NOTICE WARNING CONCERNING COPYRIGHT RESTRICTIONS:

The copyright law of the United States (title 17, U.S. Code) governs the making of photocopies or other reproductions of copyrighted material. Any copying of this document without permission of its author may be prohibited by law.

Multistep, Newton-Type Control Strategies for Constrained, Nonlinear Processes

by

.

• • .

.

.

W.C. Li, L.T. Biegler

EDRC 06-68-89 Carnegie Mellon University

MULTISTEP, NEWTON-TYPE CONTROL STRATEGIES FOR

CONSTRAINED, NONLINEAR PROCESSES

W. C. LI and L. T. Biegler*

Carnegie-Mellon University Department of Chemical Engineering Pittsburgh, PA 15213

Submitted to Chemical Engineering Research and Design May, 1989

.

.

*Author to whom correspondence should be addressed

Financial support from the National Science Foundation, under Grant ENG 8451058, is gratefully acknowledged.

Multistep, Newton-type control strategies are developed in order to deal with nonlinear, constrained process control problems. The development parallels the previous development of single step strategies based on operator theory, and this extension includes input and output constraints.

In this paper we consider the development of moving time horizon strategies where optimal controller moves are determined from a model linearized about a nominal trajectory, and only the first step is implemented. In a nonlinear analogy to Quadratic Dynamic Matrix Control (QDMC), this approach solves a single quadratic program (QP) over the time horizon and easily incorporates bounds on control inputs and outputs.

By invoking concepts from operator theory such as attraction regions for contraction mappings and descent directions, we also derive sufficient conditions for stability of these methods; these conditions can also be checked on-line. Finally, the effectiveness of this approach is demonstrated on two nonlinear, reactor examples.

1. Introduction

The effectiveness of Quadratic Dynamic Matrix Control (QDMC) has been demonstrated for multivariable linear process models with input and output constraints (Prett and Garcia, 1988). Recently, the extension of this approach to nonlinear process models was proposed by a number of researchers (Morshedi, 1986; Patwardhan, et al, 1988). Since minimization (over a time horizon) of the setpoint deviation for linear models can be formulated as a QP, the natural extension for nonlinear models is to formulate a nonlinear program for each time horizon. While this approach shows considerable promise, it can sometimes be expensive for large models, especially since the standard approach is to solve quadratic programs recursively until convergence.

The approach considered in this paper is simply to linearize the nonlinear model around a nominal trajectory and to solve a QP once over the horizon. As the controller moves are implemented and the time horizon moves forward, successively smaller deviations from the setpoint are observed and this procedure thus converges as it moves forward in time.

This approach is motivated by recently developed single-step Newton-type methods (Li et al, 1989). By treating the control algorithm as a nonlinear operator, analogies can be made to stability, i.e. convergence of the method, through contraction mappings (Economou, 1985). Moreover, through the action of a line search, global convergence of the method can be enforced as long as the method exhibits descent directions. Descent properties for the single-step Newton method that guarantee monotonic convergence to the setpoint were shown in Li et al (1989). With these two properties, one can demonstrate, under mild conditions, the stability of this single step, Newton-type algorithm.

The single step algorithm was derived on the assumption that a linearization of the process reaches its setpoint at the end of the first step. However, if the process has time delays or inverse responses slower than one sampling time interval, the single step algorithm experiences difficulties. In addition,

> University Libraries Carnegie Mellon University Pittsburgh, Pennsylvania 15213

1

when an optimal time profile needs to determined (e.g. in a batch process) a multistep predictive algorithm is required. Finally, even if a process does not have these characteristics, controller performance benefits from a multistep algorithm in a moving time horizon.

In the next section, a multistep algorithm for controlling a continuous process with a constant setpoint is developed. The algorithm requires the solution of one (or, if desired, several) quadratic programming (QP) problems for each time horizon. Controller moves are implemented only after a line search is performed. Here a sufficiently small stepsize is found from the QP-generated search direction. Finally, the algorithm is also modified from the moving time horizon format to directly handle the determination of optimal process profiles, in which we are only interested in the system outputs at the end of the process time.

Section three then deals with the extension of this method to handle a restricted class (for illustration purposes) of state and control variable time delays. Since the solutions of time delay systems are not only dependent on the initial condition at the beginning of the sampling time, but also dependent on the initial path function in the previous time interval, a new formulation needs to be developed to discretize the systems and to derive the Newton-type control strategy. The results of this analysis show that our approach can be applied directly to general classes of time delay problems.

Section four develops sufficient conditions for the stability (or global convergence) of this multistep, moving time horizon approach. By showing that the optimal controller moves generate descent directions for the norm of the setpoint deviations, one can guarantee, through the application of a line search, that the setpoint is approached monotonically. For both unconstrained and constrained controllers we will show that for sampling times sufficiently large, these descent properties are always obtained. The existence of descent properties also has implications for other recently developed multistep, optimization-based approaches. In particular, Patwardhan et al (1988), Peterson et al (1989) and Brengel and Seider (1989) have developed similar nonlinear multistep controllers that have characteristics related to our approach.

Finally, section five demonstrates the effectiveness of our approach on two nonlinear reactor control problems, while section six concludes the paper. With these examples we show the ability of our multistep approach to generate optimal operating profiles as well as perform as a moving time horizon controller. Moreover, the second example demonstrates the controller's ability to deal with time delays.

2

2. Derivation of the General Constrained Newton-Type Control Algorithm

The constrained nonlinear control problem typically can be formulated as follows:

$$S.t \quad \underbrace{\pounds}_{\mu t} = f(x,\mu(t)) \tag{1a}$$

$$\mathbf{y} \leq \mathbf{y}\mathbf{i}\mathbf{t} \quad \mathbf{z} \quad \mathbf{y}^{\mathbf{z}} \tag{1c}$$

$$a^* \pounds u(\mathbf{r}) \pounds u^{\mu}$$
 (1d)

$$\mathbf{u}'(0^7 \wedge u|t) \leq \mathbf{u}'(t)^{\boldsymbol{u}} \tag{1e}$$

$$JC_0 = known$$

where $x \in \mathbb{R}^n$ is the state of the system, and for every $t \in (0, \sim)$, $u(t) \in \mathbb{R}^m$ is the input, with the corresponding output map $(y \in \mathbb{R}^p)$ and $p \notin \dots u'(t)$ is the derivative of system inputs with respect to t. y' is a constant setpoint. All the inequalities are represented by simple bounds without loss of generality. Here $|| \cdot ||$ can be any weighted norm in time and y.

The system inputs are also assumed to be piecewise constant functions and the moving time horizon (see Figure 1) is used in the development of the multistep control algorithm. The following notation will be used:

I — the number of predictive steps

s+i ~ superscript; the (s+i)* sampling time interval extends from t^{6*1} to t^{6*i+1}

- T ~ the constant sampling time
- u^{s+i} the system inputs held constant over (t^{8*1} , t^{s+i+1})
- x^{s+i} the solution of equation(1 a) at time t^{s+i+1}

Also the following convention is introduced; $\overline{y}^{**2} \ll (x(i^{**1}; \Lambda^1))$. i.e. the system outputs at t • t^{8*2} if the inputs were held at a nominal value such as \overline{u}^{**1} over the $(s+i)^*$ sampling interval. Similarly, $y^{**3} - (x(f^{**2}; \overline{x}^* + ^2)u^* + ^2))_t$ etc. The bar indicates that these are nominal system states, inputs, and outputs. The nominal values of control variables can be defined in any method which is suitable for problem (1). For instance, if problem (1) needs to be solved by iterative methods, the nominal values of

control variables can be those calculated from the previous iteration. In the moving time horizon approach, the control variable at previous sampling time, u^s , is used as the nominal control variable, i.e. $\overline{u}^{s+i} = u^s$ (i = 1, 2, ...l). Then the first order approximation of system outputs, at the end of every subinterval in the predictive time horizon, becomes:

$$\hat{y}^{s+2} = \overline{y}^{s+2} + C^{s+1}\Gamma^{s+1}\Delta u^{s+1}$$
(2a)
$$\hat{y}^{s+3} = \overline{y}^{s+3} + C^{s+2}\Phi^{s+2}\Gamma^{s+1}\Delta u^{s+1} + C^{s+2}\Gamma^{s+2}\Delta u^{s+2}$$
(2b)

where

$$\Delta u^{s+i} = u^{s+i} - \overline{u}^{s+i}$$

$$y^{s+2} = y^{s+2} + O(||\Delta u^{s+1}||^2)$$
(2c)

 $y^{s+3} = \hat{y}^{s+3} + O(||\Delta u^{s+1}, \Delta u^{s+2}||^2)$ (2d)

Here the hat "" is used to indicate system outputs as the first order approximations linearized around the nominal trajectory. Φ^{s+i} and Γ^{s+i} are sensitivity functions. They are similar to, but more general than, those defined in Li et al (1989), since more sampling intervals are involved. Since the sensitivity functions are also based on nominal trajectories, a bar should also be put over these sensitivity functions. Here, however, the bar is suppressed for the sensitivity functions in order to simplify the following definitions.

$$\Phi^{s+i} = \Phi(t^{s+1+i}, t^{s+i}) = \frac{\partial \overline{\chi}^{s+i}}{\partial \overline{x}^{s+i}}$$
(3a)

$$\Gamma^{s+i} \equiv \Gamma(t^{s+1+i}, t^{s+i}) \equiv \frac{\partial \overline{\chi}^{s+i}}{\partial \overline{u}^{s+i}}$$
(3b)

$$C^{s+i} \equiv \frac{\partial \overline{y}^{s+1+i}}{\partial \overline{u}^{s+i}}$$
(3c)

Computation formulae for calculating Φ^{s+i} and Γ^{s+i} are presented below. These computation methods for sensitivity functions are similar to those discussed in Li et al (1989).

$$\frac{\partial \Phi(t, t^{p+i})}{\&} = \frac{\partial f(\zeta(t), \xi(t))_{i}}{\partial C(O} \Phi(t, t^{p+i})$$
(4a)

initial condition: $(r^{**1}, t^{*+i}) = I$

.1

a,

$$\Phi^{s+i} = \Phi(t^{s+i}+T; t^{s+i})$$

$$\underbrace{\operatorname{an}^{*}, \mathbf{O}}_{\partial t} = \frac{\partial f(\boldsymbol{\zeta}(t), \boldsymbol{\xi}(t))}{\partial \boldsymbol{\zeta}(t)}|_{(\bullet)} \Gamma(t, t^{\bullet+1}) + \frac{\partial f(\boldsymbol{\zeta}(t), \boldsymbol{\xi}(t))}{\partial \boldsymbol{\xi}(t)}|_{(\bullet)}$$
(4b)

initial condition: H^{1*1} , $i^{\text{res}} = 0$

.

$$\mathbf{I}^{**i} = \Gamma(\mathbf{I}^{**i} + T; \mathbf{I}^{**i})$$

where the following notation is defined as:

$$= \bigcup_{i=1}^{n} (t; \quad \overline{X}^{p+i}, \overline{u}^{p+i}), \xi(t) = \overline{u}^{p+i}$$

To simplify the notation, as well as make it more compact, the coefficients $B_{j^{n}}^{1}$ are defined as follows:

$$BI^{+1} = C^{\Lambda} T^{"*} \qquad * = i \qquad (5a)$$

$$B_{k}^{i+1} = C^{\sigma+i} (\prod_{j=k}^{i} \Phi^{\sigma+1+i-j}) \Gamma^{\sigma+k} \qquad * = 1, 2, ... 0-1) \qquad (5fc)$$

$$i = 1, 2, 3, ... /$$

Using this newly defined notation, Eq. (2) can be written as:

_____.

$$\hat{\mathbf{y}}^{*+1+i} = \overline{\mathbf{y}}^{*+1+i} + \sum_{\overline{feel}}^{i} B_{\underline{k}}^{i+1} \Delta u^{*+k}$$
f • 1, 2, ... /
* - 1. 2. ... i

An alternate, but equivalent, representation of linearized system outputs can also be generated without Φ^{s+i} , which can be expensive to compute if many states are present. Here we define the input change in

.

the s^{*} interval as: $5u^{8+i} - u^{8+i}$, the step change from interval (s+i-1)^{*} to (s+i) ^{*}.

The u^{8+i} can be found from the following recursive formula:

2

By substituting for $u^{*+i} \cdot u^{84} \cdot 1 + 8u^{8+i}$ and continuing the process, Eq. (7) becomes:

$$\boldsymbol{u}^{s+i} = \mathbf{u}^{*} + \underset{j=1}{\overset{i}{\pounds}} \mathbf{u}^{\wedge} \tag{8}$$

The derivation of $\bar{\mathbf{x}}^{**'}$ with respect to $\bar{\boldsymbol{u}}^{*+k}$ is now defined as follows:

$$\Gamma_{k}^{s+i} = \Gamma(t^{s+i}, t^{s+k}) = \frac{\partial \overline{\chi}^{s+i}}{\partial \overline{u}^{s-1+k}}$$
(9)

$$k = 1, 2... i$$

The sensitivity matrix rg⁺ⁱ is obtained from the solution of this set of linear time-variant ODE's is:

$$\frac{\partial \Gamma(t, t^{s+k})}{\partial t} = \frac{\partial f(\zeta, \xi)}{\partial \zeta}|_{(\bullet)} \Gamma(t, t^{s+k}) + \frac{\partial f(\zeta, \xi)}{\partial \xi}|_{(\bullet)}$$
(10)

with the initial condition: $r(i^{***}, *^{\bullet}+^{*}) \bullet 0$

$$\Gamma_k^{s+i} = \Gamma(t^{s+i}; t^{s+k})$$

where

Then the step response coefficients $D\dot{E}^1$ can be defined as:

$$D_{k}^{i+1} = C^{\bullet+i} \Gamma_{k}^{\bullet+i} \tag{11}$$

The first order approximation of system outputs in terms of step response coefficients can be

written as:

٠,

$$\mathbf{\hat{y}}^{5*1'} \mathbf{s} \quad \mathbf{\hat{y}}^{*+1+'} + \mathbf{\underline{V}}^{i} D^{*+l} \mathcal{E} u^{*+*}$$

$$\mathbf{i} = 1, 2, ... /$$

$$* = 1, 2, ... \mathbf{\hat{i}}$$

$$(12)$$

Note that equations (6) and (12) can be thought of as nonlinear analogs to the well-known impulse and step response models, respectively. The equivalence between these linear models can be found, for example, in Garcia and Prett (1986). Now, if the first order approximation of system outputs Eq. (6) is used, problem (1) can be represented as the following QP problem:

Here bounds on changes in system inputs are used, which is equivalent to having the ability to bound the derivative of u(t) with respect to t when sampling time is small. Note that in the above QP problem, the Hessian is positive semi-definite, which guarantees a global minimum value for problem (13).

The algorithm for the multistep nonlinear control problem within a moving time horizon is stated below. For this paper we will assume no model mismatch and simple parameter estimation, for example, (see, e.g. Morshedi, 1986) can be used to estimate unknown disturbances as well as model parameters.

Algorithm

1. Start with an initial condition x^{8*1} , u^* and process measurements, y^{8*1}

1

2. a) Set j * 0 (subscript j is used to indicate the j* iteration)

b) $u_0^{s+i} = U^s$, i = 1, 2, ..., 1c) Solve for χ_0^{s+i} , C_0^{s+i} , Φ_0^{s+i} , Γ_0^{s+i} , i=1, 2, ..., 13. a) Solve QP (13) to get Δu_i^{s+i} (i = 1, 2, ..., 1)

b) Choose a stepsize that gives a sufficient decrease of $\sum_{i=1}^{l} \|y^{s+1+i}-y^*\|^2$ based on the Armijo line search. (This involves a model solution over the time horizon for each set of trial controller moves.)

1

4.
$$\overline{u}_{j}^{s+i} = \overline{u}_{j-1}^{s+i} + \lambda \Delta u^{s+i}$$

If $\sum_{i=1}^{l} || \overline{u}_{j}^{s+i} - \overline{u}_{j-1}^{s+i} ||^2 \leq \varepsilon$

where ε is a small predetermined positive number, update $u^{s+1} = \overline{u}_j^{s+1}$, i=1,2,...I and go to step 5.

Else

a) Set
$$j = j+1$$
.
b) $\overline{u}_{j-1}^{s+i} = \overline{u}_{j}^{s+i}$, $i = 1, 2, ..., l$
c) Solve for χ_{j-1}^{s+1} , C_{j-1}^{s+i} , Φ_{j-1}^{s+i} , Γ_{j-1}^{s+i} , $i=1, 2, ..., l$
d) Go back to step 3.

5. Implement the controller move for the first time step, set s = s+1, and return to step 1.

It is worth noting that it is not really necessary to solve the QP problem in step 3 repeatedly, especially when the algorithm only predicts a few steps ahead. Here, when only a few predictive steps are involved, the sensitivity functions can reflect the system dynamics quite well. Therefore, it is possible to find an optimal solution for the control problem after solving the QP problem once. Of course, the line search is employed to control the step size and guarantee improvement toward the setpoint. The simulation results in section five support the above arguments.

In addition to moving time horizon applications, the above control algorithm can also be modified to generate optimal operating profiles, such as those required for batch processes. For example, when controlling a batch process, one may be only interested in the system output at the end of a batch. These problems can be written as follows:

Here we assume that the entire batch time is equally divided into /time intervals. If the notation in Eq. (6) is used, the system outputs at the end of batch time can be approximated by:

$$\hat{y}^{s+1+i} = \bar{y}^{s+1+i} + \sum_{k=1}^{i} B[^{*1} \Delta u^{s+k}$$

$$k = 1, 2, ... /$$
(15)

Now problem (14) becomes:

÷

. 4

This problem can then be solved by looping through steps 3 and 4 of the above control algorithm (and deleting step 5). Moreover, problem (16) can actually deal with more general objectives than the weighted norm objective function of problem (2). For instance, when the objective function includes an integral term such as:

9

$$\int_{t_0}^{t_f} F(\mathbf{y}(t), u(t)) dt$$
(17)

The above objective function can be converted to the weighted norm as in problem (2) by defining a new variable y_{p+1} and writing:

$$f'_{-^{\wedge}} \ll F(y(t), \ll 0)$$
 (18)
 $y_{p+1}(0) = 0$

This relation is then incorporated into problem (16). It is interesting to note that this optimization application is the same as proposed by Morshedi (1986) with the added advantage that a general purpose nonlinear programming solver is not required. Instead, the above algorithm takes advantage of the weighted norm structure of the objective function and converges rather quickly (in the manner of a Gauss-Newton method).

3. Extension to Time-Delay Systems

Because most chemical industrial processes have transport lags in pipes, long recycle loops, and analysis delay, time delays frequently need to be introduced into the overall control problem. These time delays can be a serious obstacle to good process operation and prevent high controller gains from being used, thus leading to offset and sluggish system response.

In designing linear multivariable control systems, one may choose one of the following two approaches for time delays:

1). Time delay compensation methods

Here a prediction device in the control loop is first used to compensate for the time delays. Then the standard multivariable controller design procedure is employed to complete the design. This approach is confined to unconstrained, linear systems, i.e, input-output transfer function matrices in the Laplace or frequency domain. These were developed by Smith (1957) for SISO systems, extended to multivariable systems by Ogunnaike and Ray (1979) and refined by and Jerome and Ray (1986).

2). Optimal control methods

The control objective is first formulated as an optimization problem. The optimum conditions need to be derived to find the optimal control variable trajectory. This approach always deals directly with

differential equations in the time domain, but often leads to equation systems and control laws that are very difficult to solve. Studies that employ this state space approach include Soliman and Ray (1971), Mee (1973) and Donoghue (1977).

In addition to these control schemes, Wong (1984) and Russell and Perkins (1987) defined a *generic* minimum necessary time delay for multivariable systems using only time delay information incorporated in a delay matrix, <u>D</u>. In particular, Russell and Perkins (1987) computed the generic minimum necessary delay, t_{ming} of delayed DAE systems by finding an output set for a matrix derived from <u>D</u>. From this property, it becomes relatively easy to determine the minimum necessary predictive horizon for a Newton-type controller.

. •

Time delay systems considered in this study are modeled by the following delay differential equations:

£ = /WO. *(i-a). «(0. *0-P)	i < h	(19a)
y(t) = g(x(t))	$t < t_0$	(19 <i>b</i>)
$\mathbf{x}(0 = \mathbf{K}\mathbf{t})$	$t \in [\mathbf{f}_0\text{-}\mathbf{a}, t \mathbf{\pounds}]$	
$u(t) * \mathbf{v}(0)$	<i>t</i> € [/ ₀ -P, /J	

For the special case of linear systems, the linear time-invariant differential equations are

$$A_1 x(t) + A_2 x(t-\alpha) + B_x u(t) + B_2 w(t-p)$$
 (20a)

$\begin{array}{c} t < 0 \\ yd \end{array} = cxd$	$t < t_0$	(20b)
$\mathbf{x}(0 = hjj)$	<i>i e</i> [/ ₀ -a, /J	
$u(t) = v_t(t)$	$t \in [t_0 - \beta, t_0]$	

Unlike the state and sensitivity equations derived in the previous section, these delay systems present a number of difficulties. First, the initial condition is no longer a point property, i.e. the system states in the future are not only dependent on the state variables at $t \cdot to$. but also on the initial state function in the time period, t e [to-a, t]. These conditions create some difficulties when defining the discrete system required by the Newton-type controller. Secondly, the sluggishness of system responses requires a longer predictive time horizon, since it takes time before the effects of delayed states and control variables are reflected in the system outputs. Finally, because delayed states and inputs increase the system dimensions, and the profile of these delayed states needs to be interpolated when computing the sensitivity functions and states, the computational burden of controlling time delay systems is much larger than for normal systems.

In this study we illustrate some difficulties of dealing with time delay systems for Newton-type controllers by considering a restricted class of time delays. In general, one can always develop step response models of the form of equation (16) by linearizing (19) about a nominal trajectory. However, in order to simplify our derivation, we consider systems where:

- The sampling time T equals β , the time delay in control variables.
- $\alpha < \beta$, i.e. the time delay in state variables is less than time delay in control variables.

We emphasize that the above assumptions do not restrict our proposed control algorithm. Instead, the purpose here is to establish a basic structure to design a constrained Newton-type controller for nonlinear time delay systems. The following derivation can be easily generalized to systems without the above assumptions. For instance, if the sampling time does not equal β , the delay system inputs may change their values within the time interval. The sensitivity function Γ_d^{ϵ} (see Eq. (22) for the definition) can be defined separately, corresponding to these delay system inputs. This case has also been derived in Li (1989). In addition, if $\alpha > T$, i.e., the time delay in states is larger than the sampling time, the delay states in current sampling interval, $x(t-\alpha)$ ($t \in [t^{\epsilon}, t^{\epsilon+1}]$), cannot affect the solution of the system at the end of this sampling time, χ^{ϵ} . However, it will affect the solution of the system at the end of some future sampling time, χ^{s+i} , depending on the length of α . Here, χ^{ϵ} is the solution of equation (19) at time $t^{\epsilon+1}$ for $u(t) = u^{\epsilon}(t^{\epsilon} < t < t^{\epsilon+1})$, $u(t-\beta) = u^{\epsilon-1}$ ($t^{\epsilon} < t < t^{\epsilon+1}$), and $x(t^{\epsilon}) = x^{\epsilon}$.

$$\chi^{s} \equiv \chi^{s+1} = \chi(t^{s}+T; \chi^{s}, \chi(t^{s}-\alpha), \mu^{s}, \mu(t^{s}-\beta))$$
 (21a)

In general, the following notation is defined:

$$\overline{\chi}^{s+i} \equiv \overline{\chi}^{s+i+1} = \chi(t^{s+i}+T; \overline{\chi}^{s+i}, \overline{\chi}(t^{s+i}-\alpha), \overline{\mu}^{s+i}, \overline{\mu}(t^{s+i}-\beta))$$
(21b)

where the bar is used to indicate that the solution is based on the nominal value. The derivative of $\overline{\chi}^{s+i}$ with respect to $u(t^{s+i}-\beta)$ for system (19) is defined as:

$$\Gamma_{d}^{s+i} \equiv \Gamma_{d}(t^{s+i+1}, t^{s+i}) \equiv \frac{\partial \overline{\chi}^{s}}{\partial \overline{u}(t^{s+i}-\beta)}$$
(22)

The sensitivity matrices Φ^s , Γ^s , and Γ^s_d are obtained from solutions of three sets of linear time-variant ODE's.

$$\frac{\partial \Phi(t, t^{s})}{\partial t} = \frac{\partial f(\bullet)}{\partial \zeta(t)}|_{(\bullet)} \Phi(t, t^{s}) + \frac{\partial f(\bullet)}{\partial \zeta(t-\alpha)}|_{(\bullet)} \Phi(t-\alpha, t^{s})$$
(23a)
with initial conditions: $\Phi(t, t^{s}) = 0$ $t < t^{s}$
 $\Phi(t^{s}, t^{s}) = I$
 $\Phi^{s} = \Phi(t^{s}+T; t^{s})$

$$\frac{\partial \Gamma(t, t^{p})}{\partial t} = \frac{\partial f(\bullet)}{\partial \zeta(t)}|_{(\bullet)} \Gamma(t, t^{p}) + \frac{\partial f(\bullet)}{\partial \zeta(t-\alpha)}|_{(\bullet)} \Gamma(t-\alpha, t^{p}) + \frac{\partial f(\bullet)}{\partial \zeta(t)}|_{(\bullet)}$$
(23b)

initial condition: r(/, f) = 0 $P \ll r(^+r; f)$

$$\frac{\partial \Gamma_d(t, t')}{5} = \frac{\partial f(\bullet)}{\partial \zeta(t)} \int_{(\bullet)} \Gamma_d(t, t') + \frac{\partial f(\bullet)}{\partial \zeta(t-\alpha)} \int_{(\bullet)} \Gamma_d(t-\alpha, t') + \frac{\partial f(\bullet)}{\partial \xi(t-\beta)} \int_{(\bullet)} (23c)$$

initial condition:

rrf(r, 0 * 0

$$rj = \Gamma_d(t^d+T; t^d)$$

Where the following notation is defined as:

Similarly the sensitivity formula corresponding to a linear system, (20), can be found in Li (1989). Note that in the above derivation, the initial state path function is not included in the argument of the system solution x. even though the solution is dependent on the initial state function. However, all sensitivity functions of both linear and nonlinear systems are independent on the initial state path functions. Therefore, in order to simplify the notation, we remove the initial state function from the argument without losing mathematical rigor.

Halanay (1966) derived the sensitivity equations for the linear system (20) fbr continuous system inputs. We can easily extend his results to discrete system input models by using sensitivity functions. The basic idea is that solution of both the linear system (20) and nonlinear system (19) at t^{+1} can be partitioned into two parts. The first part is the solution, assuming the initial path function is zero. This is allowable, since sensitivity equations fbr both linear and nonlinear systems are independent of the initial path function. The second part is the solution, assuming that the initial path function is nonzero, and the x^{s} and u^{*} are both zero. The first order approximations of system outputs linearized around the states and system inputs at the previous subinterval are:

 $t \leq t^3$

150

$$\mathbf{\hat{y}}^{*+2} = C^{*+1} \Phi^{*+1} \mathbf{x}^{*+1} + (T^{*1} \wedge 1 + a^{*1}!)^{*1} + C^{**1} \mathbf{x}^{*+1} + C^{**1} \mathbf{x}^{*+1}$$
(24a)

$$\hat{y}^{s+3} = C^{s+2} \Phi^{s+2} x^{s+2} + C^{s+2} \Gamma^{s+2} u^{s+2} - C^{s+2} \Gamma^{s+2} u^{s+1} + C^{s+2} W^{s+2}$$
(24b)

where the following notation is defined:

$$W^{a+i} = \int_{p^{a+i}-\alpha}^{p^{a+i}} \Phi(t^{a+1+i}, \tau+\alpha) \frac{\partial f(\bullet)}{\partial \zeta_{a}(t-\alpha)} |_{(\bullet)^{a+i}} x(\tau) d\tau$$
(24c)

$$W^{\mathfrak{s}+2} = \int_{t^{\mathfrak{s}+2}-\alpha}^{t^{\mathfrak{s}+2}} \Phi(t^{\mathfrak{s}+3}, \tau+\alpha) \frac{\partial f(\bullet)}{\partial \zeta(t-\alpha)} I_{(\bullet)^{\mathfrak{s}+2}} x(\tau) d\tau \qquad (24d)$$

$$\partial f(\bullet) = \partial f[\zeta(t), \zeta(t-\alpha), \xi(t), \xi(t-\beta)]$$

 $|_{(\bullet)^{k+1+i}} = |_{\zeta = \chi[t; x^{k+i}, x(t^{k+i}-t), u^{k+i}, u(t^{k+i}-\beta)], \zeta(t-t \wedge (t-t; x^{k+i}, x(t^{k+i}-t), u^{k+i}, u(t^{k+i}-\beta)), \zeta(t) = u^{k+i}, \xi(t-\beta) = u^{k-1+i}}$

The first order approximation of system outputs linearized around fixed states and system inputs at the previous subinterval is not very useful to develop our control algorithm. Our primary interest is the first order approximation of system outputs linearized around the nominal trajectory, i.e. the system outputs are represented by changes of system inputs from the nominal trajectory. The first part of solution represented by the sensitivity functions in Eqs. (24) can be easily converted to the representation linearized around the nominal trajectory. When converting the second part of the solution, the derivative of the integral term with respect to nominal system inputs needs to be computed. For nonlinear systems, the sensitivity functions, which are the integrand in the integral term, are dependent on the states and system inputs. However, we are only interested in the first order approximation. The derivatives of sensitivity functions with respect to the nominal system inputs can thus be truncated because they are second order with respect to changes of system inputs from the nominal trajectory, and the following representation is obtained:

 $\hat{y}^{p+2} = \bar{y}^{n+2} + C^{p+1}\Gamma^{p+1}\Delta u^{p+1}$ (25a) $\hat{y}^{p+3} = \bar{y}^{p+3} + C^{p+2}\Gamma^{p+2}\Delta u^{p+2} + C^{p+2}\Phi^{p+2}\Gamma^{p+1}\Delta u^{p+1} + C^{p+2}\Gamma^{p+2}\Delta u^{p+1} + C^{p+2}\Gamma^{p+2}\Delta u^{p+1}$ (256) where the following notation is defined by:

$$\overline{\Omega}_{1}^{s+2} = \frac{\partial \overline{W}^{s+2}}{\partial W} = \frac{\partial}{\partial u^{s+2}} \int_{t^{s+2}-\alpha}^{t^{s+2}} \Phi(t^{s+3}, \tau+\alpha) \frac{\partial f(\bullet)}{\partial \zeta(t-\alpha)} |_{(\bullet)^{s+2}} \overline{x}(\tau) d\tau$$

$$= \int_{t^{s+2}-\alpha}^{t^{s+2}} \Phi(t^{s+3}, \tau+\alpha) \frac{\partial f(\bullet)}{\partial \zeta(t-\alpha)} |_{(\bullet)^{s+2}} T(T, f^{-1}(\tau)) d\tau$$

$$= \int_{t^{s+2}-\alpha}^{t^{s+2}-\alpha} \Phi(t^{s+3}, \tau+\alpha) \frac{\partial f(\bullet)}{\partial \zeta(t-\alpha)} |_{(\bullet)^{s+2}} T(T, f^{-1}(\tau)) d\tau$$

$$(25c)$$

To simplify notation, as well as make it more compact, the coefficients $M \hat{\mathfrak{L}}^1$ are defined as follows:

$$M_{k}^{i+1} = C^{r+i} \Gamma^{r+i} \qquad k = r \qquad (26a)$$

$$M_k^{i+1} = C^{a+i} \Phi^{s+i} \Gamma^{a+k} + C^{s+i} \Gamma_d^{a+k} + C^{s+i} \overline{\Omega}_k^{s+k}$$

$$k = \mathbf{i} - \mathbf{l} \tag{26b}$$

$$M_{k}^{i+1} = C^{s+i} (\prod_{j=k}^{i} \Phi^{s+1+i-j}) \Gamma^{s+k} + C^{s+i} (\prod_{j=k+1}^{i} \Phi^{s+1+i-j}) \Gamma_{d}^{s+k} + C^{s+i} \wedge i \qquad * = 1.2...0-2)$$
(26c)

where

$$\overline{\Omega}_{k}^{s+i} = \frac{\partial \overline{W}^{s+i}}{35^{s+*}}$$

Now Eq. (25) can be rewritten using our newly defined compact coefficients:

$$\hat{y}^{s+1+i} = \bar{y}^{s+1+i} + \sum_{k=1}^{i} M_{k}^{i+1} \Delta u^{s+k}$$
(27)
 $i \ll 1, 2, ... /$
 $* \ll 1, 2, ... i$

After the approximation of system outputs is represented, the algorithm of section two can be used with Equation (27) substituted for Equation (6). Note also that Eq. (27) is a *general* form that represents the first order approximation of system outputs in the predictive time horizon linearized around the nominal trajectory, and is independent on the assumption of a < p and p \ll r.Of course, without

these assumptions, M_k^{i+1} has to be defined differently.

4. Stability Analysis

In a previous paper, Li et al (1989) considered the stability of closed-loop nonlinear systems for a *single step* Newton-type control algorithm. Here the descent property is guaranteed when the open-loop system is *asymptotically stable in the large* and the sampling time is chosen to be sufficiently long. The basis for this state-space analysis comes from properties of nonlinear operators. Economou (1985) applied a contraction mapping theorem to a family of single step Newton-type control laws; for a system within a region of attraction, he showed that the control law is stable and converges to the setpoint. However, the attraction region is difficult to determine *a priori* for nonlinear systems and a global stabilizing procedure is needed. Li et al (1989) therefore considered a global convergence procedure by enforcing a line search which guarantees improvement toward the setpoint. A sufficient condition for this procedure is that the controller moves (in this case, the QP solution) provide a descent direction for the objective function.

Unconstrained Properties

Li et al (1989) showed that this descent property holds for the unconstrained, single step Newtontype controller if a sufficiently long sampling time is chosen. In this study we extend these results to the multistep algorithm for both unconstrained and constrained nonlinear systems. First, we consider the unconstrained case and develop the following theorem.

Theorem 1

If an open-loop unconstrained nonlinear system is asymptotically stable in the large, then a descent direction of the system outputs in the predictive time horizon of the closed-loop system is guaranteed for $\|y^{s+1}-y^{*}\| \ge \delta$, where $\delta > 0$, with a sampling time T large enough but finite and full rank coefficients B_{k}^{i+1} . (Note this last assumption is always satisfied for systems with unique steady states if the sampling time is sufficiently large.) Thus, we have:

$$\|y^{s+i} - y^{*}\| - \|y^{s+1} - y^{*}\| \le -\frac{\delta\lambda}{2}$$
(28)
$$i = 1, 2, ... l$$

The proof for this theorem is presented in Appendix A. It is worth mentioning that when a moving time horizon strategy is used, only the first step is implemented. Therefore, only the descent property for the first step, i = 2, is really useful. Although the proof is somewhat restrictive, it can be extended to all time

delay systems if $T > x_{mUig\%}$ the minimum necessary time delay defined by Russell and Perkins (1987). Here only the representation of Ec (27) needs to be substituted for Eq (6). Also, it can be seen from the proof that the theorem can be specialized to single time delay systems to yield the same result with a shorter sampling time.

Theorem 1 guarantees that the deviation between the setpoint and system outputs at the end of every subinterval in the predictive time horizon decreases up to IIKO-/II * 8 for systems without and with time delay. If we assume for $II/*^1-?*!! \pounds$ & that S is chosen so that it is within an attraction region for a Newton-type method and if the setpoint is the only unique equilibrium point in that region, the system output will converge to the setpoint monotonically (see Li et al, 1989).

Theorem 1 shows that the descent direction can be guaranteed as long as T is large enough and X is small enough. When the OP problem is solved repeatedly i.e., the controller is converged to optimality, then $||/*^2 - /11^2$ is optimized directly. Thus this descent property holds without depending on the relaxation factor X. Theorem 2 shows the descent property for this optimal, unconstrained case.

Theorem 2

If an open-loop unconstrained nonlinear system is *asymptotically stable in the large* and if the QP problem is solved repeatedly, then the descent direction of the system outputs in the predictive time horizon of the closed-loop system is guaranteed for $11/*^{1}/11 \ 2 \ 5$, where 5 > 0 and the coefficients always have full rank. Thus, we have:

 $||/+^2 - y|| * ||y||^1 - y||$

The proof of this theorem is also presented in Appendix A.

Theorem 2 shows that if the QP problem is solved repeatedly, the norm of the difference between the system output and the setpoint can be monotonically reduced up to $II/*^{1}-/!!$ 2 S.

Constrained Properties

The descent property analysis shown above can be extended to systems with constraints on both system outputs and control variables. This analysis becomes more difficult and only very restrictive cases can be shown. Nevertheless, the following theorems give useful sufficient conditions for stability properties of constrained, multistep controllers.

Before considering the multistep case, we first consider stability properties of the constrained, single step Newton-type controller. This controller was first considered by Li and Biegler (1988) and is a special case of the multistep algorithm that follows from setting /, the number of predictive steps in the time horizon, to one.

Theorem 3

If an open-loop nonlinear system is *asymptotically stable in the large* and if the QP generated controller moves never allow a zero solution, then the *constrained*, closed-loop system with a *single step constrained Newton-type controller* converges monotonically for $IIy^{"1}-/!!$ * &> where 8 > 0, with a sampling time T > T\ where T* is some finite critical sampling time. Thus, we have:

$$\|y^{s+2} - y^{*}\|^{2} - \|y^{s+1} - y^{*}\|^{2} \le -\frac{\delta\lambda}{2}$$

The proof can be found in Appendix B. Theorem 3 shows that transforming Newton-type control law to an optimization (QP) problem with control variable constraints does not destroy the closed-loop system stability if the open-loop system is *asymptotically stable in the large,* the sampling time is large enough, and the relaxation factor *X* is small enough.

The dependence on X can be eliminated by considering an iterative QP algorithm where the single step controller move is determined *optimally* from the nonlinear model for each time step. In this case, we state Theorem 4 as follows:

Theorem 4

If an open-loop nonlinear system is *asymptotically stable in the large*, and if the NLP-generated controller moves never allow a solution of zero, then the *constrained*, closed-loop system with a single step constrained Newton-type controller, where each controller move is determined optimally at each step, converges monotonically for IIy^{**1} -/!! * 5 > 0, with a sampling time T > T\ where T[#] is some finite critical sampling time. Thus, we have:

$$||y^{s+2} - y||^2 - ||T^l - y||^2 * -$$

The proof for this theorem is similar to Theorem 3 and can also be found in Appendix B. The extension of these properties to the muttistep case builds on both single step theorems. Also, the following theorem can only be proved if we delete bounds on *changes* in system inputs and thus represents a restriction on the stability property.

Theorem 5

If an open-loop nonlinear system is asymptotically stable in the large with constraints:

$$y \le /*^w \le y$$
 (29a)
 $u! \ \ u''^l \le u^u$ (29b)
 $i = 1, 2, ... /$

and if controller moves generated by a QP or an NLP never allow a zero solution, then by applying the multistep algorithm of section 2, either once per horizon or iteratively to optimality for each horizon, the descent property of the closed-loop system is guaranteed for $||/+^{1}-/11 \pm 8>0$, with a sampling time T large enough but finite. Thus, we have:

$$|b^{*+2} - y || < |t/^{*1} - y ||$$
 (30)

The proof of this theorem can be found in Appendix C. Theorem 5, however, only considers a very restrictive case, i.e. when the sampling time is large enough, all appropriate control correction to minimize $IW0-/II^{canbe}$ achieved in the first sampling interval. Although, it gives a sufficient stability condition, the sampling time may be much too large to use in practice.

However, the descent property, $||/^{*2}-/|| < ||f+'-y|$ for unconstrained systems without time delays, or a similar property, $||y^{nu'}-y^*|| < Wf^{n-y}W$ for systems with constraints or time delays, can easily be checked on-line. Here if the descent direction cannot be found, the sampling time can be increased until the descent condition is satisfied. For example, an easy way to double the sampling this is to hold over the current input for the next sampling time, and to execute the multistep controller over a longer time horizon.

5. Test Problems

In this section the proposed control algorithm is tested by solving two examples. Both examples were taken from Ray (1981). The first one is a start-up problem for a nonlinear continuous stirred tank reactor (CSTR). The second example is the open-loop control of a CSTR with time delay in both states and system inputs. In addition, the first problem is also considered by Renfro (1986).

Here our simulation results are compared with those solutions to demonstrate the effectiveness of our proposed algorithm. It needs to be emphasized that the first example is not a moving time horizon problem. The purpose of solving this problem is twofold. First, we demonstrate that if the QP problem is solved repeatedly, the optimal solution can be obtained with this multistep algorithm in the same way as with a parameterized optimal control algorithm. Secondly, we modify this problem so that it can be treated by the moving horizon approach. In this case, we demonstrate the performance of the multistep method

as a moving time horizon controller.

In the second example, the sampling time is assumed to equal the time delay in system inputs. Here, a moving time horizon approach is used, and we need to predict at least two steps ahead in order to observe the delay system inputs affecting the system outputs. Therefore, the predictive time horizon consists of two steps in our simulation. Since the number of predictive steps is quite small, the first order approximation of system outputs represents the system dynamics reasonably well and the QP problem is only solved once to find the system inputs.

۰.

Example 1: CSTR Optimal Open Loop Control

With this example problem we find the optimal start-up control scheme for a nonlinear CSTR in which the exothermic, first-order reaction

A -→ B

occurs. The control objective is to minimize the deviation between system outputs and setpoints, and between the system input and its steady state value in the start up time period (pp. 103-104, Ray 1981; pp. 82-86. Renfro, 1986). The following optimization problem is formed to represent the control objective:

S.u
$$\overline{dt}^{T} = 0.1(1.0 - x_{x}) - k(x_{2})x_{l}$$

 $\frac{dx_{2}}{dt} \ll 0.1(3.0 - \%) + kfy \$ x_{x} - 0.195u(xj - 2.90)$
 $\frac{dx_{3}}{2} \approx 106o_{s} - 0.408)^{2} + 2.0(x_{s} - 3.298)^{2} + (\ll -0.370)^{2}$
 dt
 $x_{s}(0) \ll 1.0$
 $x_{2}(0) \approx 3.0$
 $x_{3}(0) \approx 0.0$
 $k(x_{2}) = 300.exp(-252)/x_{2}$
 $0 = f u(t) = 15$
(31)

where

. •

 x_1 — dimensionless concentration of A.

 x_2 — dimensionless temperature in the reactor.

 x_3 — dimensionless variable represented the original objective function.

u — overall heat transfer coefficient.

Here the third state is added in order to reflect the original objective function presented by Ray (1981):

$$Min \int_{0}^{20} 10^{3} \left\{ 10^{3} (x_{1} - 0.408)^{2} + 2.0 (x_{2} - 3.298)^{2} + (u - 0.370)^{2} \right\} dt$$
(32)

Also, the objective function is rescaled to avoid the numerical difficulties.

Optimal Control Formulation

For this case, the objective function requires the profile of system inputs to be optimized in the entire time region. The control algorithm needs to predict a number of steps ahead. Since a first order approximation linearized around a nominal trajectory is used to present the system outputs, the approximation errors are increased with the number of predictive steps. Thus, in order to get an optimal solution, the QP problem needs to be solved repeatedly. To speed up the convergence, a single step algorithm over the entire batch time is used to initialize a nominal trajectory, i.e. the system inputs are assumed to be the same in the entire region. For the optimal control formulation, the entire time horizon was divided into ten subintervals. Here the sampling time of the first and last subinterval was 6 units while the sampling time of the remaining subintervals was 1 unit. This subinterval pattern matches the one chosen by Renfro (1986). For Figures (2) to (4), Curve 1 shows the simulation results using Renfro's approach; Curve 2 shows the single step initialization; and Curve 3 shows the multistep algorithm solution. Here Figure (2) shows the objective function values versus time while Figure (3) plots the reactant concentration versus time. Figure (4) is the control profile in the time horizon. The objective functional value calculated by our multistep algorithm is 1.01×10^6 , which is within 1.3 % of the solution obtained by Renfro (1986). The objective functional value obtained by a single step method is 1.12×10^6 . Thus, while it was not solved to a tight tolerance, the multistep Newton-type algorithm yields a guite reasonable solution and requires only 3 QP iterations and 50.1 CPU seconds on a MicroVax II workstation.

Moving Horizon Formulation

For the equations given above we also applied a moving time horizon controller, as given by the multistep algorithm in section 2. Here the sampling time is taken as one minute and a three step horizon is chosen. The objective function, x_3 , is shown in Figure (5) for this approach; controller moves (for the first step in the time horizon are given in Figure (6). For both figures, Curve 2 represents the solution with

21

our moving horizon approach while Curve 1 represents Renfro's optimal solution. Note that the curves for x_3 are almost indistinguishable. The objective function value for this problem at final time was 1.00×10^6 , or slightly better than the above approach with the preassigned subinterval pattern. Note also from Figures (4) and (6) that the optimal controller moves are not unique and differ from those reported by Renfro. Finally, the moving horizon approach required the solution of 20 QP's and approximately three CPU minutes on a MicroVax II workstation.

Example 2: CSTR with State and Input Time Delays

To demonstrate the proposed control algorithm for time delay systems, an example of the openloop control of a continuous stirred tank reactor (CSTR) shown in Figure (7) (pp. 231-235, Ray, 1981) is modified and treated here. Based on the material and energy balances, the following describing equations can be formulated:

$$V|\pounds_{f} \ll 14 \ (c_{f} - c) - K_{0}VexfK \wedge)\overline{c}c \qquad c(0) \ll c_{0}$$

$$V_{-p}^{d\overline{c}} \approx 0-Y) \approx 4 \ C-P^{1}) \cdot T\text{-ufcO} - \overline{c}u_{3}^{f} \qquad \overline{c}(0) \ll \overline{c}_{0} \qquad (33)$$

$$\rho C_{p}|\pounds_{di} = \rho C_{p}u \setminus (7) - 7) \cdot (iJf)K_{0}Vexp\{ \pm T)\overline{c}c \qquad (hA \cdot kJCOPV-cO - T_{s}))(T - T_{c}) \qquad T(0) = T_{0}$$

The following assumptions are made:

1. The chemical reaction A_1 -» A_2 is first order in both the catalyst \overline{c} and reactant c.

2. The catalyst feed u^is made up of two parts (see Figure (7)): a fraction *y* entering the reactor directly, and (1-f) mixed with the feed a time P' upstream of the reactor.

3. The temperature is controlled by a feedback controller which uses continuous temperature measurements at time t'-a' to adjust the coolant flow rate, where u; is a time-variable proportional gain.

4. The molar feed rate of catalyst u'_2 is negligible compared with reactant feed rate $u' \sim so$ that the physical properties are unaffected by catalyst addition.

5. a and £, time delay parameters, are constant and independent of the states and system inputs.

To simplify the notation and calculation, the following dimensionless variables are defined:

$$\begin{aligned} x_1 &= \frac{c - c_s}{c_s} & x_2 = \frac{\overline{c} - \overline{c}_s}{\overline{c}_s} & x_3 = \frac{T - T_s}{T_s} & \theta_h = \frac{V}{F_s} \\ t &= \frac{t'}{\theta_h} & u_1 = \frac{u'_1 T_s}{\overline{F}_s} & u_2 = \frac{u'_2}{\overline{c}_s F_s} & u_3 = \frac{u'_3}{\overline{F}_s} \\ \Theta &= \frac{E}{RT_s} & \beta = \frac{\beta'}{\theta_h} & \alpha = \frac{\alpha'}{\theta_h} & Q = \frac{hA}{\rho C_p F_s} \\ P &= K_0 \theta_h e^{-\Theta} \ \overline{c}_s & J = \frac{(-\Delta H)\overline{c}_s}{\rho C_0 T_s} & x_{3c} = \frac{T_c - T_s}{T_s} \end{aligned}$$

Using the above newly defined dimensionless variables, Eq.(33) becomes:

$$\frac{dx_1}{dt} = -u_3 x_1 - P[(1.0+x_1)(1.0+x_2) \otimes P(\frac{\Theta x_3}{1.0+x_3}) - u_3]$$

$$\frac{dx_2}{dt} = (1.0-\gamma) u_2(t-P) + 1^{(0)} - U \otimes 2 + 1.0) \qquad (34)$$

$$\frac{dx}{dt} = u_3 x_3 + JP[(1.0+x_1)(1.0+x_2) \otimes P(\frac{\Theta x_3}{1.0+x_3}) - u_3]$$

$$- Q[x_3(t) - x_{3c}(1.0-u_3)] - u_1 x_3(t-\alpha)[x_3(t) - x_{3c}]$$

$$u_1 \leq u \leq u'$$

Table (1) shows the values of parameters, bounds, and the initial conditions.

In Ray's original problem, the control objective is to minimize the summation of states as well as the differences between the system inputs and their steady state values in the entire time horizon. Instead, we modify the control objective auch that the system outputs are forced to the setpoint as closely as possible at the end of every subinterval within the predictive time horizon. To simplify the control algorithm, we choose the sampling time, T, to equal p, the time delay of catalyst feed rate, i.e., T - 0.20.. Then the control algorithm needs to predict at least two steps ahead in order to observe the influence of delay system input on the system outputs. Values of delayed states and sensitivity functions are saved at equally-spaced points with the subintervals. Lagrange polynomials are used to interpolate delayed states and sensitivity functions.

e - 25.	Q«r«i.	J «li5	X£4.125		
0 - 0.02	• - 04	•i»-foo	•*1« 500.		
o - 0.015	3-1	∙ _s -wi	• ₂ « «, « 2 .		
Y - 0.1	« _t (0).M9	x_<0)«tJM02	i^0)«.«.©2		
j⊑(t) « 4X2 . O<1 < 0 «j (t) « 1. •p<1 < 0 •JO « 1p <t 0<="" td="" «=""></t>					

Table 1: Values of Parameters, Bounds, and Initial Conditions for Example 2

Figures (8) through (10) show dimensionless reactant concentration, dimensionless catalyst concentration, and dimensionless temperature in the reactor versus time, respectively. We observe that all system outputs approach the setpoints, even though x_2 and x_3 exhibit some oscillation.

Ray (1981) solved this problem as an optimal control problem by a conjugate gradient technique, which involves solving a set of partial differential equations with two point boundary values. Although Ray (1981) considers a slightly different objective function, and solves an optimal control problem over the entire time domain, we present his results for contrast.

With Ray's solution, x, takes less time to reach the setpoint. (about 02 time units by using our control algorithm versus about 0.1 time units by using Ray's approach). Also, while ^ oscillates with our approach, before it settles to the setpoint in Figure (9) at about 0.6 time units, x_2 remains at the setpoint virtually all the time with the optimal control solution. Finally, It takes a similar amount of time for x_3 to reach the setpoint for both methods, which is about 02 time units. However, the maximum offset of x_3 by using our algorithm, 0.10, is smaller than the one by using Ray's approach, 0.12.

As expected, optimal control performance is better than that of our suboptimal, moving horizon

algorithm. Here the optimal control minimizes the setpoint deviations in the entire time region $(0 \le t \le 0.4)$ while with our approach the *linearized* system error is minimized in the predictive time horizon, which only consists of a small part of that region. However, this example clearly demonstrates that the multistep, Newton-type control algorithm can effectively drive the system outputs to the setpoint with quite short predictive horizons, as proven by the above simulation results.

Figures (11) through (13) show dimensionless coolant flow rate, dimensionless molar feed rate, and dimensionless reactant feed rate versus time, respectively. From these figures, we observed that the system inputs have zigzag shapes. A possible explanation for this is that since our predictive time horizon is very short (two steps ahead) the system dynamics cannot be fully predicted and the control algorithm tends to overcorrect the system errors.

Finally, because of the computational burden of calculating and interpolating the sensitivity equations for time delays, it takes about one CPU hour on a Microvax II to simulate this moving horizon problem.

6. Conclusions

÷

. •

This study develops a multistep, moving horizon, Newton-type control algorithm for constrained nonlinear processes. The algorithm first evaluates the first order approximation of system outputs (around some nominal trajectory) at the end of every subinterval in the predictive time horizon by using sensitivity functions. Then a QP problem is constructed which can be solved in a similar manner as the single-step algorithm (see Li and Biegler, 1988). Here discrete linearized models can be constructed that are similar to the well-known impulse response and step response models for linear systems. Moreover, bounds on inputs, controller moves and outputs can easily be added to the problem as constraints in the QP formulation.

However, special precautions must be taken in order to extend this approach to systems having time delay. This limitation is due to the fact that when systems have time delay in control variables, the prediction time horizon needs to be increased in order to observe how these delayed control variables affect the system outputs. In addition, when systems have time delay in states, future system states are not only dependent on the state variables at the point $t = t_0$, but also on the initial state path function in the time period, $t \in [t_0-\alpha, t]$ (where α is the time delay in the state). Therefore, the discrete forms of system outputs are more difficult and time-consuming to derive. Here the solution of the system states and sensitivities was partitioned into two parts. First, we find the solution, assuming the initial path function is zero. It is possible to do this since all sensitivity functions for both linear and nonlinear systems are independent of the initial path functions. Second, we find the solution assuming that the initial path function is possible due to the linearity of the sensitivity equations.

Once developed, properties of the multistep algorithm were analyzed in the context of nonlinear

operator theory. Here we assume a region of attraction around the setpoint for which a Newton contraction mapping can be shown. Next we add a line search step to guarantee improvement toward the setpoint from outside of this region. A sufficient condition for this is a descent property for the controller moves and can be found under the following conditions.

If the system is *asymptotically stable in the large* and all gradients with respect to the nominal control variables and states are continuous and bounded, the descent properties of the multistep algorithm were shown for sufficiently long sampling times for the following control problem classes:

- 1. Unconstrained nonlinear systems with or without time delay using linearized response models to determine controller moves.
- Unconstrained nonlinear systems with or without time delay where controller moves are determined by iteratively solving QP problems.
- 3. Input and output bounded nonlinear systems with or without time delay using linearized response models to determine controller moves (single QP per step).
- 4. Input and output bounded nonlinear systems with or without time delay where controller moves are determined by iteratively solving QP problems.

Finally, two example problems are considered with our proposed control algorithm. The first is a start up problem and demonstrates the use of our multistep controller in order to determine optimal operating profiles over a fixed time horizon. For comparison this problem is also solved using a moving time horizon formulation. Results show excellent agreement with these approaches and a parameterized optimal control solution. The second problem, a CSTR model with time delays in both state and control variables, demonstrates the use of this multistep algorithm with time delays. Again, the results of our multistep, moving horizon controller, although suboptimal, compare well with an optimal control solution reported in the literature. Thus, the simulation results demonstrate the effectiveness of the proposed control algorithm.

Appendix A

Proof of Theorem 1

The following assumptions are made to prove the theorem:

- 1. The system is asymptotically stable In the large for all feasible control variables
- 2. All gradients with respect to $P+^*$ and \overline{u}^{*+} are bounded and continuous.
- 3. The coefficients B¹ are of full rank.

The first order approximation of system outputs linearized around the nominal trajectory at the end of every subinterval is :

$$\mathbf{\tilde{y}} \gg M \quad m \quad \overline{\mathbf{y}}^{\mathbf{s}+1+i} + \sum_{k=1}^{i} B_{k}^{i+1} \Delta \boldsymbol{u}^{\mathbf{s}+k} \tag{A.1.1}$$

The difference between the real solution and the first order approximation of system outputs is second order with respect to changes of system inputs:

$$y^{s+1+i} = \hat{y}^{s+1+i} + O(||\Delta u^{s+1}, \Delta u^{s+2}, \dots, \Delta u^{s+i}||^2)$$
(A.1.2)
$$i = i, 2, 3, \dots, i$$

For a system which is *asymptotically stable in the large,* the sensitivity functions ($$£^{**}$)? approach 2ero when sampling time approaches infinity.

The multistep unconstrained OP problem is:

 $u^{*+k} - u^{*+k}$

÷

$$Min \sum_{k=1}^{l} ||^{\lambda_{k}^{1+i}} - \sum_{k=1}^{l} ||^{2}$$

S.t $\$ > u^{ui} \ll \ge * *^{1+i} + \sum_{k=1}^{l} B_{k}^{i+1} \Delta u^{p+k}$ (A.1.3)

At the optimal solution, the following condition is satisfied:

$$\sum_{i=1}^{l} 2(\hat{y}^{p+1+i} - y^{i})^{T} (\frac{\partial \hat{y}^{p+1+i}}{\partial \Delta u}) = 0$$
 (A.1.4)

i « 1, 2, ... /

To satisfy the above condition, we have for full rank $B\dot{E}^1$:

This means:

$$B_{i}^{i+1}\Delta u^{s+i} = -(\overline{y}^{s+1+i} - y^{*} + \underbrace{Y}_{i=1}^{i-1} B^{A} li^{*})$$
(A.1.6)

Assuming large enough sampling times for nonsingular coefficients, the Au^{*+i} can be generated recursively. When the relaxation factor is added, the Au^{*VI} is defined by:

$$B_{k}^{i+1}\Delta u^{s+i} = -\lambda (\bar{y}^{s+1+i} - y^{*} + \sum_{k=1}^{k} B_{k}^{i+1}\Delta u^{s+k})$$
(A.1.7)

The nominal system outputs $\mathbf{\tilde{y}}^{*+Ui}$ can be related to the initial system output \mathbf{y}^{**1} by the following equation:

$$\overline{y}^{s+1+i}x^{y+1} + C^{s+i}\Phi(t^{s+i}, t^{s})(\overline{x}^{s+i}x^{s+1}) + \frac{1}{2!}(\overline{x}^{s+i}x^{s+1})^{T}\Phi_{x}(t^{s+i}, t^{s})(\overline{x}^{s+i}x^{s+1})$$

+ $O(|\overline{x}^{s+i}-\overline{x}^{s+1}||^3)$ (A.1.8)

$$\mathbf{y}^{\mathbf{x}+\mathbf{i}+\mathbf{i}} = \mathbf{y}^{\mathbf{x}+\mathbf{i}+\mathbf{k}} + \mathbf{y}^{\mathbf{B}} \mathbf{A} \mathbf{K}^{\mathbf{v}+\mathbf{x}} \cdot \mathbf{O}(\mathbf{A} \mathbf{w}^{2} \mathbf{r})$$
(A.1.9)

For the first step, we have:

$$B_{1}^{2} \Delta u^{s+1} = -\lambda (\overline{y}^{s+2} - y^{*})$$
 (A.1.10)

$$y^{s+2} = \overline{y}^{s+2} + B_1^2 \Delta u^{s+1} + O(\Delta u^{s+1})^2 \qquad (A.1.11)$$

Plugging Eq. (A.1.10) into Eq. (A.1.11) and subtracting y^e from both sides, we obtain:

$$y^{s+2}-y^{*} = \overline{y}^{s+2} - y^{*} - \lambda(\overline{y}^{s+2}-y^{*}) + O(\lambda^{2})$$
$$= (1-\lambda)[(y^{s+1}-y^{*}) + (\overline{y}^{s+2}-y^{s+1})] + O(\lambda^{2}) \qquad (A.1.12)$$

Taking the norm of both sides of Eq. (A.1.12) and rearranging, we have:

$$||y^{s+2}-y^{*}|| - ||y^{s+1}-y^{*}||$$

$$\leq -\lambda ||y^{s+1}-y^{*}|| + (1-\lambda) |\overline{|y^{s+2}-y^{s+1}||} + O(||\lambda^{2}||) \qquad (A.1.13)$$

We know:

$$\overline{y}^{s+2} - y^{s+1} = C^s \Phi^s (x^{s+1} - x^s) + \frac{1}{2!} (x^{s+1} - x^s)^T \Phi^s_x (x^{s+1} - x^s) + O(||x^{s+1} - x^s||^3)$$
(A.1.14)

For an asymptotically stable in the large system, it can be proven:

$$\lim_{T \to \infty} (\Phi_x)^p = 0 \tag{A.1.15a}$$

$$\lim_{T \to \infty} \overline{y^{s+2}} = y^{s+1} \tag{A.1.15b}$$

١

Therefore, when T and X are chosen such that $(i - \lambda) | [j^{2} + 2 - y^{2} + || + O|| \lambda^{2} ||) < 8X/2$. where 8 is a positive small number, the descent direction is guaranteed.

$$\|y^{s+2}-y^{*}\| - \|y^{s+1}-y^{*}\| \le -\lambda \|y^{s+} \vee \| = O(\|\Phi^{s}\|) + O(\|\lambda^{2}\|)$$

$$\le \frac{JK}{2}$$
(A.1.16)

* in *e whole predictive time horfcon and the sampling time is large enough, we have:

$$\|y^{s+1+i}-y^*\| - \|y^{s+1}-y^*\| \le -\lambda \|y^{s+1}-y^*\| + \|\overline{y}^{s+1+i}-y^*\| + O(\|\lambda^2\|)$$
(A.1.17)

and since

$$\lim_{T \to \infty} \overline{y}^{s+1+i} = \lim_{T \to \infty} \overline{y}^{s+2} = y^{s+1}$$
(A.1.18)

Therefore, $^{mou. *n*r.in_{B}}$. he descem direct exists .0, he s^ern ou,pu* a. me end o. every subinterval:

$$\|y^{y+1+i}-y^*\| - \|y^{y+1}-y^*\| = \delta\lambda$$
 (A.1.19)

me above descent property » va,« lor systems wHh or without «me delay because T can be chosen much larger than the delay in control variables, p.

Proof of Theorem 2

The assume of *s*m**o*«ca»y «*»* In the large system and continuous and bounded Bradients In Theorem 1 still hold here, except tor Assumption 2.

Now. the multistep unconstrained NLP problem is:

where y^{8*1*i} is given by a (perfect) model.

At the optimal solution, the following condition is satisfied:

$$\sum_{n=1}^{l} 2(y^{n+1+i} - y^{*})^{T} (\frac{\partial y^{n+1+i}}{\partial \Delta u}) = 0$$
 (A.2.2)

To satisfy the above condition, we have for full rank B_{\pm}^{1} :

$$/+**^{-} - / = 0$$
 (A23)

which means that the setpoint is satisfied for all predicted steps in the time horizon, and obviously:

$$||y^{s+2}-y^{*}|| \le ||y^{s+1}-y^{*}||$$
 (A.2.4)

Appendix **B**

Proof of Theorem 3

A constrained Newton-type controller has the following form:

$$\begin{array}{lll} Min & \mathcal{C}^{T} \Delta u^{s} + \frac{1}{2} (\Delta u^{s})^{T} H \Delta u^{s} = \mathcal{Q}(\Delta u^{s}) \\ & SJ. \quad a^{\prime\prime} \quad \& \ Atif \quad \& \quad a^{\prime\prime} \end{array} \tag{B.1.lfl)} \end{array}$$

where

$$C^{T} - [C^{A}Qf^{*I} - JiO + / \cdot' - /](CT0$$
(B.1.16)
$$H = (C^{T}\Gamma)^{T}(C^{T}\Gamma)$$
(B.1.1c)

$$\begin{array}{lll}
& Min & C^{T} \Delta u^{s} + \frac{1}{2} (\Delta u^{s})^{T} H \Delta u^{s} = Q(\Delta u^{s}) \\
& a^{\mu} \leq A \Delta u^{s} \leq a^{\mu} \\
\end{array} \tag{B.1.1a}$$

where

$$C^{T} = [C^{*}\Phi^{*}(x^{s+1} - x^{s}) + y^{s+1} - y^{*}](C^{*}T^{*}) < -^{BUb}$$

$$H = (C^{*}T^{*})^{T}(C^{*}T^{*}) \qquad .1c)$$

Expanding the system output y^{+2} in a Taylor series around the state x « x^{*}. u « u»:

$$\begin{aligned} \|y^{s+2}-y^*\|^2 &= \|y^{s+1}-y^*\|^2 + 2(y^{s+1}-y^*)^T [C^s \Phi^s (x^{s+1}-x^s) + C^s T^s \Delta u^s] \\ &+ 2(x^{s+1}-x^s)^T (C^s \Phi^s)^T C^s T^s \Delta u^s + (x^{s+1}-x^s)^T (C^s \Phi^s) (x^{s+1}-x^s) \\ &+ (\Delta u^s)^T (C^s T^s)^T (C^s T^s) \Delta u^s + higher order terms \\ &= \|y^{s+1}-y^*\|^2 + \|C^s \Phi^s (x^{s+1}-x^s)\|^2 + 2Q(\Delta u^s) \\ &+ 2(y^{s+1}-y^*)^T [C^s \Phi^s (x^{s+1}-x^s)] + higher order \ \text{ermi} \end{aligned}$$
(B.1.2)

Sine the Hessian H * po*e * * * * by ft. way £ « " ' ' J ' ' J ' ' ' J ' ' ' S A * wmmttrt with, nonz.ro sollionover the f.a_s«.r.Qion I M,n Q _w | rf_s « »• s A * »

C(0) «	0	•	(B .1.3 <i>a</i>)
C(U) «	0		(B.1.3b)
Q(∆نة)	< 0		(- ,)

If Au*# 0, **the** following relationship can be obtained:

 $Q(XAuO < X\pounds(Au) < 0$ for X 6 (0,1] (B.1.4)

where the λ is relaxation factor and its value is determined by line search. Also we assume $Q(\Delta u^2) < -\delta$, where δ is a small positive number. Else if $Q(\Delta u^2) > -\delta$, no improvement can be made toward the setpoint. If T is large enough and λ is small enough (referring the proof of Theorem 1), the descent direction is guaranteed:

Proof of Theorem 4

Since we have $||y^{s+1}-y^*|| \ge \delta$, with large enough sampling time, the iterated, constrained, single step control algorithm with a *nonzero* solution yields a control variable u^{s+1} satisfying the following relation:

$$\|y^{s+2} - y^{s}\| < \|\overline{y}^{s+2} - y^{s}\|$$
 (B.2.1)

As in Appendix A the bar is used to indicate that the system output is integrated with the control variable held at the value of a previous sampling time, u^s. Also, we know:

$$\|\overline{y}^{s+2} - y^{*}\| = \|y^{s+1} - y^{*}\| + O(\Phi)$$
(B.2.2)

In order to get the descent property, we choose T large enough so that:

$$O(\Phi) \leq \frac{1}{2} (|\overline{y}^{s+2} - y^{*}|| - ||y^{s+2} - y^{*}||)$$
 (B.2.3)

which leads to:

$$||y^{s+2}-y^{*}|| < ||y^{s+1}-y^{*}||$$
 (B.2.4)

Appendix C

Proof of Theorem 5

The assumptions of *asymptotically stable in the large* system and continuous and bounded gradients are still hold here.

The constrained control problem indicated in Theorem 5 can be formulated as follows:

Appendix C

Proof of Theorem 5

The assumptions of *asymptotically stable in the large* system and continuous and bounded gradients are still hold here.

The constrained control problem indicated in Theorem 5 can be formulated as follows:

There is no constraint on the rate of changes of control variable Au^{8*i} . The nominal system outputs in the predictive time horizon has the following relationship with the current system output, y^{6*1} :

$$\overline{y}^{s+1+i} = y^{s+1} + \Phi(t^{s+i}, t^{s})(\overline{x}^{s+i} - \overline{x}^{s}) + O(||\Phi(t^{s+i}, t^{s})||^{2})$$
(C.1.2)

Let T be large enough so that Au^{*1} is found that gives:

$$\begin{array}{l}
\text{Min} & \&^{**} - y' \mathbf{P} \\
\text{S.I.} & & y^{p+2} = \overline{y}^{p+2} & B_1^2(u^{p+1} - u^p) \\
\text{(C.1.3)} \\
\text{od} & \in u^{p+1} & \in u^n
\end{array}$$

an optimal solution for the above system, i.e. Hy^{**^2} -/II is minimum in the feasible region. Then a lower bound is obtained:

$$\eta y^{*+2} - y^* \Pi * j_{i=1}^{i} fl y^{*+1*} - y |$$
 (C.1.4)

When T approaches infinity, we have:

.

$$\lim_{x \to \infty} y^{M} \ll \lim_{x \to \infty} I/x^{1} \cdot O(\Phi(t^{*}+tT; t^{*}))$$

$$(C.1.5)$$

Then the optimal solution of system (C.1.1) is :

$$Aw^{TM} \rightarrow 0 \tag{C.I.6}$$

The proof for a descent direction now follows from the single step case of Theorem 4. For the recursive solution of (C.1.1) to be optimal, we can find $||/*^2 - /11 \ll$ Min Hy-/||, the minimum in the feasible region. Again, as $T \to \infty$, Ai/"ⁱ -4 0, i • 2,... I and the proof follows from the single step case of Theorem 4.



Figure 1: Moving Time Horizon Representation



Figure 2: Example 1: the Original Objective Function Value, x3, vs. Time

.



2

Figure 3: Example 1: Reactant Concentration, xv vs. Time



Figure 4: Example 1: Overall Heat Transfer Coefficient, u, vs. Time

36 A



Figure 5: Example 1: Objective Function, x₃ vs. Time, Moving time horizon formulation



Flgura 6: Example 1: Overall Heat Transfer Coefficient, u. vs. Time. Moving time horizon formulation



Figure 7: A CSTR System with Time Delay in Both States and System Inputs

•



Figure 8: Example 2: Reactant Concentration, x1, vs. Time



Figure 9: Example 2: Catalyst Concentration, x2, vs. Time

•



÷

Figure 10: Example 2: Temperature in the Reactor, x_3 , vs. Time



Figure 11: Example 2: Coolant Row Rate, $u_v vs$. Time



Figure 12: Example 2: Molar Feed Rate. u₂, vs. Time



Figure 13: Example 2: Reactant Feed Rate. u₃, vs. Time

References

- 1. Brengel, D.D. and W.D. Seider. "Multistep Nonlinear Predictive Controllers",, Presented at 1989 ACC Meeting,.
- 2. Donoghue, J. F., "Review of Control Design Approaches tor Transport Delay Processes", ISATrans.*. 1977, pp. 27.
- 3. Economou, C.G., *An Operator Theory Approach to Nonlinear Controller Design,* PhD dissertation, California Institute of Technology, June 1985.
- 4. C.E. Garcia and D.M. Prett, "Advances in Industrial Model Predictive Contror\C/wnca/ Process Control - CPC III. M. Moran and T. J. McAvoy.ed., CACHE and ELSEVIER, Amsterdam,.
- 5. Halanay, A, Differential Equations. Oscillations, Stability, rime Lags. Academic, New York, 1966.
- 6. Jerome., N. F. and W. H. Ray, "High-Performance Multivariable Control Strategies for Systems Having Time Delays", *Journal of the American Institute of Chemical Engineers*, Vol. 32, No. 6,1986, pp. 914.
- 7. Li, Wei-chong, A Mathematical Programming Approach for Control of Constrained Nonlinear Systems. PhD dissertation, Carnegie Mellon University, 1989.
- 8. Li, W.C. and L.T. Biegler, "Process Control Strategies for Constrained Nonlinear Systems",/nd. *Eng. Chem. Research*, Vol. 27,1988, pp. 1421.
- 9. Li, W.C, L.T. Biegler, C. G. Eoonomou and M. Morari, "A Newton Type Control Strategy for Nonlinear Systems '\Comp. Chem.Engr., accepted for publication, Vol., 1989, pp. .
- 10. Mee, D.H., "An Extension of Predictor Control tor Systems with Control Time-Delays", *IntJ.Controf*, Vol. 18, No. 6,1973, pp. 1151-1168.
- 11. Morshedi, A. M., "Universal Dynamic Matrix Control", *Chemcal Process Control CPC III,* M. Morari and T. J. McAvoy.ed., CACHE and ELSEVIER, Amsterdam, 1986.
- 12. Ogunnaike, B. A. and W. H. Ray, "Multivariable Controller Design for Linear Systems Having Multiple Time *Delays*' *VAIChE J.*, Vol. 25, No. 6,1979, pp. 1043.
- 13. Patwardhan, A., J. B. Rawlings and T.F. Edgar, "Model Predictive Control of Nonlinear Processes in the Presence of Constraints", Presented at AIChE National Meeting, 1988.
- 14. Peterson, T._t E. Hernandez, Y. Arkun and FJ. Schork, "Nonlinear Predictive Control of a Semibatch Polymerization Reactor by Extended DMC",, Presented at 1989 ACC Meeting,.
- 15. Ray, W. H., Advanced Process Control, McGraw-Hill, New York, 1981.
- 16. Renfro, J. G., Computational Studies In the Optimization of Systems Described by Differential/Algebraic Equations, PhD dissertation, University of Houston, 1986.
- 17. Russell, L. W. and J. D. Perkins, ^Towards a Method for Diagnosis of Controllability and Operability Problems in Chemical Plants ".*Chem. Eng. Res. DEs.*, Vol. 65,1987, pp. 453.
- 18. Smith, O. J. M, "Closer Control of Loops with Dead *Ttme"jChem. Eng. Prog.*, Vol. 53,1957, pp. 217.
- 19. Soliman, M. A. and W. A. Ray, "Optimal Control of Multivariable Systems with Pure Time Delays", *Automatics*, Vol. 7, 1971, pp. 681-689.
- 20. Wong, M. P. F., *The Assessment of Controllability of Chemical Processes,* PhD dissertation, Imperial College, London, 1984.