . In this formulation one can obtain necessary conditions (to use as a basis for computational schemes) via application of the operator theoretic optimization framework with abstract multiplier rule developed by Neustadt (e.g., see Chap. 7 of [3]).

The above formulation essentially involves the assumption that "changes" (or more precisely "rates of changes") in s_0, a_0 are the controls. This can be viewed as a special case of a reformulation for the continuous version problems. Consider the full "0-dimensional medium" problem and adjoin to the state equations (6) additional equations

$$\frac{ds_0}{dt} = v$$

$$\frac{da_0}{dt} = w$$

(12)

with control constraints $|v| \leq M_1, |w| \leq M_2$. The "states" for the problem are then taken as s_0, a_0, s, a with "controls" given by v, w . In addition to the natural control restraints, one imposes mixed state-control (so-called "phase-control" constraints) inequality constraints which restrict the choices of v and w in the event one is in the region Γ in (s_0, ρ) space (see Fig. 4). These constraints are defined so that one rules out control policies that yield paths in the (s_0, ρ) plane that travel along the "singular" arc containing CA (see Figs. 2, 3, 4). That is, one rules out via constraints on v, w policies such as those depicted in Fig. 3. Hence, while one does not prohibit crossing of the Γ region, one restricts carefully the types of trajectories one allows while passing through this region. The resulting constraints will thus be joint in the "states" s_0, a_0 and the "controls" v, w .

Finally, we point out that one can also use these reformulation ideas to take a linear programming approach (function minimization problems with linear inequality constraints) to these problems as opposed to the optimal control approach (multiplier rule for constrained control problems) sketched above. For example we illustrate briefly with the quasi-steady approximation to the "0-dimensional medium" problem.

We approximate the arc containing CA above and below by straight lines with slope m . With this fixed slope m , we construct a family of parallel and equidistant lines $\{\rho = ms_0 + b_i\}_{i=0}^k$ in the (s_0, ρ) plane as depicted in Figure 5. The admissible

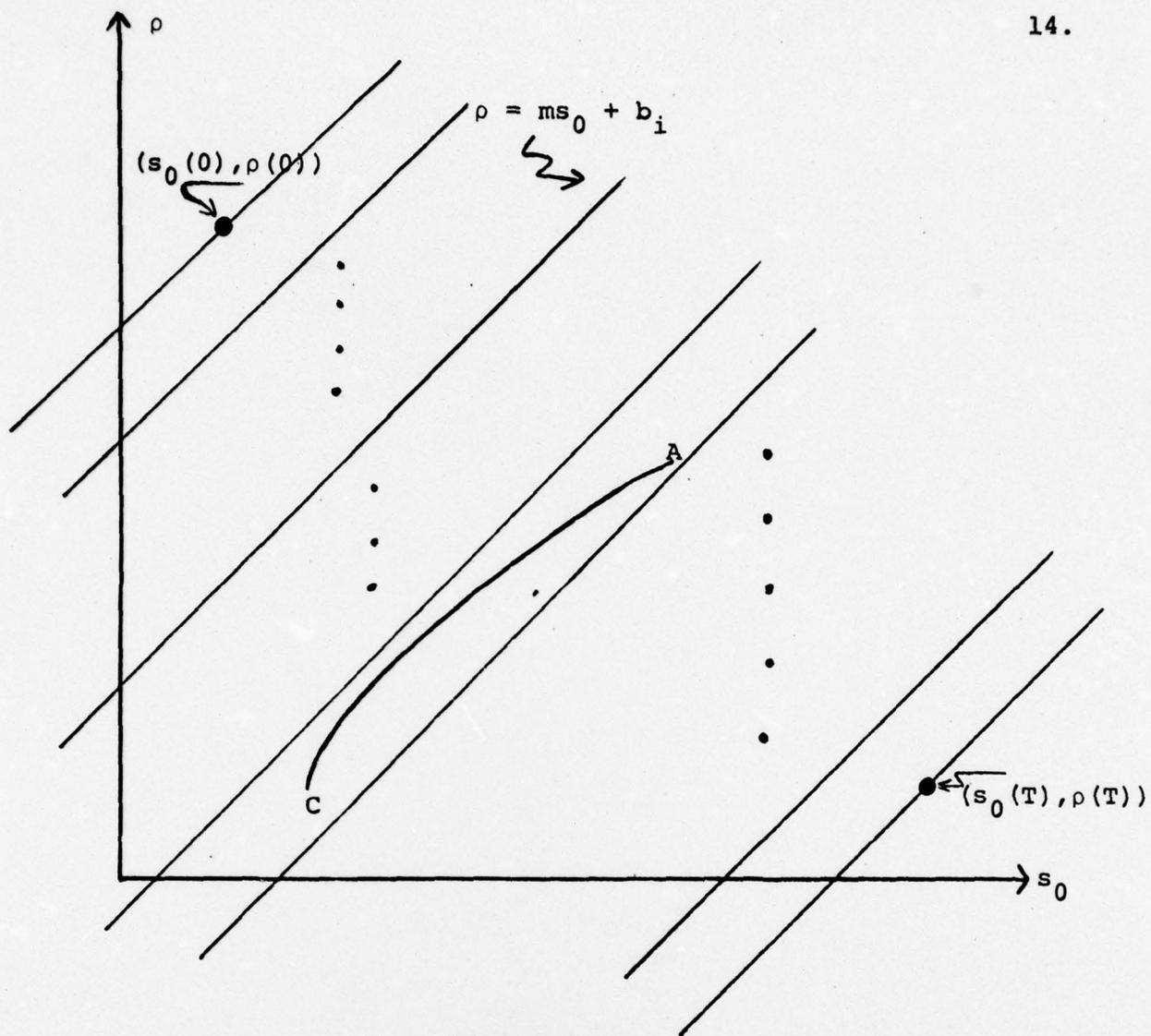


Figure 5

"states" are then required to lie on these lines. (The construction is made so that the arc CA lies between two of these lines, $(s_0(0), \rho(0))$ lies on $\rho = ms_0 + b_0$, and $(s_0(T), \rho(T))$ lies on $\rho = ms_0 + b_k$.) A "trajectory" will then consist of a sequence of points $(s_0(t_i), \rho(t_i), s(t_i))$ satisfying (11) with $(s_0(t_i), \rho(t_i))$ belonging to the line $\rho = ms_0 + b_i$. One can take as control policies the collection of sequences

$$U = (\rho_1, t_1, \rho_2, t_2, \dots, \rho_{k-1}, t_{k-1})$$

with $t_0 = 0$, $t_k = T$ and corresponding "state" equations

$$s_0(t_i) = (\rho_i - b_i)/m$$

$$s_0(t_i) - s(t_i) - \rho_i F(s(t_i)) = 0 .$$

In addition to making appropriate modifications to the payoff J , one constrains the analogues of equations (12), i.e.,

$$\left| \frac{s_0(t_i) - s_0(t_{i-1})}{t_i - t_{i-1}} \right| \leq K_1 \tag{13}$$

$$\left| \frac{\rho_i - \rho_{i-1}}{t_i - t_{i-1}} \right| \leq K_2 .$$

One must also add positivity constraints for s_0, ρ given by

$$\rho_i \geq \max\{0, b_i\} . \tag{14}$$

By defining suitable coefficient matrices E and D , one can write the constraints (13), (14) as

$$EU^T \geq D . \tag{15}$$

The problem then becomes one of minimizing a function J subject to the linear inequality constraints (15) and standard computa-

tional techniques (e.g., descent methods such as the Davidon-Fletcher-Powell schemes) are applicable.

A more detailed discussion of theoretical aspects of the above different formulations and approximations along with our numerical findings will be presented in a forthcoming manuscript.

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