1988

Simultaneous strategies for optimization of differential-algebraic systems

S Vasantharajan
Carnegie Mellon University

J Logsdon

Lorenz T. Biegler

Carnegie Mellon University.Engineering Design Research Center.

Simultaneous Strategies for Optimization of Differential-Algebraic Systems

by

S. Vasantharajan, J. Logsdon, L.T. Biegler

EDRC 06-65-89

Carnegie Mellon University

SIMULTANEOUS STRATEGIES FOR OPTIMIZATION OF DIFFERENTIAL-ALGEBRAIC SYSTEMS

by

S. Vasantharajan, J. Logsdon and L.T. Biegler

Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, Pa 15213

Paper 173 e
1988 Annual AIChE Meeting
Washington, DC
November, 1988
Unpublished

Financial support from the Engineering Design Research Center, an NSF sponsored center, and the Department of Energy is gratefully acknowledged.

Abstract

A Simultaneous approach to the optimization of problems involving both Differential and Algebraic equation models (DAE) is developed. The equations that result from a discretization of a DAE model using orthogonal collocation on finite elements (OCFE), are incorporated directly into the optimization problem, and the combined problem is then solved using an efficient large-scale optimization strategy. In formulating this simultaneous strategy, profile constraints can be incorporated and handled automatically as part of the optimization problem. Moreover, since the DAE model is solved only once as the optimization problem converges, this approach can have a significant impact on the efficiency and reliability of the algorithm.

To ensure accuracy of the solution of the Simultaneous strategy, reliable error estimates have been developed which not only permit an assessment of the validity of the results obtained, but also allow for an adaptive refinement of the mesh on which the solution is computed Criteria which permit such estimates are discussed, and the concept of "equidistribution" is outlined

When control profiles are introduced, the error criteria become considerably more complicated. Here, we relate optimal control problems to the well-known index problem of DAE systems. A number of examples are presented that illustrate the difficulties of DAE systems and strategies are outlined for solving these problems.

Finally, the Simultaneous strategy will be demonstrated on several optimization problems, which require determination of continuous, possibly constrained state profiles, as well as optimal parameter values and control profiles.

1. Introduction and Outline

The role of differential and algebraic equation models (DAEs) in characterizing chemical process systems cannot be overemphasized. The optimization of such process problems described by DAEs has numerous references in chemical engineering annals. Typical examples are reactor design and optimization, optimization of batch processes, process control and parameter estimation.

Although these systems are commonplace, until recently no general and accurate method was available for handling these differential algebraic optimization models. This was, in spite of the availability of precise methods for solution of general algebraic equations and differential equations separately. An efficient fusion of these disparate techniques to yield a sufficiently general and accurate method for handling differential algebraic optimization problems (DAOPs) had not been achieved.

In this paper, we first examine the conventional technique for optimizing DAE systems, and present the drawbacks of such an approach. Then we present a new and promising Simultaneous strategy to solve such systems, and outline its derivation in detail. This strategy incorporates principles from finite element methods (FEM) and sophisticated large-scale optimization techniques.

In the subsequent sections, we address the topic of analyzing the quality of the results obtained with this Simultaneous approach. As this technique solves an approximation to the original system, there is a need for sensitive error estimates, which permit an evaluation of the solution computed Here, we present and derive new, reliable error estimates and deal with minimizing the approximation error. A sufficiently general strategy is derived, which satisfies tight error bounds. Moreover, for problems with control profiles we explore the problem of solving DAE systems. Depending on the structure of the control problem, higher index problems can easily be formulated and need to be dealt with. Here, these concepts will be analyzed and solution strategies for optimal control problems will be presented

The Simultaneous approach and the related principles outlined have been combined in an optimization environment efficiently. An implementation to handle large, sparse problems based on Range and Null spaces (Vasantharajan and Biegler (1988)) has been developed, implemented and extensively tested. The effectiveness of this Simultaneous algorithm in solving optimization problems is demonstrated on several difficult process examples.

General Differential-Algebraic Optimization Problem [DAOP]

A general DAOP can be stated as follows:

Min x. U(lZU)	*(X.U(£).Z{£))	(DAOP)
s.t.	$c(x_t \backslash Jtt), Z(t)) = 0$	
	$g(x, U(t), Z(t)) \le 0$	
	$\dot{Z}(£) = F(x, U(£), Z(t)X)$ $t \in [0,1]$	
	$Z(0) = Z_o$	
	$x^L \le x \le x^u$	
	$U^L \le \backslash J(£) \le U^u$	
	$Z^L \le Z(£) \le Z^U$	

where

$	=	objective function
g	=	design inequality constraint vector
c	=	design equality constraint vector
x	=	parameter, decision variable vector
$Z(£)$	=	state profile vector
$U(£)$	=	control profile vector
x^L, x^u	=	variable bounds
Z^L, Z^U	=	state profile bounds
U^L, U^U	=	control profile bounds

In this formulation, the system of ODE's are written as initial value problems for convenience and include a possible dependence on some scalar parameters which can be lumped in the decision variable subvector of x.

Review of Previous Work

In this section, we will first examine the tools and techniques available for the solution of differential equations and algebraic equations. We will then evaluate some of the existing strategies for optimization of DAE systems. Then, we will introduce and outline the newly proposed Simultaneous solution approach, and present its advantages over the conventional approaches.

Nonlinear programming problems (NLPs) can be handled by robust and efficient strategies like Successive Quadratic Programming (SQP) (Han (1977), Powell (1977)) and Reduced Gradient techniques (Murtagh and Saunders (1978)). Likewise, variational calculus (Bryson and Ho (1975)) is applicable for optimization of differential equation problems. But neither of these techniques is individually capable of handling DAOPs efficiently. While the NLP approaches have to resort to an often expensive numerical integration scheme, techniques based on optimal control theory have difficulty in handling even simple types of algebraic equations.

One established approach in solving DAOPs is the equivalent of a "Feasible path" technique (Sargent and Sullivan (1977)), where the optimization and solution of ODE models are performed in a two tier approach. The optimization is treated as an "outer" problem, and the ODE model is solved in an "inner" loop for each estimate of the parameters of the problem. However, this involves repeated numerical integration (often with implicit methods), and hence an inordinate amount of expensive function evaluations.

An alternate approach would be to discretize the differential equations using polynomial approximation and orthogonal collocation. The resulting algebraic equations (usually nonlinear) are then made part of a nonlinear program (NLP). The NLP is then solved with a SQP technique, which is among the most efficient optimization routines available. In addition, in order to ensure accuracy of approximation a set of finite element knot placement equations are employed, which represent sufficient conditions for error minimization. These equations accordingly refine the mesh on which the problem is solved.

This "Simultaneous" approach can represent a more efficient strategy than the conventional "Feasible path" solutions for differential-algebraic optimization. Large and stiff systems of ODEs can now be handled without unduly expensive function evaluations. Constraints on state variables are handled in a direct manner by bounding the coefficients of the approximating polynomials. Further, since the exact ODE model never needs to be solved at intermediate points, but rather a linearized set of the approximating equations solved at each iteration, difficulties associated with intermediate ODE solutions can be avoided.

This approach, originally proposed by Cuthrell and Biegler (1987), was able under certain conditions, to solve general DAOPs precisely. This formulation is however handicapped because of the nonconvexities involved in these mesh refinement constraints. Considerable caution had to exercised in initializing the example problems solved. A reformulation of this strategy, which in some way eliminated some of the nonlinearities is warranted. We will address this topic in this paper, and present new mesh refinement criteria and formulations, that ensure the accuracy of the state profile approximations, and preciseness of the optimization, without introducing nonconvexities.

This approach is then extended to problems with control profiles, as well as parameters to be optimized Solution strategies for DAE systems will be introduced and applied to optimal control problems. Here, we will show how certain classes of optimal control problems show the same difficulties attributed to DAE systems.

Also, during the implementation of this strategy very large NLPs had to be solved, which are computationally expensive and require considerable core storage. Thus there is a need for an efficient decomposition strategy, a topic which has been addressed successfully in Vasantharajan and Biegler (1988).

The effectiveness of the mesh refinement or knot placement equations proposed, and the decomposition strategy developed will then be demonstrated within the context of an optimization environment with the help of suitable examples.

2. Discretization of ODE Models

The optimization probiem as stated above, requires the solution of the set of equations,

$$\dot{Z}tt) = Fix.UM.ZWlA \qquad <€[0,1] \qquad (D$$

$$2(0) = Z_o \ .$$

where Z represents the models state variables and *Hx.U(t)Z(t).t)* represents the modelling expressions which usually depend on the decision variables. For example, in a tubular reactor, the above ODE's would represent the differential mass and energy balances determined from reaction kinetics. For instance, *£* could be the length of *a* reactor and the state variable Z, the conversion for each reaction or temperature of the reactor.

The solution of the model above is approximated by a polynomial written in Lagrange interpolation form:

$$z_{K+1}(t) = \sum_{i=0}^{K} z_i \, \phi_i(t) \qquad \phi_i(t) = \prod_{k=0,i}^{K} \frac{(t - t_k)}{(t_i - t_k)}$$

$$\sum_{i=1}^{K} \qquad \prod_{k=1,i}^{K} \frac{(t - t_k)}{(t_i - t_k)}$$

where *Z^^AJQ* and $u_{,x1}$ are (K+1)th order (degree < K+1) and Kth order polynomials, respectively. Here, the notation k=0,i indicates that k=0,...,i-1,i+1,...,K. A desirable property of the Lagrange form polynomial is that (for *z.. At)* for example)

$$z_{K+1}(t_i) = z_i$$

which is due to the Lagrange condition. Thus the coefficients z_i and u_i now become the decision variables in the optimization problem. Since the states represent quantities like temperature or conversion in chemical engineering problems, using the Lagrange form of the polynomial, produces coefficients whose physical significance is apparent. As a result constraints on the state and control variable trajectories can be enforced explicitly by writing the bounds on the associated coefficients z_i and u.

Substitution of (2) into (1) yields the Residual or Collocation equations, which with the Lagrange condition, yields the discretized form of the ODE model,

RU.) = T" Z. *$.(£)* - *FUM.Z.X.)* = 0   i=1.....K
1^g J J i I I I

with $z_0 = Z_o$.

Orthogonal Collocation can also be applied over NE finite elements (OCFE) of length AC*, i=1,..,NE, along the reactor distance (Vasantharajan and Biegler (1988)). The residuals discretized on finite elements can now be written as:

$$R(t_{[i\ell]}, \Delta\alpha_i) = \sum_{j=0}^{K} z_{ij} \dot{\phi}_j(t_\ell) - F(x, u_{i\ell}, z_{i\ell}, t_{[i\ell]})\, \Delta\alpha_i = 0 \qquad \begin{matrix} i=1,\dots NE \\ \ell=1,\dots K \end{matrix}$$

with $z_{1Q} = Z_Q$.

Here, the initial condition for all but the first element is taken as extrapolation of the states from the previous elements.

3. Error Estimates in Collocation

A detailed analysis of polynomial approximation using collocation at Legendre roots by de Boor and Swartz (1973) and de Boor (1974) showed that the *global error e(t)* = Z(t) - z(t) satisfies the local inequalities

$$\| e \|_i \leq C_1 \Delta\alpha_i^k \| T(t) \|_i + O(\Delta\alpha^{k+1}) \qquad 1 \leq i \leq NE \qquad (3)$$

where $\Delta\alpha = \max(\Delta\alpha_i)$ and the function T(t) depends on the true solution Z(t) and is independent of the mesh on which the problem is solved C_1 is a generic constant

If the functions are sufficiently smooth, which we shall assume, the error bound of eqn. (3) can be replaced by the following equality (Russell and Christiansen (1978)):

$$\| e \|_i = C\Delta\alpha_i^k \, \|Z^{(k)}(t)\|_i + O(\Delta\alpha^{k+1}) \qquad 1 \le i \le NE \qquad (4)$$

which involves the derivative of the solution Z(t). C is a computable constant which depends only on k and the order of the ODE's for a given collocation method. Ideally we would like to consider an expression like (4) for the global truncation error, but in general such an expression, given the local dependency with respect to the mesh size, will not be available for general boundary problems. Hence, by noting that the additional term $O(\Delta\alpha^{k+1})$ is hard to quantify and is negligible for small elements, we can neglect this term and concentrate on the local term in eqn. (4).

The error bound of eqn. (4) can be used to minimize the maximum error resulting from the approximation. For all $k<K+1$, this can be formulated as the following minimax problem:

$$\min_{\Delta\alpha_i} \; \max_j \; \Delta\alpha_j^k \, \|T(\bar{t})\|_j \qquad i=1,\ldots,NE \quad j=1,\ldots,NE$$

$$\text{s.t.} \quad \Delta\alpha_i \ge 0 \qquad i=1,\ldots,NE$$

$$\sum_{i=1}^{NE} \Delta\alpha_i = C$$

The objective of this optimization is to relocate the knots so as to minimize the maximum error estimate computed over all the finite elements. In this context, $T(\bar{t})$ is used to denote generically either the kth derivative of Z(t) in eqn. (4) or any other bound for the terms in the eqn. (3) which can be directly estimated from the problem and will be used to devise an adaptive mesh. Using the standard transformation in optimization literature, the minimax problem can be reformulated as a minimization problem as follows:

$$\min_{\delta, \Delta\alpha_i} \; \delta \qquad \text{(NLP 1)}$$

s.t $\quad AC^{**}_i \; |jT\bar{l}t|_i - 6 \leq 0 \qquad\qquad i=1....NE$

$\quad Aa_i \geq 0 \qquad\qquad i=1....NE$

$$\sum_{i=1}^{NE} AOC_i = C.$$

Under mild assumptions of regularity, the necessary and sufficient conditions for minimizing the approximation error for (NLP1) can be represented by,

$$Att^{fe}\; T(\bar{t}) = \text{constant} \qquad\qquad i=1....NE$$

These conditions, enforced as equalities in an optimization problem, require that a certain function T(T) be distributed equally over a number of intervals. This is the underlying principle of *equidistribution,* which was first proposed by Pereyra and Sewell (1975). The function being equidistributed in the knot placement equation is the local term in the estimate for the global truncation error in polynomial approximation (5.2). The idea of using truncation error for equidistribution was first proposed by de Boor (1974) and fully investigated by him in (1978).

In this section, we propose two choices for the error estimating function T(T), which is some form of computable approximation to the true solution Z(t).

One choice is an approximation to the higher derivative $Z^{(K+1)}(t)$ which is involved in the error bound (4) for fe=K+1 by divided differences using the highest available derivative $z^{(K)}(t)$, which by assumption is equal to $Z^{(K)}(t)$. Proposed originally by de Boor (1978), it was enforced through equality constraints by Cuthrell (1986), with good results. However, severe nonlinearities in this formulation limited its domain of applicability considerably. Careful initialization, especially for the knots, close to the solution was essential to guarantee the convergence of this method. Further, the non-convexities and non-differentiabilities introduced by the presence of absolute-valued terms in the knot placement equations made gradient calculations computationally difficult

In order to overcome these limitations, we propose a new formulation based on the residual function (see Russell and Christiansen (1978)). Since as part of collocation, the model is solved exactly only at the collocation points, an obvious estimate for error would be the residual computed at a non-collocation point Assuming even point collocation procedure, we can employ, for example, the residual at the midpoint $t_{1/2}$, of each element as an estimate for the local truncation error. Thus, the equations governing knot placement would now be

$$|R_i(t_{1/2})| = \text{constant} \qquad i=1....NE.$$

An advantage of this formulation is that it also permits direct quantitative local error estimates. Thus, if sufficient elements are available, one can relax the stringent requirement of equidistribution, and instead enforce the constraints: Using the ODE model, the error constraints become:

$$\|R_i(t_{1/2})\| \le \epsilon \qquad i=1....NE.$$

where C is a computable constant and 6 is any desired tolerance. Thus, the knot placement procedure can be tailored to satisfy tight error bounds.

The final NLP formulation to solve DAOPs, which includes the discretized equations and the mesh refinement constraints can be represented as:

$\min_{x, u_{i\ell}, z_{i\ell}, \Delta\alpha_i}$	$\phi(x, u, p, z, p)$		(NLP2)
S.t	$C(x, u_{i\ell}, z_{i\ell}, p) = 0$		
	$g(x, u_{i\ell}, z_{i\ell}) \le 0$		
	$R(t_{[i\ell]}, \Delta\alpha_i) = 0$	$i=1,...,NE$ $\ell=1,...,K$	
	$z_{10} = z_0$		
(Direct Enforcement)	$\|R_i(t_{i/2})\| \le \epsilon$	$i=1.....NE$	
(Equidistribution)	$\|R_i(t_{1/2})\| - \|R_{i-1}(t_{1/2})\| = 0$	$i=2....NE$	
	$\Delta\alpha_i \le e$	$i=1....NE$	
	$z^i_{K+1} = z^{i-1}_{K+1}$	$i=2,..NE$	

$$\sum_{i=1}^{NE} \Delta\alpha_i - C = 0$$

$$x^L \le x \le x^u$$

$$U^L \le U_i \le U^u$$

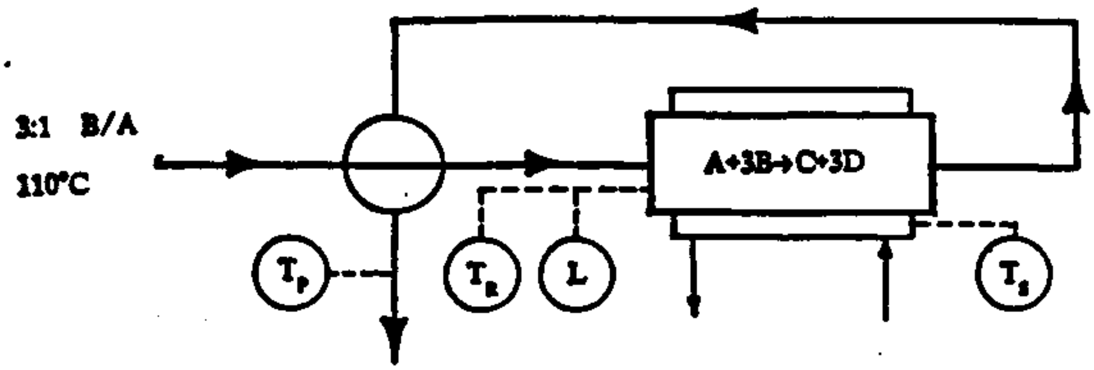
where € is a small tolerance to satisfy some error bound £ is a small lower bound, which is used in conjunction with the equidistribution constraints to ensure that the elements do not vanish.

4. Optimization with Adaptive Mesh Refinement

In this section we will present a reactor optimization problem solved with (NLP2). This involves embedding the discretized modelling equations for a packed bed reactor along with the set of knot placement equations in an optimization environment. The intent of this problem is to demonstrate that: 1.) A differential-algebraic problem can be efficiently solved using (NLP2), 2.) Adaptive knot placement ensures that a suitable accuracy of the ODE model at the optimum is obtained, and 3.) Bounds on the continuous state profile can be enforced easily.

Problem Statement

The reactor optimization problem illustrated in Figure below involves a simple heat exchanger and a packed bed reactor. A 3:1 ratio of the two reactants B and A is first preheated by the reactor effluent This stream is then fed to a packed bed reactor where the reaction A + 3B -» C + 3D takes place. The reactor is jacketed to allow the heat of reaction to be used to raise steam for the rest of the process. The differential-algebraic optimization problem for this reactor design is given in detail in Vasantharajan (1987).



Reactor Optimization Problem

The system of ODE's which mode! the reactor were taken from Finlayson (1971) and Hlavacek (1970). The objective function represents maximizing the production of steam (utility profit) from this reactor while minimizing the capital cost represented by the length of the reactor. Equal normalized unit prices were used to weight each term in the objective function. The optimization is done with respect to four design parameters, T_P, T_R, L and T_S as well as the two continuous profiles q(t) and $\bar{T}(t)$.

Three different cases were considered *as* part of this optimization problem:

Case Ia - reactor optimization problem (P1) with a hot spot appearing in the temperature profile.

Case Ib - Same as Case Ia except with T(t) £ 1.45 imposed, in the temperature profile.

Case II - reactor optimization problem (P1) <u>without</u> a hot spot

Although cases I and II employed the same reactor model by the use of different stating points and imposing different constraints (e.g., a shorter length) the hot spot was avoided in case II.

Using equidistribution constraints, the solution and the final profiles are presented in the following Figures 1, 2 and 3, and the optimization results in Table 1. As shown in these Figures, the knot placement equations are very effective in grouping the elements in regions with steep gradients, thereby ensuring good approximations to difficult profiles. This is evident from the final mesh distribution in Table 2, where, the knots are concentrated near the hot spot in the reactor, where the profiles are steep.

S. Solving Optimal Control Problems

The determination of the optimal control policy for a unit operation has economic signifigance in the process industries. Examples of unit operations of interest are batch reactors, fixed bed reactors , and distillation columns. Consider the determination of the optimal temperature policy for a batch reactor maximizing the yield of one of the components. An example of this problem is given in Ray (1981) and is discussed by Biegler (1984) and Renfro (1986). This problem is of interest because the control profile becomes saturated. The optimal control problem is

$$\text{Max} \quad y_2(1.0)$$

$$\text{s.t.} \quad \dot{y}_1 = -\left(u + \frac{u^2}{2}\right) y_1$$

$$\dot{y}_2 = (u)\, y_1$$

$$y_1(0) = 1. \quad y_2(0) = 0$$

$$0 \leq u \leq 5$$

The optimal control profile shown in Figure 4 is a smooth, continuous curve for the temperature trajectory. However, certain classes of optimal problems are more complicated because the control profiles contain discontinuites and/or singular arc segments. Also, the state variable constraints may influence the control policy and are thus difficult to solve using a variational calculus approach.

Numerical Problems In Solving Differential Equations

Numerical problems occur when the discretized differential equations are solved in conjucture with the algebraic constraints. Here, the control of the integration error must be enforced in order to keep the method stable. Methods will fail due to incorrect error control strategies or instabilites resulting from the error propogation during the integration. In this section we will consider these difficulties in light of recent theory developed for solutions of Differential - Algebraic Equations (DAE's). First, we present some basic concepts and background on DAE's. Methods which handle higher index DAE systems will also be discussed. Finally, a detailed relation of higher index of DAE systems to optimal control problems will be presented in the next section.

These numerical problems are characteristic of classes of DAE's equations and can be classified by the index of the system. To illustrate the index of a problem , consider the special case of semi-explicit DAE's - (Petzold and Lötstedt (1986), Brenan (1983)) :

$$\dot{z} = f(z, v, t)$$
$$0 = g(z, v, t)$$

The index of this system is simply the number of times the algebraic constraints have to be differentiated to obtain a standard form ODE system. As an example, consider the mechanical system of a simple pendulum.(See Figure 5)

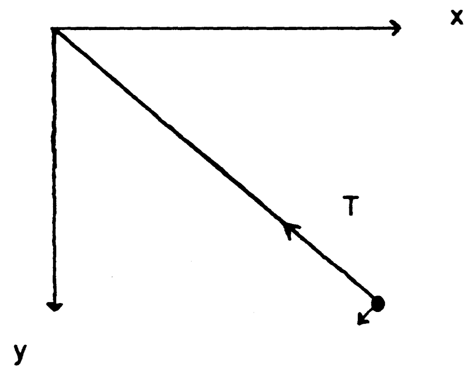


Figure 5. Pendulum System

For the case of a unit mass on a unit length of string, the following system of equations describe the model:

$$\dot{x} = u \qquad (a)$$
$$\dot{y} = v \qquad (b)$$
$$\dot{u} = -Tx \qquad (c)$$
$$\dot{v} = g - Ty \qquad (d)$$
$$1 = x^2 + y^2 \qquad (e)$$
$$x(0) = x_0$$
$$y(0) = y_0$$

This is an index three system because (e) has to be differentiated (and ODE's substituted) three times to yield a first order ODE in T. The first differentiation yields

$$0 = xu + yv \qquad (f) \qquad \text{Index } 2$$

Differentiating (f) gives:

$$0= -T+yg + u + v \quad (g) \qquad \text{index } 1$$

And differentiating again leads to :

$$f = 3vg -2Tux -2Tvy \quad (h) \qquad \text{index } 0$$

Using the index 0 formulation , one can, in principle, solve this problem with any standard ODE solver. The solution of this problem in the higher index forms has been studied for linear multistep methods such as the BDF (backward - differentiation formulas) first proposed by Gear (1971) and used currently in codes such as DASSL (1982) and LSODE (1980). Convergence proofs have been established for fixed step-size BDF methods for index 2 and index 3 problems (Lötstedt and Petzold (1986), and Brenan and Engquist (1985)). The variable step-size BDF for index 2 systems was established by Gear, Gupta, and Leimkuhler (1985).

Runge-Kutta method's for DAE's have been studied by Petzold (1986), März (1981), Brenan and Petzold (1986), and Burrage and Petzold (1988). Petzold (1986) showed that the Runge-Kutta methods can suffer order reduction for index one problems. Brenan and Petzold (1986) studied the order, stability, and convergence of implicit Runge-Kutta (IRK) methods applied to differential-algebraic systems. Burrage and Petzold (1988) established the convergence and stability properties of index 1 systems solved by IRK methods.

Two point orthogonal collocation falls into the class of IRK methods which are stable and have good error control (i.e., they converge to the solution as h => 0) for index 1 systems.

The higher index problem is of concern however because it is desirable to solve the DAE system directly rather than the differentiated form. Moreover, for optimal control problems, the solution may be governed by different sets of constraints over different parts of the trajectory and the reformulation is difficult to implement. Also the differentiation may introduce additional constants of integration which may not remain invariant under integration. As an example, consider the index 1 problem

$$0 = y - t^2 \qquad (5)$$

Differentiate to get

$$\dot{y} = t \qquad (6)$$

Even with the correct initial condition y(0) « 0, integration errors due to truncation and roundoff errors could cause the numerical solution of (6) to differ from (5). We would prefer to use the formulation of the DAE's in the higher index form because this is the natural statement of the physical models. Moreover, with optimal control problems where inequality constraints are active for only a portion of the problem, reformulation to an ODE system is usually impossible.

We tested the stability of collocation methods on the pendulum problem. The " analytical" solution was generated by using the index 0 formulation and LSODE was used for the solution . Further, two point collocation solved the index 1 system, but it failed for the index 3 formulation. Here four point (nonorthogonal) collocation was found to converge the index 3 formulation. However, when orthogonal roots were used the error propogation caused the solution to become unstable as the integration proceeded forward. The method with non-orthogonal roots remained stable. These results (Table 3) follow the stability properties shown by Brenan and Petzold (1986).

Table 3. Pendulum Results

Index	x	y	u	v	T	
after 100 elements						
0	0.391044	0.920376	-3.91109	1.661727	27.086565	
1	0.391048	0.920369	-3.91104	1.661734	27.086487	+
3	0.391048	0.920369	-3.91104	1.661736	27.086496	*
3	0.391048	0.920369	-3.91106	1.661705	31.684719	"
after 2000 elements						
0	0.275085	0.961419	•4.175598	1.194742	28.294455	
3	0.275087	0.961419	-4.175598	1.194749	28.294575	*
3	-0.137607	0.951803	40924.18	-283047	1.068e12	**

Key + two-pointA-stable (orthogonal)

* four point L-stable (nonorthogonal)

** four point A-stable (orthogonal)

Note that the A-stable cases are obtained by using orthogonal collocation and the L-stable cases are obtained by also collocating at the endpoint. Also we see from the table that the error propogates in the algebraic (control) variable and as the error grows with time it causes the differential variables to become unstable. The above results were obtained by careful selection of the integration step size.

The theoretical properties of collocation have thus been established and illustrated (Brenan and Petzold (1986)). By using the proper order of a stable method we can therefore solve systems of equations that are higher index by controlling the integration error.

The minimum requirements are listed below

1. Index 1 problems - two point collocation
2. Index 2 problems - three point collocation
3. Index 3 problems - four point collocation

However, optimal control problems may be mixed index problems due to the appearance of path constraints caused by state variable constraints and conditions for singular arcs. Here control variables are the "higher" index variables if the algebraic constraints do not explicitly contain them. As mentioned above, it is not desirable to reformulate these constraints because, over the solution trajectory, different constraints may be active and we do not know , a priori , where the higher index constraints will be active. Also, the issue of numerical errors from the differentiation would have to be dealt with. In the next section , we will investigate the path constraints and singular arc cases after reviewing the optimal control formulation.

6. Optimal Control Problem Formulation

Consider the following optimal control problem

$$\text{Mn} \quad J$$
$$\text{s.t} \quad \dot{x} \; * \; f(x(t),u(t),t) \quad _t \; x(t_o) = x_o$$

Here we form the adjoined cost function

$$J = *(x(t,),t,) + f\,\{L[x(t),u(t),t] + X^T(t)[(f(x(t),u(t),t)-\dot{i}(t)\}dt$$

with the Hamiltonian being defined as:

$$H[x(t),u(t),X(t),t] - L[x(t),u(t),t] + X^J i[x(t),u(t),t]$$

It can be shown from variational calculus:

$$\dot{\lambda}^T(t) = -\frac{\partial H(x(t),u(t),\lambda(t),t)}{\partial x} \qquad (7)$$

$$\lambda^T(t_f) = \frac{\partial \Phi(x(t),t)}{\partial x}\Big]_{t=t_f} \qquad (8)$$

$$\frac{\partial H[x(t),u(t),\lambda(t),t]}{\partial u} = 0 \qquad (9)$$

Equations (7 to 9) are the Euler-Lagrange equations and are necessary conditions for optimality when the final time is fixed. Note that the optimization of the cost function subject to a dynamic constraint is a split boundary problem for state and adjoint variable equations. In addition, an algebraic equation (9) must be solved. The alternative to repeatedly solving the ODE's forward and backwards is to solve the discretized equations (with the Kuhn-Tucker conditions) simultaneously. Also, by using the math programming formulation, inequalities can easily be enforced when they become active. The relationship between the Kuhn - Tucker conditions and the optimality conditions from the calculus of variations was shown by Cuthrell and Biegler (1988).

Path Constraints and Singular Arcs

Bryson and Ho (1975) developed the case for an equality path constraint as a q^{th} order state variable constraint when the equation is a function of states only (the control is implicit in the equation). Consider

$$S(x,t) = 0$$

For this condition to hold for a section of the path, $t_o \le t \le t^*$, its time derivative along that section of the path must vanish, i.e.,

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \frac{\partial S}{\partial x} f(x,u,t) \qquad (10)$$

The order of (10) is defined as the number of times that (10) has to be differentiated in order to recover the dependence of the control - u. As an example , consider the problem of starting and stopping a car in the minimum time for a fixed distance (300 units). The problem description is:

$$\begin{aligned}
&\text{Min } t_f && && \text{(CP)}\\
&\text{s.t. } \dot{z}_2 = z_1 && z_1(0) = 0\ ,\ z_2(0) = 0 &&\\
&\qquad \dot{z}_1 = u && z_1(t_f) = 0\ ,\ z_2(t_f) = 300 &&\\
&\qquad -2 \le u \le 1 && &&
\end{aligned}$$

The analytical solution is the expected bang-bang solution shown in Figures 6 - 8. This problem is index 1 because one differentiation is needed to obtain an expression for $\dot{u}$ (from the active inequality constraint bounding u). Next lets place a path constraint on the problem by setting an upper bound on the speed limit of 10 units. When this speed limit comes into effect, then the problem is index 2 for that portion of the solution trajectories. The problem is index 2 because the speed can not exceed 10 units and the control has to be adjusted accordingly (or two differentiations are needed to obtain $\dot{u}$ from 2 ^ 1 0) . The solution profiles for this problem are shown in Figures 9 - 1 1 . Notice that the path constraint forces the control off of the bounds even though the problem is linear in the states and the control.

Another way for the index of the DAE system to increase is due to the existence of a singular arc.

To review the conditions for a singular arc, consider the following optimal control problem

$$\text{Min} \quad <\&(x_{tf})$$

$$\text{s.t} \quad \dot{x} = f(x) + g(x)u \qquad (11)$$

$$¥(x_{I(})-0 \quad , \quad t_o \leq t \leq t,$$

The Hamiltonian is linear in u and assumed to be non-linear in x

$$H = M^T \; f(x)+g(x)u] \qquad (12)$$

Necessary conditions include

$$\frac{|i}{du} = X^T g(x) - 0 \qquad (13)$$

$$i = -[M^T \; Ix + 0x)I \qquad 04)$$

$$M^T t_f) = (*_x + v^T 4\backslash)_{wf} \qquad (15)$$

Note that (13) does not determine the control u (x, X) directly; additional conditions are needed to find u(t) so that (13) is satisfied. If this happens then

$$\frac{d}{dt}\frac{\partial H}{\partial u} = \lambda^T \dot{g} +$$

$$= \lambda^T \frac{\partial g}{\partial x}\dot{x} + \dot{\lambda}^T g = 0$$

Substituting (11) and (14) into (13) yields

$$\frac{d}{dt}\left(\frac{\partial H}{\partial u}\right) = \lambda^T \frac{\partial g}{\partial x}[f + gu] - \lambda^T\left[\frac{\partial f}{\partial x} + \frac{\partial g}{\partial x}u\right]g$$

$$= \lambda^T q(x) = 0$$

where $$q(x) = \frac{\partial g}{\partial x} f - \frac{\partial f}{\partial x} g$$

Note that the terms in u cancel each other so we are forced to take the second derivative of &-) du

in order to recover u.

$$\frac{d^2}{dt^2}\left(\frac{\partial H}{\partial u}\right) = \lambda^T \dot{q} + \dot{\lambda}^T q = \lambda^T \frac{\partial q}{\partial x}(f+gu) - \lambda^T \left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial x} u\right) q$$

$$= \lambda^T \left(\frac{\partial q}{\partial x} f - \frac{\partial f}{\partial x} q\right) + \lambda^T \left(\frac{\partial q}{\partial x} g - \frac{\partial g}{\partial x} q\right) u = 0$$

Then, for a single singular control profile :

$$u = \frac{-\lambda^T \left(\frac{\partial q}{\partial x} f - \frac{\partial f}{\partial x} q\right)}{\lambda^T \left(\frac{\partial q}{\partial x} g - \frac{\partial g}{\partial x} q\right)} \quad \text{if} \quad \lambda^T \left(\frac{\partial q}{\partial x} g - \frac{\partial g}{\partial x} q\right) \neq 0$$

Therefore, singular arcs that occur for the above type of problems would normally be index 3 because at least three differentiations of $\partial H / \partial u$ would be required to obtain an expression for $\dot{u}$.

As an example, consider the mixed catalyst problem solved analytically by Jackson (1968).

$$\text{Min} \quad P(t) = 1 - x(t_f) - y(t_f) \quad , t_f \text{ specified}$$

$$\text{s.t.} \quad \frac{dx}{dt} = u(k_2 y - k_1 x)$$

$$\frac{dy}{dt} = -u(k_2 y - k_1 x) - (1-u)k_3 y$$

$$x(0) = 1.0$$

$$y(0) = 0.0$$

The Hamiltonian for this system is

$$H = \lambda_1 u(k_2 y - k_1 x) + \lambda_2[u(k_1 x - k_2 y) - (1-u)k_3 y]$$

and the adjoint equations are

$$\dot{\lambda}_1 = u k_1(\lambda_1 - \lambda_2)$$

$$\dot{\lambda}_2 = -u k_2(\lambda_1 - \lambda_2) + (1-u) k_3 \lambda_2$$

Taking the first time derivative yields :

$$\frac{d}{dt}\left(\frac{\partial H}{\partial u}\right) = k_3(\lambda_2 k_1 x - \lambda_1 k_2 y) = 0$$

which does not exhibit any control dependence.

The second time derivative is

$$\frac{d^2}{dt^2}\left(\frac{\partial H}{du}\right) = \dot{\lambda}_2 k_1 x + \lambda_2 k_1 \dot{x} - (\dot{\lambda}_1 k_2 y + \lambda_1 k_2 \dot{y})$$

from which one can obtain the control as in the general derivation above . The problem is index 3 over the singular arc section. The analytical solution is shown in Figure 14.

7. Example Problems

Orthogonal collocation (with Lagrange polynomial basis functions) on finite elements was used to construct the control profiles by using math programming techiques, as described in sections 2 and 3 . The control of the integration error was achieved by defining a residual at non-collocation point.

The first example to consider is the car problem (CP) given above. Without a speed limit constraint, (CP) is an index 1 problem and two-point collocation solves this problem without any problems, matching the analytical results shown in Figures 6 - 8. Next, we placed the speed limit constraint on the problem and changed the problem from one of index 1 to a mixed problem of index 1 and index 2. The trajectory where the control moves off of the bound is index 2. We obtained a solution without controlling the error in the index 2 segment using two-point collocation and the control profile is shown in Figure 12. This solution was unsatisfactory, and we added the residual constraints as inequalities to the formulation. The numerical result obtained matched the analytical result. Note that we solved a mixed index 1 - index 2 system using two-point collocation which does not have algebraic order for index 2 systems but that we controlled the error to achieve the solution.

Figure 13 shows the comparison between the speed limit problem and the unconstrained car problem . As expected the speed limit constraint required a longer time to cover 300 distance units.

The next example, the mixed catalyst problem (Jackson (1968)), raises more questions. The problem has a singular arc solution for a fixed time of 1 hour. This is a mixed index 1 - index 3 problem and was found to be very difficult to achieve a solution . We achieved a solution using two-point collocation by controlling the integration error in each element individually as inequality constraints in the math programming formulation. Table 4 shows the final residuals and error tolerances.

Table 4. Mixed Catalyst Results

Element	$\Delta\alpha_i$	Controls u_1	u_2	Final Residual	Error Tolerance
1	.07924	1.0	1.0	2.241e-5	2.5e-5
2	.05750	1.0	1.0	7.075e-7	9.0e-7
3	.29830	.2264	.2267	1.320e-10	9.0e-11
4	.29311	.2252	.2249	4.360e-11	9.0e-11
5	.27182	0.0	0.0	1.006e-8	1.9e-8

Note that different error tolerances are exhibited in each element ; these were set by trial and error until the solution matching the analytical profile (singular arc section - u = 0.2272) was achieved (See Figure 15). Other strategies would either terminate due to line search failures or they would converge to sub-optimal solutions. This method of solution is not very robust because the trail and error procedure required setting the residual weights based on solutions obtained using two-point collocation for a mixed index 1 - index 3 problem.

We then converted the catalyst problem from an index three problem to an index zero problem by parameterizing the control profile. We required that the control variables be the same within each element, in effect, lining up reactors in sequence and asking what catalyst blend for a given reactor length would optimize the problem? The solution using this approach matched the analytical solution within numerical tolerances (See Figure 16).

8. Conclusions

This paper considers efficient formulations for simultaneous solution and optimization of Differential - Algebraic systems. After applying collocation on finite elements to this problem, knot placement equations are added to the nonlinear program. In this way the solution of the DAE system, accurate placement of the knots , the determination of optimal parameters, and control profiles are found simultaneously.

This concept was introduced by Cuthrell and Biegler (1986). To extend the knot placement strategy, this paper presents a more reliable residual - based formulation that simplifies the intialization procedure in Cuthrell and Biegler (1986). The knot placement constraints can be formulated in two ways. If sufficient elements are available, the residual error can be enforced directly to be below a certain tolerance, e . With equidistribution, on the other hand, the residual error is minimized for a given number of elements. To demonstrate the concept of knot placement, the optimization of a hot spot reactor is presented.

Optimal control problems , on the other hand, present another class of difficulties compared to parameter optimization problems. By writing the Kuhn - Tucker conditions for both problems (see Cuthrell and Biegler (1988)), one can consider the parameter optimization problem as a boundary value problem, while the optimal control problem becomes a DAE system. To study these problems more closely we presented some properties and difficulties in solving DAE's. These properties were applied to optimal control problems and examples were presented to show how these difficulties are carried over. Finally, a number of small examples were solved to demonstrate the effectiveness of this approach.

For simultaneous solution of parametric optimization problems, an open question remains regarding selecting the number of finite elements. Work is currently being done with LP relaxation strategies that adaptively add elements during the solution strategy. For optimal control problems that result in higher index systems of DAE's , future work will address the derivation of appropriate error criteria for state and control profiles.

References

1. Biegler, L.T., " Solution of Dynamic Optimization Problems by Successive Quadratic Programming and Orthogonal Collocation," Computers and Chemical Engineering, Vol. 8 No. 3/4 pp. 243-248 (1984)

2. Brenan, K. " Stability and convergence of difference approximations for higher index differential/algebraic equations with applications to trajectory control", Ph. D. Disseration , Math Dept. UCLA , Los Angeles (1983)

3. Brenan.K.E., and L.R. Petzold ," The Numerical Solution of Higher Index Differential/Algebraic Equations by Implicit Runge - Kutta Methods M , UCRL - 95905. preprint, Sandia National Laboratories, Livermore, Ca. (1986)

4. Bryson, A.E. and Y-C Ho , Applied Optimal Control, Hemisphere Publishing, Washington D. C. (1975)

5. Campbell, S.L.Singular Systems of Differential Equations, Research Notes in Mathematics 40, Pitman Advanced Publishing Program (1980)

6. Cuthrell, J.E.,Ph. D. thesis, Carnegie - Mellon University, Oct. (1986)

7. Cuthrell, J. E., and L.T. Biegler, " On the Optimization of Differential - Algebraic Process Systems ", AICHE J. 33(8),1257 (1987)

8. de Boor, C.," Collocation at Gaussian Points", SIAM J. Numerical Anal. 10(4) pp. 582 - 606 (1973)

9. de Boor, C. , * Good Approximation by Splines with Variable Knots. II", Dundee conf. on Numerical Solution of Differential Equations, Lecture Notes in Math #363 (1974)

10. de Boor, C, A Practical Guide to Splines, Springer - Veriag (1978)

11. Finlayson, B.A.," Packed Bed Reactor Analysis By Orthogonal Collocation", Chem. Eng. Sci., 26, pp. 1081 -1091 (1971)

12. Gear, C.W.. , "Simultaneous numerical solution of differential algebraic equations", IEEE Trans. Circuit Theory CT-18 (1971), pp.89-95.

13. Gear ,C.W., B. Leimkuhler, and G.K. Gupta ," Automatic Integration of Euler - Lagrange Equations with Constraints", Journal of Computational and Applied Mathematics 12 and 13 (1985) pp.77-90

14. Han , S- P.," A Globally Convergent Method for Nonlinear Programming", J. Opt. Theory and Cont., 22, 3 p.297 (1977)

15. Hindmarsh, A.C.," LSODE and LSODI, Two New Initial Value Ordinary Differential Equation Solvers", ACM - SIGNUM Newsletter, Vol. 15, No. 4 (1980) pp. 10-11

16. Hlavacek, V.," Aspects in Design of Packed Catalytic Reactors", Ind. & Eng. Chem., 62 (7) (1970)

17. Jackson , J.," Optimal Use of Mixed Catalysts For Two Successive Chemical Reactions", Journal of Optimization Theory and Applications , Vol. 2, No.1 (1968)

18. Lötstedt, P. ," On the Relation Between Singular Perturbation Problems and Differential - Algebraic Equations", Report No.100 , Department of Computer Science , Uppsala University (1985)

19. März. M. ," Multistep Methods for Initial Value Problems in Implicit Differential - Algebraic Equations" Preprint No. 22, Humboldt - Universitat, Berlin , Sektion Matematik (1981)

20. Murtagh, B.A. and M. A. Saunders, * Minos / Augmented Supplementary User's Manual", Report OR / 78 / 6, The University of New South Wales, Australia (1978)

21. Pereyra, V. and E.G. Sewell," Mesh Selection for Discrete Solution of Boundary Problems in Ordinary Differential Equations", Numer. Math., 23, pp. 261 - 268 (1978)

22. Petzold, L.R., " A description of DASSL: A differential/ algebraic system solver", SAND82-8637, Sandia National Laboratries, Livermore, Ca. (1982)

23. Petzold, L.R.," Order Results for Implicit Runge - Kutta Methods Applied to Differential/ Algebraic", SIAM Journal on Numerical Analysis, No. 4, pp. 837-852 (1986)

24. Petzold, L.R., and P. Lötstedt," Numerical solution of nonlinear differential equations with algebraic constraints I: convergence results for backward differentiation formulas ", SIAM J. Sci. and Stat. Computing (July 1986), Vol. 7, No. 3, pp. 720 - 733

25. Powell, M. J. D.,* A Fast Algorithm for Nonlinearly Constrained Optimization Calculations", Dundee Conf. on Num. Analysis (1977)

26. Ray, W.H.,Advanced Process Control, McGraw-Hill , New York (1981)

27. Renfro.J.G., Computational Studies in the Optimization of Systems Described by Differential - Algebraic Equations . Ph. D. Dissertation, University of Houston , Texas (1986)

28. Russell, R.D. and J. Christiansen," Adaptive Mesh Selection Strategies for Solving Boundary Value Problems", SIAM J. Numerical Anal., 15(1), pp. 59 - 80 (1978)

29. Sargent, R.W.H. and G.R. Sullivan, " The Development of an Efficient Optimal Control Package", Proceedings of the 8th IFIP Conference on Optimization Techniques Pt. 2 (1977)

30. Vasantharajan, S. and L.T. Biegler," Large - Scale Decomposition for Successive Quadratic Programming", (Accepted for publication), Comp. and Chem. Eng. (1988)

31. Vasantharajan, S. and L.T. Biegler," Simultaneous Solution of Reactor Models", Chem. Eng. Res. Des., 66, pp. 396 -407 (1988)

32. Vasantharajan, S., Ph. D. Proposal Report, Carnegie Mellon University (1987)

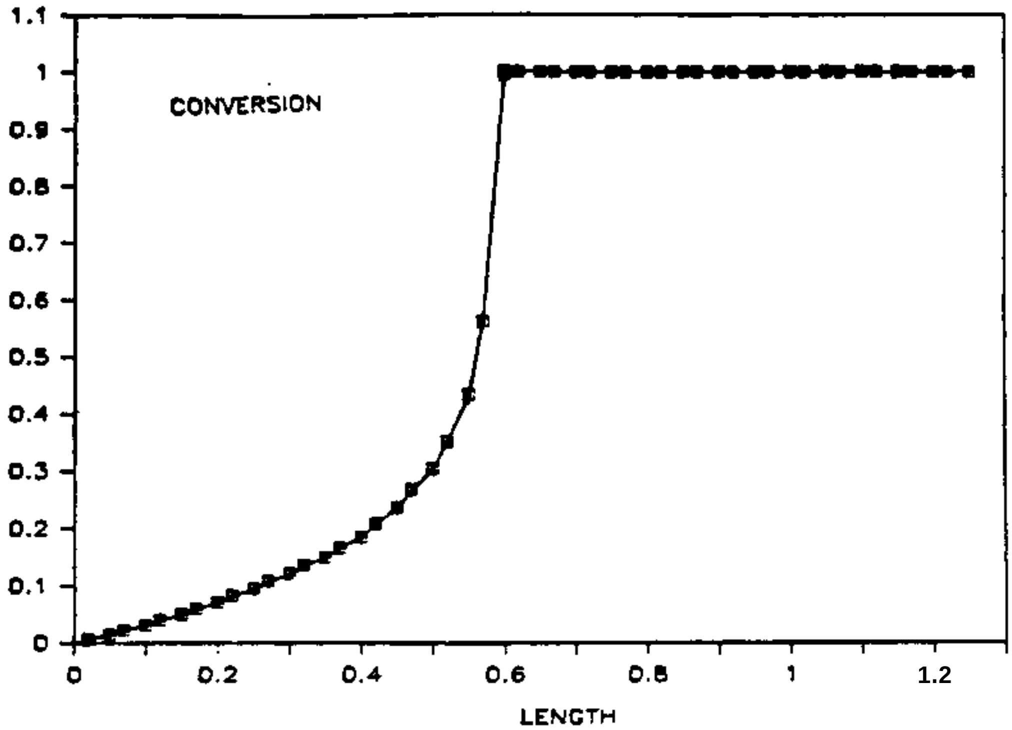
	Case Ia	Case Ib	Case II
T/C)	500	500	500
L	1.25	1.25	1.0
T/C)	470.1	450.5	448.4
T_p(°C)	188.4	232.1	345.2
$\|q^{err}(t)\|$	0.01101	0.01093	0.02028
|-r^r«f	0.0065S2	0.006488	0.01256
# SQP iterations	44	23	45
4>*	-172.967	-148.473	-82.524
KT error	10"^{5}	10"^{5}	10"^{13}
CPU/iter (sec)$^{+}$	11.98	11.69	7.46
CPU/QP (sec)$^{+}$	6.05	5.97	3.6

t Micro VAX II

Table 1: Results for Reactor Optimization Problem

	Case Ia	Case Ib	Case II
a . initial	0,0.167,0.333,0.500	same as Ia	0,0.134,0.268,0.402
i=1.....NE+1	0.667,0.692,1.0		0.536,0.67
a . final	0,0.271.0.509,0.557	0,0.450.0.649,0.833	0.0.431,0.700,0.832
i=1.....NE+1	0.589.0.618,1.25	0.884.0.934,1.25	0.921,1.0

Table 2: Initial and Final Knot Distributions for (P1)



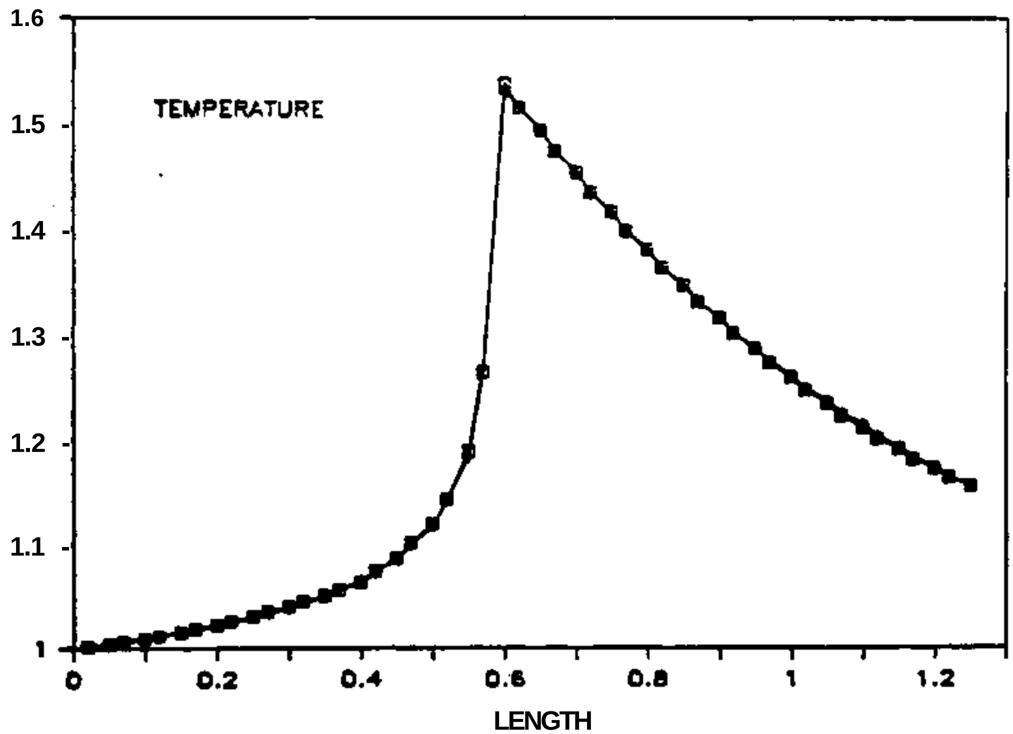


Figure 1: Final Profiles for Problem (P1): Case la

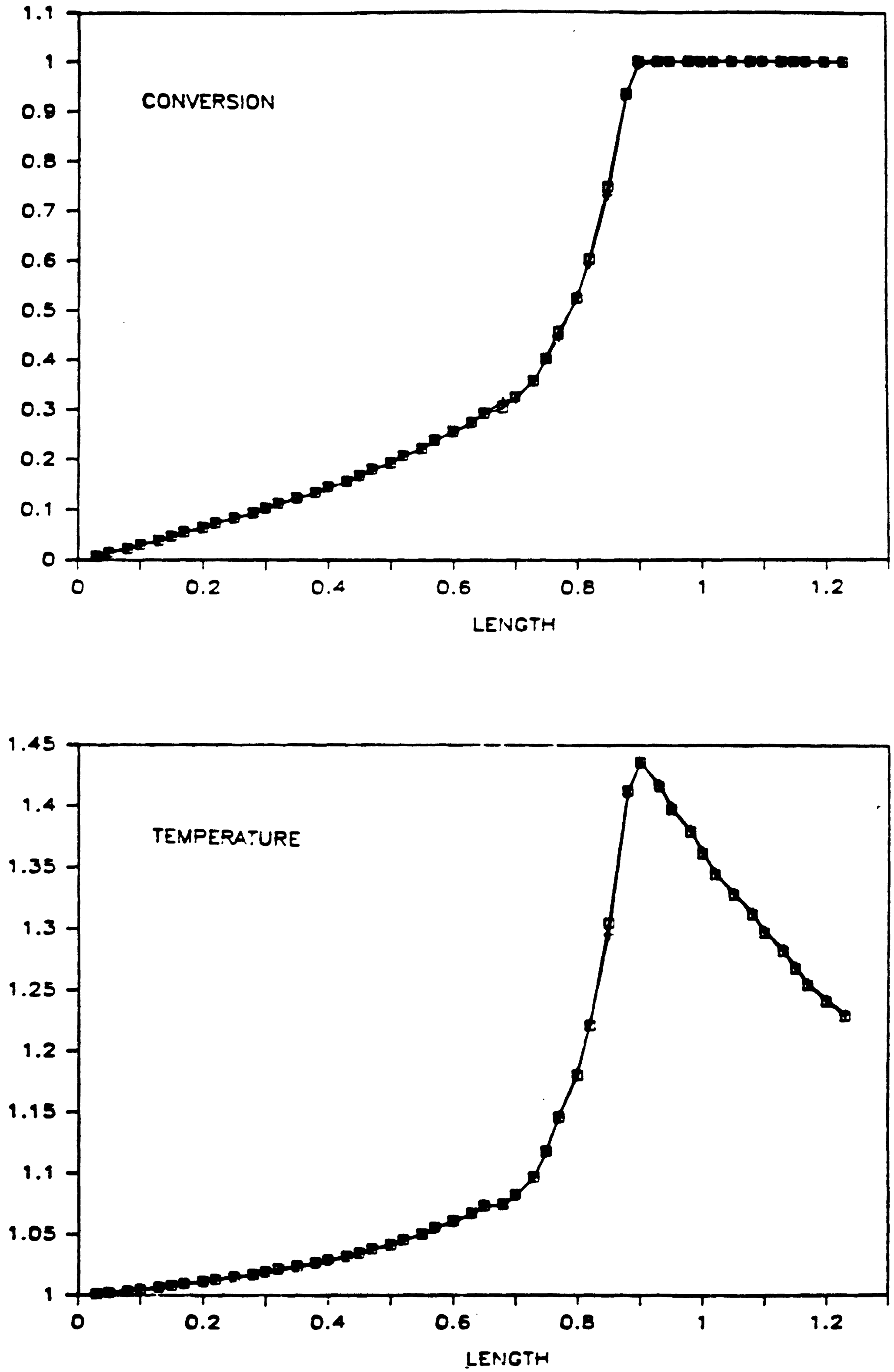


Figure 2: Final Profiles for Problem (P1): Case Ib

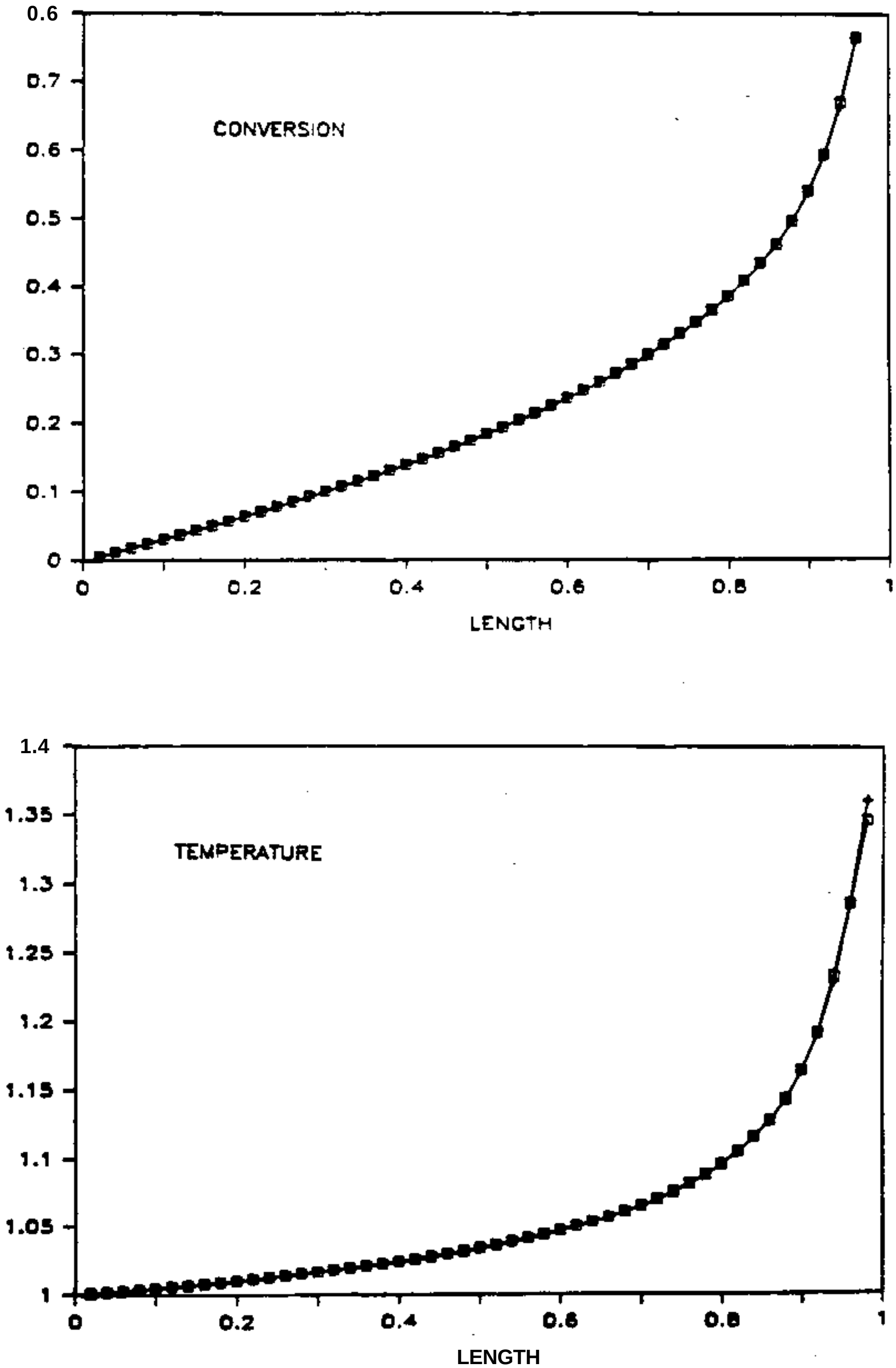


Figure 3: Final Profiles for Problem (P1): Case II

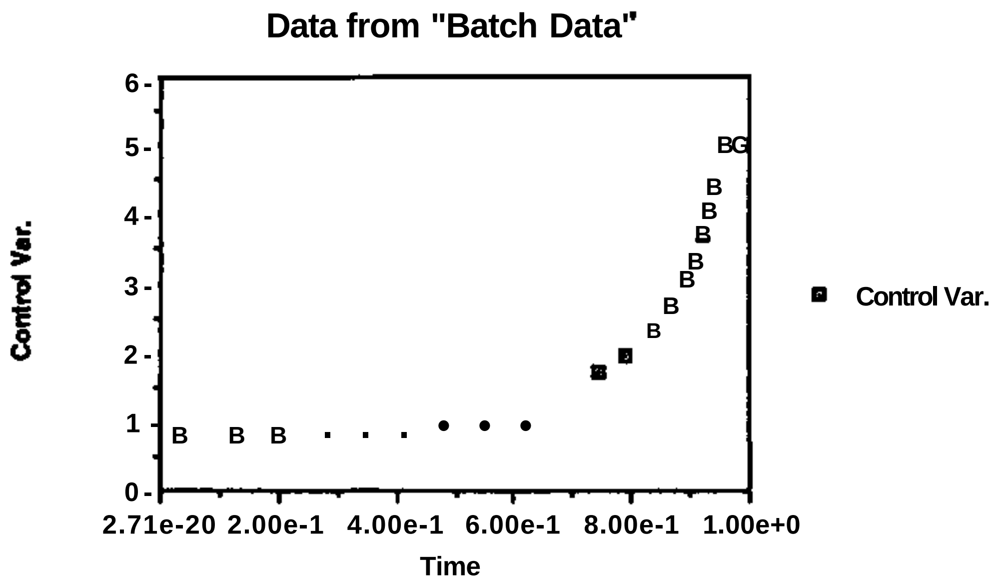


Figure 4. Optimal Temperature Profile

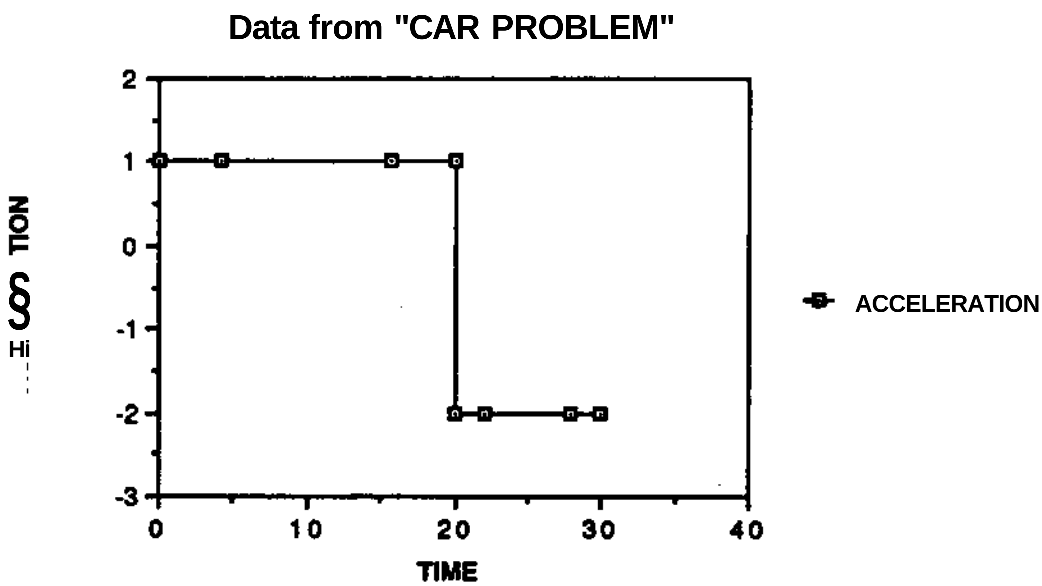


Figure 6. Analytical Control Profile

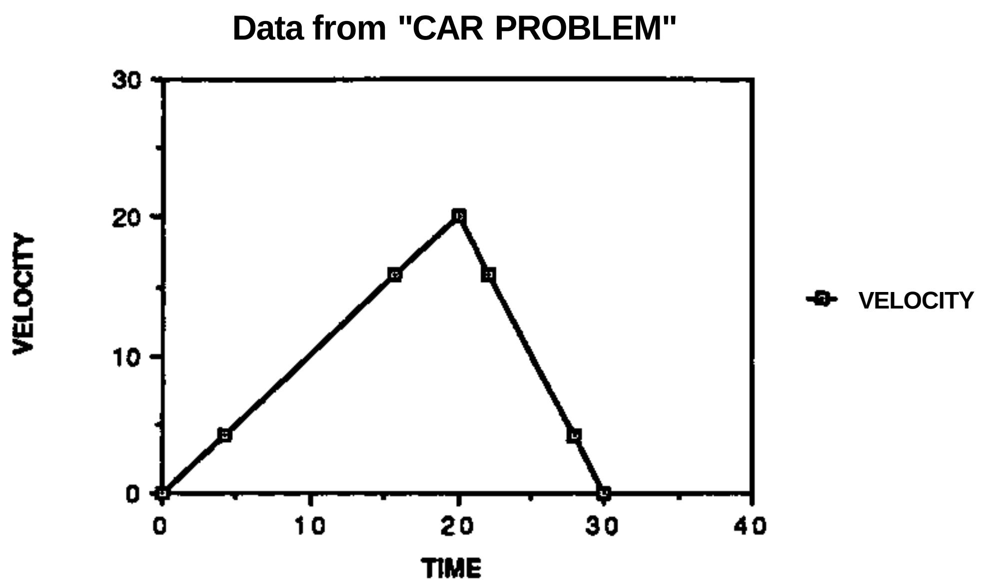


Figure 7. Analytical Velocity

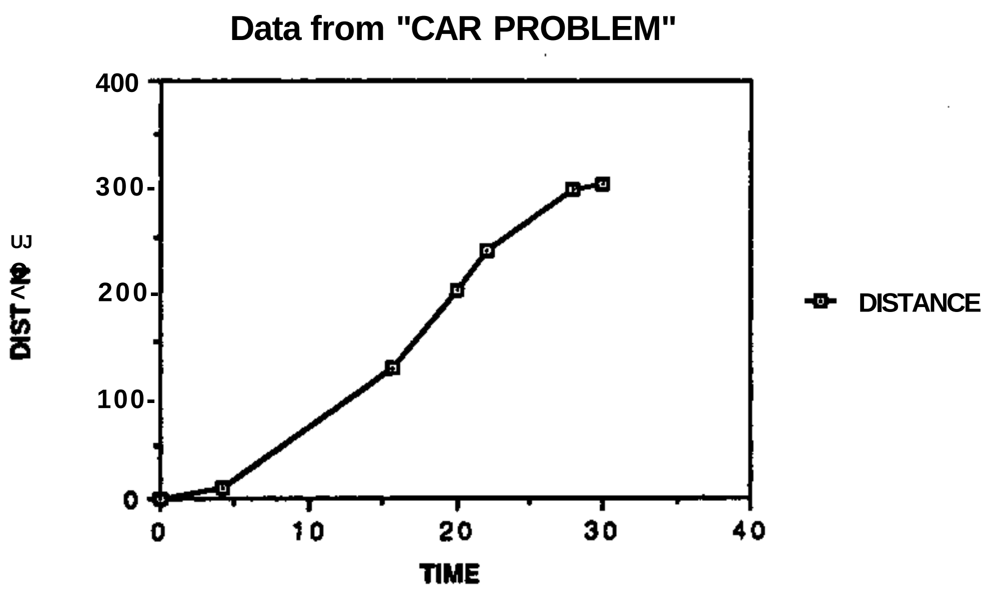


Figure 8. Analytical Distance

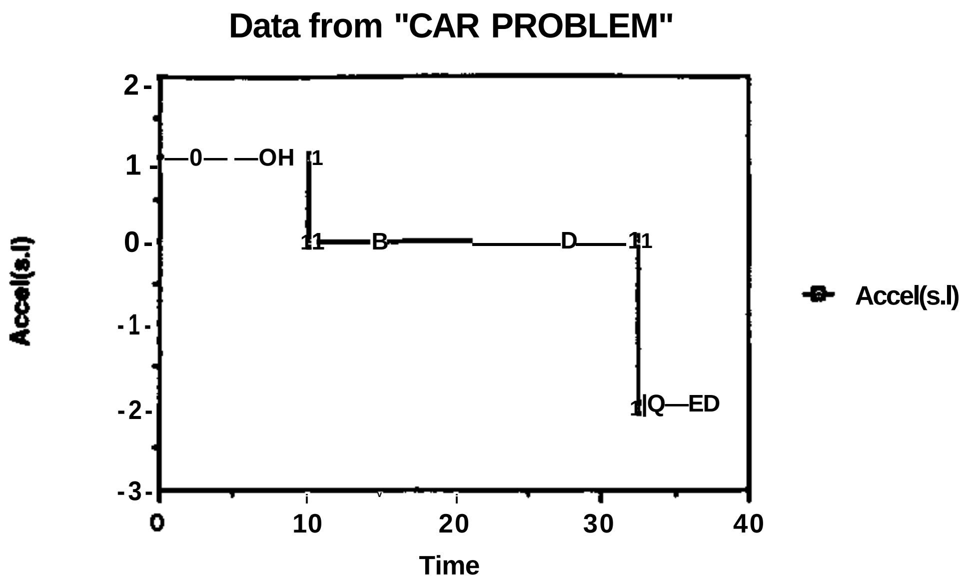


Figure 9. Speed Limit Acceleration Case

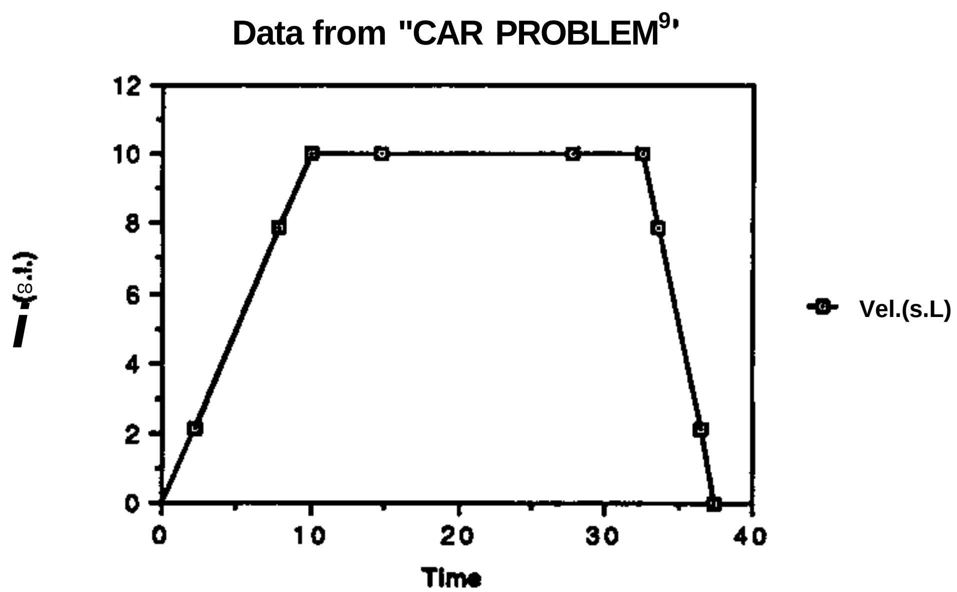


Figure 10. Speed Limit Vetocity Case

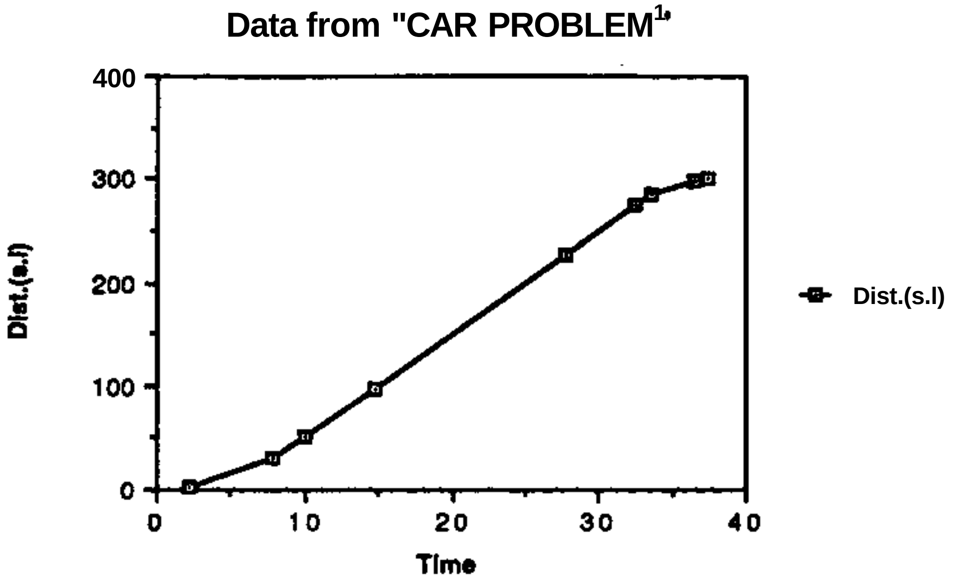


Figure 11. Speed Limit Case -Distance

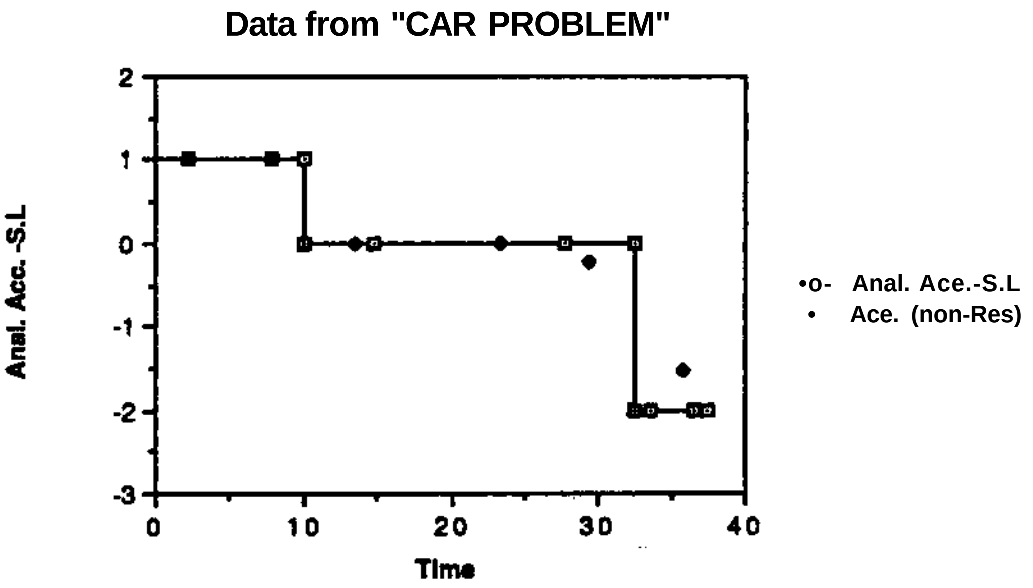


Figure 12. Acceleration Profile - Nonresidual case

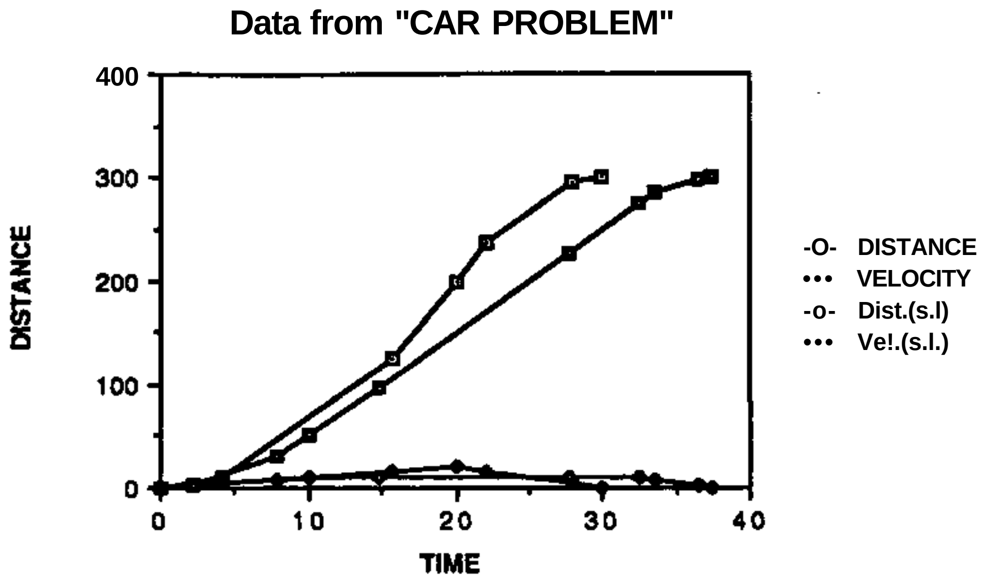


Figure 13. Comparison of Constrained and Unconstrained Cases for Car Problem

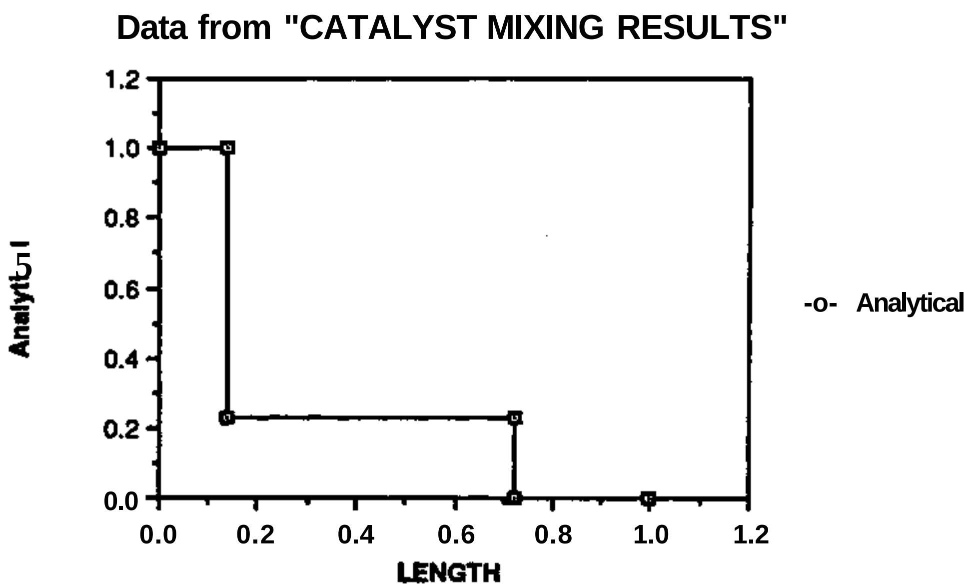


Figure 14. Analytical Profile for Blend Policy

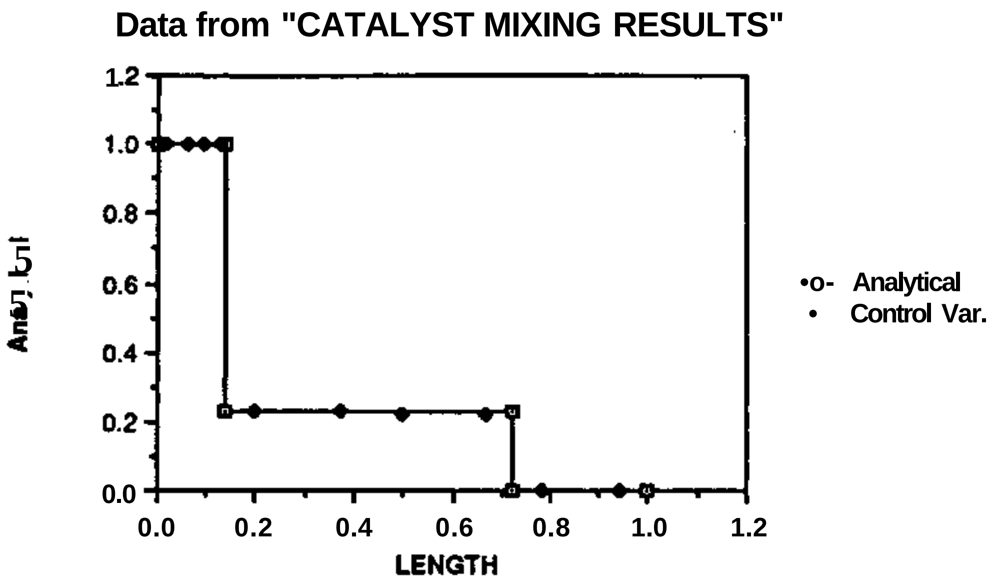


Figure 15. Catalyst Problem Two-Point Results

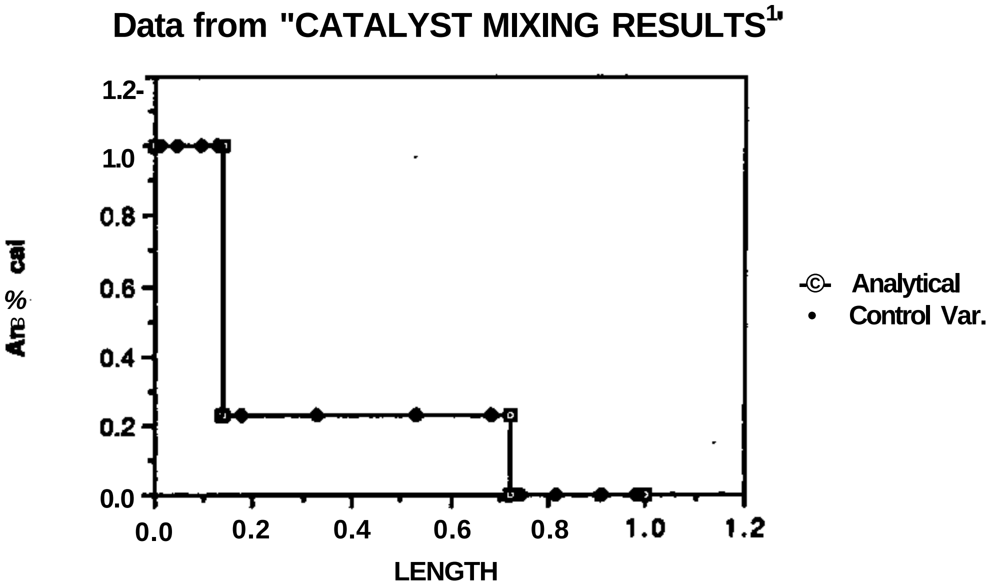


Figure 16. Mixed Catalyst Problem - Parameterized Result