Process Control Strategies for Constrained Nonlinear Systems

by

W. Li and L. Biegler

EDRC-06-33-87

PROCESS CONTROL STRATEGIES FOR

CONSTRAINED NONLINEAR SYSTEMS

WEI-CHONG LI

and

LORENZ T. BIEGLER*

Department of Chemical Engineering
Carnegie-Mellon University
Pittsburgh, PA 15213
July 1987

Prepared for presentation at Annual AIChE Meeting, New York,
November 15-20,1987

•Author to whom correspondence should be addressed

Table of Contents

List of Figures

1. ABSTRACT

Control and state variable constraints are often overlooked in the development of control laws. Although recent developments with DMC and QDMC have addressed this problem for linear systems, incorporation of state and control variable constraints for nonlinear control problems has seen relatively little development. In this paper, a nonlinear control strategy based on operator theory is extended to deal with control and state variable constraints. Here we show that Newton-type control algorithms can easily be generalized using an on-line optimization approach. In particular, a special form of a successive quadratic programming (SQP) strategy is used to handle control and state variable constraints.

Moreover, the constrained approach can be shown to fit into the IMC structure proposed by Economou and Morari. Using the small gain theory of Zames, we show that constraints on state and control variables can replace the design of a nonlinear fitter for noninvertble processes and thereby lead to stable controllers. The advantage to this approach, however, is that constraints are relatively straightforward to'apply since the limits of their response are known in advance.

After presenting a detailed description of the method, a number of scenarios are considered for the control of nonlinear reactor models. These models cannot in general be controlled using linear control strategies. With the nonlinear constrained approach, on the other hand, regulation and control can be done in a straightforward manner, and emphasis to more important parts of the system can be given with appropriate placement of constraints.

2. INTRODUCTION

The Internal Model Control(IMC) structure was proposed by Garcia and Morari (1982). They recently extended ft to multivariable systems (Garcia and Morari, 1985a, 1985b). The main attractive features in the IMC structure are as follows. First, while the controller affects the quality of the response, the filter takes care of the robustness of the control block independently. Note that a filter is a block in the feedback signal to account for the model and process mismatch reflected through the estimated disturbance and to achieve a desired degree of robustness. Secondly, the closed-loop system is stable as long as the controller and model are open-loop stable. Only robustness needs to be considered. Furthermore, this model representation is suitable for a theoretical robustness analysis.

One special case of IMC is Dynamic Matrix Control(DMC) (developed at the Shell Oil Co.) .which has been reported to perform very well in application (Cutler and Ramaker, 1979; Prett and Gllette,i979). DMC is structured such that the entire control algorithm can be put into a linearly constrained optimization problem . When the objective function for this optimization problem is of the sum-of-the-error-squared form, the algorithm becomes Quadratic Dynamic Matrix Control (QDMC), the second generation of the DMC algorithm. QDMC without constraints was found to have an IMC structure (Garcia and Morari,1982). Moreover, the DMC algorithm is the first control technique which could successfully handle general process constraints. DMC is a type of model-predictive controller, which solves a new optimal problem and produces a "new" controller at each execution. The on-line measurements which cannot be foreseen at the design stage are used to adjust controller settings and to handle the constraints. This distinguishes the algorithm from the conventional controller that uses a fixed relationship between error and manipulated variables, and is solved only once, during the conceptual design phase. Even though DMC shows certain superior characteristics among linear controllers, the inherent linear model restricts its use in highly non-linear processes. One can argue that if the nonlinear model can be linearized, then DMC can be used to control the process. N is well known however that a linearized model is only valid in a small neighborhood of the reference point. If the external forces such as unmeasured disturbances drive the system outside the valid neighborhood, the linearized model will introduce large modeling errors which can mislead control actions. Furthermore, certain nonlinear systems are almost impossible to be controlled by any type of linear controller. Two examples of this type of systems will be presented later. Therefore, a nonlinear predictor-type controller in the IMC structure should be developed to deal with these nonlinear systems.

Economou and Morari (1985,1986) extended the IMC design approach to nonlinear lumped parameter systems. Based on an operator formalism, a Newton-type control algorithm was constructed. Simulation examples demonstrated the good performance of this control algorithm and showed that the control algorithm worked well even in the case where no linear controller can yield stable behavior. On the other hand, this algorithm cannot deal with the process constraints .which limits the potential usefulness of this algorithm.

In this work, a special form of the successive quadratic programming strategy is used to handle

process constraints. A Newton-type control law in the IMC structure is briefly presented in the next section. The successive quadratic programming algorithm is developed in section 4. This approach can be shown to fit into the nonlinear IMC structure. A computing algorithm based on this strategy is outlined in section 5. In order to demonstrate the effectiveness of the strategy, two example problems are simulated in section 6. The simulation results demonstrate the good performance of the suggested algorithm. Finally, the stability of the constrained controller is briefly analyzed in section 7.

3. A NEWTON TYPE CONTROL LAW

Economou and Morari (1985,1986) extended the IMC structure to an autonomous lumped parameter Muttiple-Input-Muttiple-Output (MIMO) nonlinear system. A Newton-type method was used to construct the control law for nonlinear models. The systems considered are generated by a set of ordinary differential equations. The vector form is as follows:

$$\wedge \quad = f(x,u(t)) \tag{l}$$

where x € R^n is the state of the system, and for every t € (0, «) ,u(t) € R^m is the input, with the corresponding output form map (y € R^m)

$$y \ll tOO \tag{2}$$

In deriving this strategy, several assumptions are made. First, we assume the system exists and has a unique solution. Secondly, we assume at this point the model is perfect, in that there is no model and system mismatch. This assumption will later be relaxed for stability analysis. Finally, we assume that the system inputs are piecewise constant functions to reduce the problem at hand to a finite dimensional space. Here, the letter s Is used as a superscript to make the time discrete. The s* sampling interval •xtendsfrom t* to f^{*1}. T - t ^ - t * Is the constant sampling time; X^s is the state at t^8; u^s is the system input held constant over (t^*. t^{*+1}).

In the discrete setting of the study, $x(t_2; t_v x,u»^{+1})$ is the solution of equation (1) at time t_2 for u(t) * u» (t_t < t < tg) and initial condition $x(t_t; t_{1f}x,u^*)$ - x»; X^s will denote the state of the system at t - *+\ i.e. x^{s+1}:

$$X' \bullet^{**+1} \ll X(\wedge r_f \ tftf) \tag{3}$$

Since (1) is autonomous: $X(t_t^* T; t_{1f}x,u) \ll X(t_2+T; t_2,x,u)$ i.e. t does not have an explicit

dependence on t. Therefore time will be dropped from the parameter list and the following convention will be used:

$$X' \text{ « } X(T;\ J>*T) \text{ « } Xtf+7;\ ftfjf] \tag{4}$$

The derivatives of X* with respect to x* and u* will be defined as follows:

$$\Phi^{*} = \frac{\partial(\chi^{*})}{\partial(x^{*})} \tag{5}$$

$$p \quad . \quad \underset{30*0}{2\pounds)} \tag{6}$$

The y* > g(x') is the system output at t*, The derivative of y* with respect to x will be defined

$$ax» \quad ax^{*}$$

A computational theory for calculating 4>* and I* is presented here. The statements are proved in Economou (1985).

$$\frac{\partial\Phi(t)}{\partial t} = \frac{\partial f(\zeta,\ \xi)}{\partial\zeta}\Big|_{\zeta\ =\ \chi^{*},\xi=u^{*}}\ \Phi(t) \tag{8}$$

$$\Phi(t^{*}) \text{ « } / \tag{9}$$

$$\frac{}{\partial t} = \frac{\partial f(\zeta,\ \xi)}{\partial\zeta}\Big|_{\zeta=\chi^{*},\xi=u^{*}}\ \Gamma(t) + \frac{\partial f(\zeta,\ \xi)}{\partial\xi}\Big|_{\zeta=\chi^{*},\xi=u^{*}} \tag{10}$$

$$TOO - 0 \tag{11}$$

The Newton-Type Control law with p • 1 (where p is the number of forward steps allowed to achieve the desired output y*) is presented here. The detailed derivation is straightforward and can be found in Economou (1985).

$$c\text{^}Voc - x») \bullet (y \ -/\bullet») - (cr^{l}rw \bullet o \tag{02}$$

where Au « u " W

However, the algorithm developed by Economou and Morari cannot deal with constraints which inevitably exist in the chemical process. The process constraints can arise from various considerations, a

few of which include:

(I) Physical Limitations on Equipment: All equipment has physical limitations which cannot be exceeded during the operation.

(II) Product Specifications: Any intermediates, or marketable products need to satisfy certain specifications required for further processing, or by consumers.

(III) Safety: Many process variables should not exceed certain bounds for the sake of safety.

4. A NONLINEAR STRATEGY FOR HANDLING PROCESS CONSTRAINTS

Designing a control algorithm which has the capacity to handle the constraints is not an easy task, especially when a nonlinear system is involved. A candidate algorithm should have the following characteristics:

(I) Predict Model: A model should be based on prediction of output. Thus, any potential violation of process constraints can be foreseen, and proper corrections can be made.

(II) Optimal Input: In MIMO systems , it is often possible to trade off good performance of one output against poor performance of another; therefore, based on the relative importance of the different outputs, a set of optimal outputs needs to be determined.

(III) Easy To Analyze: The structure of the controller should be transparent enough to perform stability and robustness analysis. The nonlinear IMC structure has a framework that allows this analysis , and as a result is a viable candidate.

Linear control variable constraints can be dealt with easily, using quadratic programming. Moreover, the following quadratic programming problem without any constraints is identical to the Newton-type control law. The proof can be found in Appendix A. Note that the Hessian of the objective function is positive semi-definite, which means at least a local minimum can be found.

$$\underset{\Delta u}{Min} \quad C^T \Delta u^s + \frac{1}{2}(\Delta u^s)^T H \Delta u^s \tag{13}$$

where

$$C^T = [\, C^{s+1}\, \Phi^s\, (\, x^s - X^s\,) + (\, y^* - y^{s+1})]^{\,T}\, (\, C^{s+1}\, \Gamma^s\,) \tag{14}$$

$$H = (C^{s+1}\Gamma^s)^T (C^{s+1}\Gamma^s) \tag{15}$$

With the help of the quadratic form in the objective function, the linear equalities and inequalities constraints of control variables can be included . In this case problem (13) becomes

$$\underset{\Delta u^s}{Min} \quad C^T \Delta u^s + \frac{1}{2}(\Delta u^s)^T H \Delta u^s$$

$$sa \quad d \; £ \; AQf+Au) \; £ \; cf \tag{16}$$

where the A € k x k i s a matrix multiplying the control variables; V defines the number of constraints. When a'$_k$ equals ag , It becomes an equality constraint. For simplicity we put equality and inequality constraints together. In a real chemical process, we need to deal not only with the constraints of the control variables, but also with the constraints of the state variables. The latter are probably more important to get a desired product or to avoid failure of the production process. Simple bounds on state variables are the most common state constraints in most chemical processes. So our objective is to handle the following problem:

$$\underset{Am}{Min} \quad C^T Au^* + \frac{1}{2}(\Delta u^s)^T H \Delta u^s$$

$$SJ \quad cf \; £ \; Atf+Aif) \; £ \; of \tag{17}$$

$$x(t) \leq x^u$$

$$t^s \leq t \leq t^{s+1}$$

The moving time horizon is introduced for on-line implementation. Given the current time t[6], the immediate past control variable u^s .initial state variable x^s (x^{s,1}), and the measurement of current state x*+^{1} (x^s), we hope to find an optimal control variable u*+^{1} which can efficiently drive the process to the set point without violating the control and state variable constraints. Figure 1. shows the schematic of the moving time horizon.

In order to avoid the computational difficulties of dealing with these state constraints, a new state variable is defined to convert a path constraint into a terminal constraint (Sargent, Sullivan,i977).

$$\frac{dx_{n+1}(t)}{dt} = \sum_{i=1}^{n} [min(0, x_i(t)-x_i^l)]^2 + \sum_{i=1}^{n} [min(0, x_i^u-x_i(t))]^2 \tag{18}$$

$$x_{n+1}(t_0) \; « \; 0$$

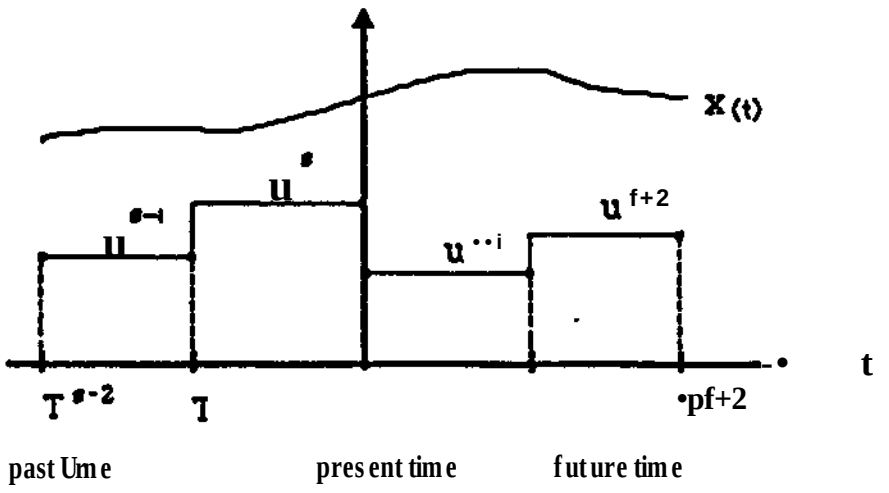


Figure 1: The moving time horizon

We then impose the constraint $x_n^{\wedge}{}_1(t_f)$ - 0 and substitute this constraint with the path constraints of state variables in (17). x» is an implicit function of u and there is no direct method to solve this kind of problem. Here an iteration algorithm is developed to deal with the above problem. We expand $x_{n4i}(t_f)$ about u£V by using Taylor series and truncating the expansion after the second term. The letter j is used as a subscript to indicate the j-th iteration .

$$x_{n+1}(t_f, \chi^{s+1}, u_j^{s+1}) = x_{n+1}(t_f, \chi^{s+1}, u_{j-1}^{s+1}) + \frac{\partial x_{n+1}}{\partial u}\Big|_{u=u_{j-1}^{s+1}} (u_j^{s+1} - u_{j-1}^{s+1}) + O(u_j^{s+1} - u_{j-1}^{s+1})^2 \quad (19)$$

Define

$$K_1^{s+1} = \frac{\partial x_{n+1}}{\partial u}\Big|_{u=u_{j-1}^{s+1}} \quad (20)$$

$$du = u_j^{s+1} - u_{j-1}^{s+1} \quad (21)$$

The calculation form of $K^{\wedge 1}$ can be found in Appendix B.

So $x_{n+1}(t|)$« 0 is linearized by the following equation:

$$x_{n+1}(t_f, \chi^{s+1}, u_{j-1}^{s+1}) + K_1^{s+1} du = 0 \quad (22)$$

The quadratic programming problem at $j*^1$ iteration is as follows:

$$\underset{\Delta u}{Min} \quad C^T \Delta u_j^i + \frac{1}{2}(\Delta u_j^i)^T H \Delta u_j^i$$

$$SJ \quad d \; £ \; A\hat{}+Aufip \qquad \text{fl"} \qquad (23)$$

$$x_{n+1}(i_j; \; \chi^{n+1} u_{j-1}^{n+1}) + K_1^{n+1} du = 0.$$

There are two types of constraints we need to consider. One is hard constraints - no dynamic violations of the bounds allowed at any time. Another is soft constraints - violations of bounds tolerated for satisfactton of other criteria, in the problem (23) only hard constraints have been considered. Let us assume the soft constraints for the control variables are

$$d \; <> \; Ajtf+bif) \; <> \; a? \qquad (24)$$

where $\backslash \in R^m i$; m_1 is the number of soft constraints. Since these constraints can be violated to satisfy the hard constraints, the slack variables S_{m_1} need to be added in the inequality (24) to increase the feasible region. On the other hand, including the summation of all elements of S_{m_1} in the objective function, the algorithm can search the optimal control strategy to satisfy soft constraints whenever it is feasible. Then the soft constraints of (24) become

$$a^l - \delta_{m_1} \; \leq \; A_s(u^i + \Delta u^i) \; \leq \; a^u + \delta_{m_1} \quad \bullet \qquad (25)$$

The objective function becomes

$$\underset{\Delta u}{Min} \qquad C^T t^* t \; + \; _z hjtufpHtot \; \; ^* \sum_{si}^{m_1} C0\& \qquad (26)$$

Since the importance of each constraint may not be same, a weighting factor o, can be included to reflect the differences. If the soft constraints involve state variables, the problem becomes more complicated. Assume $x_{\%}$ has the following soft constraint:

$$x_i^l \; \leq \; x(l)_i \; S \; af \qquad (27)$$

Similarly, as we did before, a new variable $x_{n+1+}\hat{}$ is defined as follows:

$$\frac{dx_{n+1+i}(t)}{dt} = \{\min(0.\ x_4<0\text{-}*\{)\}^2 + \{\max(0.\ x?\text{-}x,<0)\}^2 \qquad (28)$$

$$x_{n+1+i}(t_0) = 0$$

A first order approximation of the new variable is used as we did in (19) and a slack variable 5_{m_1+i} is added in the inequality to increase the feasible region. Then the soft constraint of (27) in j* iteration becomes

$$x_{n+1+i}(t_f;\ \chi^{s+1}, u_{j-1}^{s+1}) + K_{i+1}^{s+1} du \le \delta_{m_1+i} \qquad (29)$$

and dimension of soft state constraints is m_2. The vector form of these constraints is

$$N(t_f;\ \chi^{s+1}, u_{j-1}^{s+1}) \le \delta_{m_2} \qquad (30)$$

where

$$N(t_f;\ \chi^{s+1}, u_{j-1}^{s+1}) = \begin{bmatrix} x_{n+2}(t_f;\chi^{s+1}, u_{j-1}^{s+1}) \\ x_{n+3}(t_f;\chi^{s+1}, u_{j-1}^{s+1}) \\ \cdots \\ \cdots \\ x_{n+1+m_2}(t_f;\ \chi^{s+1}, u_{j-1}^{s+1}) \end{bmatrix} + \begin{bmatrix} Kf'du \\ K_3^{s+1} du \\ \cdots \\ \cdots \\ K_{1+m_2}^{s+1} du \end{bmatrix} \qquad (31)$$

$$K_i^{s+1} = \frac{\partial x_{n+i}}{\partial u}\Big|_{u=u_{j-1}^{s+1}} \qquad i = 2,\ 3,\ \ldots\ m_2 \qquad (32)$$

Including the soft constraints the quadratic programming problem at j* iteration becomes

$$\underset{\Delta u}{Min} \quad C^T \Delta u_j + h_j \Delta r_j^T H \Delta u_j + \frac{1}{2} \sum_{i=1}^{m} (0,5_i$$

$$SJ \quad tf \; S \; i4(«^j + A_{ii} J.,) \; S \; «« \qquad (33)$$

$$x_{m+1}(l_j; \chi^{s+1}, u_{j-1}^{s+1}) \cdot \mathrm{Kf} * du - 0.$$

$$a_f - \delta_{m_1} \leq A_s(u_{j-1}^s + \Delta u_{j-1}^s) \leq a^* + \delta_{m_1}$$

$$N(l_j; \chi^{s+1}, u_{j-1}^{s+1}) \leq \delta_{m_2}$$

$$6_m \; 2 \; 0.$$

where m - m , + m_2 is the dimension of alt of the soft constraints.

5. ALGORITHM

The algorithm for the nonlinear control problem follows:

1. start with an initial condition x*,u*
2. solve for X^{1*1}, $C»^{+1}.0^8$, I*. simultaneously

   a) setj-0

   b) set ug^{+1} - u*
3. a) solve QP (Eqn. 33), get $u_j»^{+1}$

   b) choose a stepsize based on the Armijo linesearch
4. If$(duf^1)^T(duf^{+1}) <$ e

   where e is a small positive number

   $u^{s+1} = u^s + \Delta u_j^s$

   go to next sampling time s - s+1 and return to step 1.
5. else(gobacktostep3.wtthj-j + 1

For clarity, the flowsheet of the algorithm for the control problem is shown in Figure 2.

An Armijo line search is introduced to control the search stepsize. We define a test function :

$$\Psi(u_j^{s+1}) = (y_j^{s+1}-y^*)^2+\sum_{i=1}^{m}\omega_i\delta_i+\sum_{i=1}^{m_1}\mu_i max\{0,\ a_i(u_j^s+\Delta u_j^s)-\delta_i-a^u,\ a^l-\delta_i-a_i(u_j^s+\Delta u_j^s)\}$$
$$+\sum_{i=1}^{m_2}\mu_{m_1+i}max(0, x_{n+1+i}(x^{s+1}, u_j^{s+1})-\delta_i) \qquad (34)$$

*(u*j*1)tethe directional derivation along the search direction. Here Hj is a penalty parameter that satisfies Uj > Xj where are Kuhn-Tucker multiplies from the QP; a, are rows of the matrix A,.

Algorithm for selecting the Armijo step size:

1. having uj*}1, and new QP solution uj*+1

   define du - $u_j^{s+1} - u_{j-1}^{s+1}$

2. a) set a - 1

   b) evaluate *(u^1 + a du). *(uf.V). *'(u$_{j-1}^{s+1}$)

   c) if

$$\Psi(u_{j-1}^{s+1} + adu) - H'dip,^1) \ ^\ aS^'d^,^1) \qquad (35)$$

   go to 3.

   d) else, use quadratic interpolation to find new value of a

$$a \ll max\ \{8,, \frac{\Psi'}{2[*'(«p^1>*4'(«p^1)H'(Jf')]}\ £L\ r-)a \qquad (36)$$

   here 8j - 63 « . 1 , a nominal value

   go to b).

3. else, go to next QP Iteration with uj*1 « u»V + adu

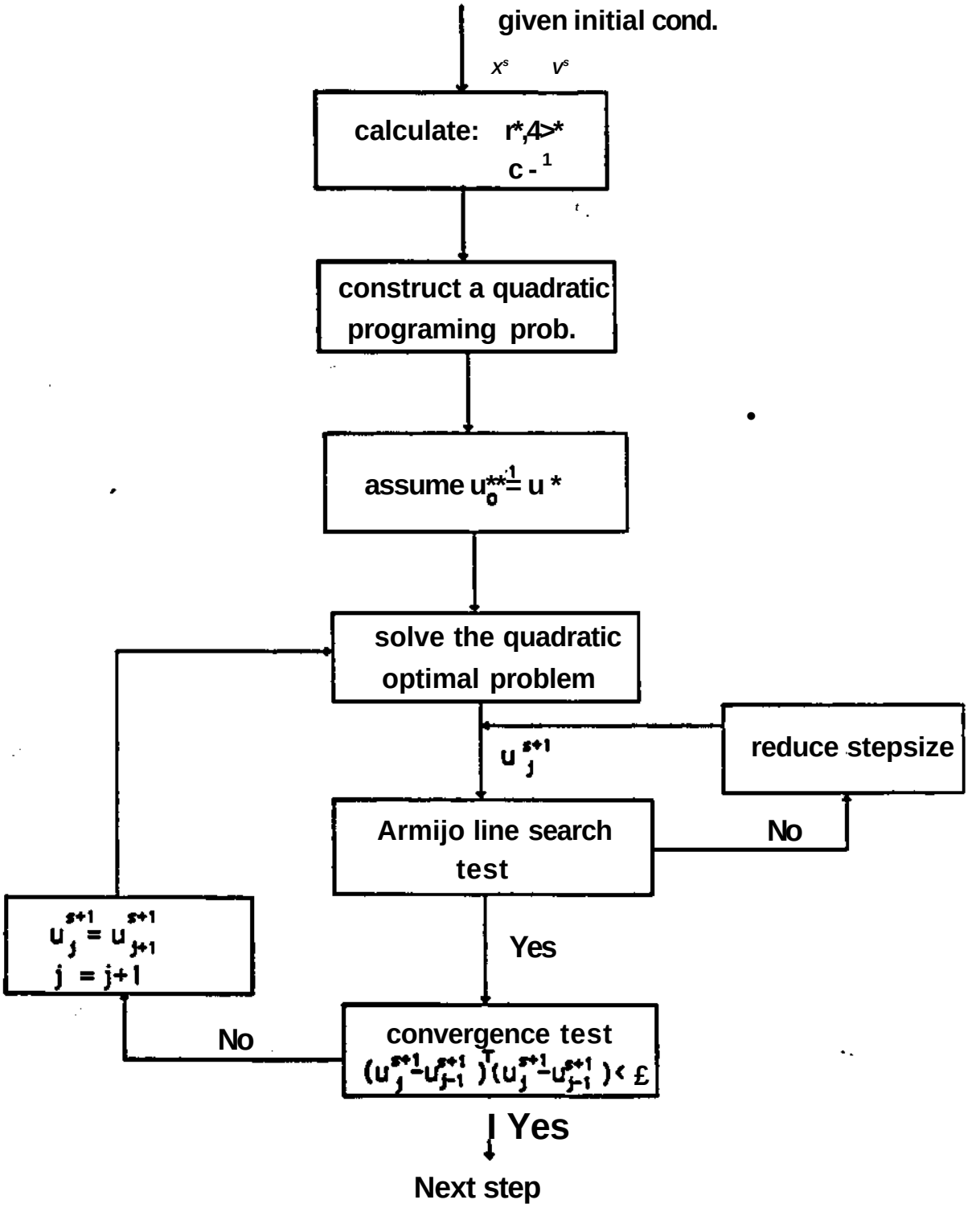


Figure 2: The flowsheet of the algorithm

The most crucial assumption which we made in developing the above algorithm is that the model be perfect. That is rarely the case in chemical processes because the model and disturbance uncertainties unavoidably exist. An on-line identification phase should be added to update the model after

a number of time steps by using the differences between measured and predicted values of outputs. An optimization problem can be constructed to estimate these uncertain parameters. The objective function is to minimize the differences between the measured and predicted values subject to the bounds of these parameters. By using a nonlinear model, the physical significances of these parameters can be recognized and it is possible to set the bounds of these parameters. If uncertain parameters are slow moving i.e. the time constants of these parameters are much larger than the time interval of control, the parameters can be assumed as constants and the updated values can be used to predict the process in a future time horizon. If variation in parameters is sufficiently large compared to the time interval of our model, the dynamic nature of these parameters should be analyzed in order to postulate some model for the variation. Jang et al. (1987) recently proposed a two-phase approach to control and operate a chemical process. A similar idea has been discussed in their paper.

6. EXAMPLES

Two example problems are simulated to demonstrate the effectiveness of the strategy proposed in this work. The first example problem was adapted from the paper of Matsuura and Kato (1967), which describes a kinetic model with multiequilibrium points at steady state. The second example problem was modified from Economou and Morari's paper (1986). Their original problem was extended to a three dimensional system with constraints. The control objective of both problems is to operate the reactor as closely as possible to the setpoint. When the system gain changes sign as the operating point changes from one side of the setpoint to the other, any linear controller with integral action cannot perform well (Morari.1983). Without integral action the linear controller will result in a large offset. Both example problems possess this feature. Therefore, the linear controller cannot be used in this type of system . On the other hand, the nonlinear controller with constraints proposed in this work controls this system very welt as seen by the results of our simulations.

Example 1: A Stirred **Tank Reactor** (1)

For the reaction

where A is in excess, a reaction rate equation can be written as follows:

$$r_B = \frac{K_1 C_B}{(1.0+K_2 C_B)} \qquad (37)$$

where C_B is the concentration of component B. The reaction occurs in an ideal stirred tank as shown in Figure 3.

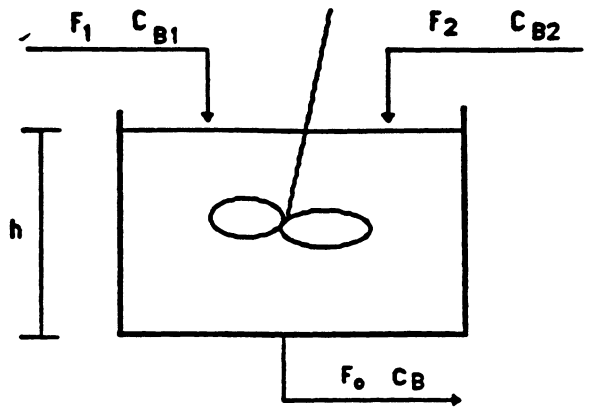


Figure 3: A stirred tank reactor (1)

The concentrations of B in the two inlet flows are assumed to be fixed: $C_{B1} = 24.9$, $C_{B2} = 0.1$. Both inlet flows contain excess amount of A. The tank is well stirred with a liquid outflow rate determined by the liquid height in the tank h, i.e., $F(h) = 0.2\ h^{0.5}$. The cross section area of the tank is 1. The sampling time of this problem is set to 1.0 min. The values of various parameters are listed in Table 1, Appendix C. After simplification, the model becomes

$$\frac{dx_1}{dt} = f_1(x;\ u) = u_1 + u_2 - .2x_1^{0.5} \qquad (38.a)$$

$$\frac{dx_2}{dt} = f_2(x;\ u) = (24.9 - x_2)u_1 x_1^{-1.0} + (0.1 - x_2)u_2 x_1^{-1.0} - \frac{x_2}{(1+x_2)^{2.0}} \qquad (38.b)$$

$$y_1 = x_1$$
$$y_2 = x_2$$

where
u_1 = inlet flow rate with condensed B (F_1)
u_2 = inlet flow rate with dilute B (F_2)
x_1 = liquid height in the tank

x_2 = concentration of B in the reactor

When the height of liquid level y, is at setpoint (y^-iOO.) and two Inlet flow rates are at the steady state (0,-1.0; u_2-1.0). the graphical solution of Eq.(38.b) is illustrated In Figure 4. The convection term in the Eq.(38.b) Is a straight line with slope i/i. t is the time constant of the reactor in the steady state. When the reaction r_B is shown as a function of C_B by the curve Indicated with $r_B(C_B)$ in the Figure 4. there are three different equilibrium points (a, p\ •$ of the system of which a, *y* are stable equilibrium points and P is unstable. Detailed discussion of the stability of this isothermal reactor was presented in Matsuura and Kato's paper (1967). Here the point p is used as a setpoint to demonstrate the proposed algorithm developed above.

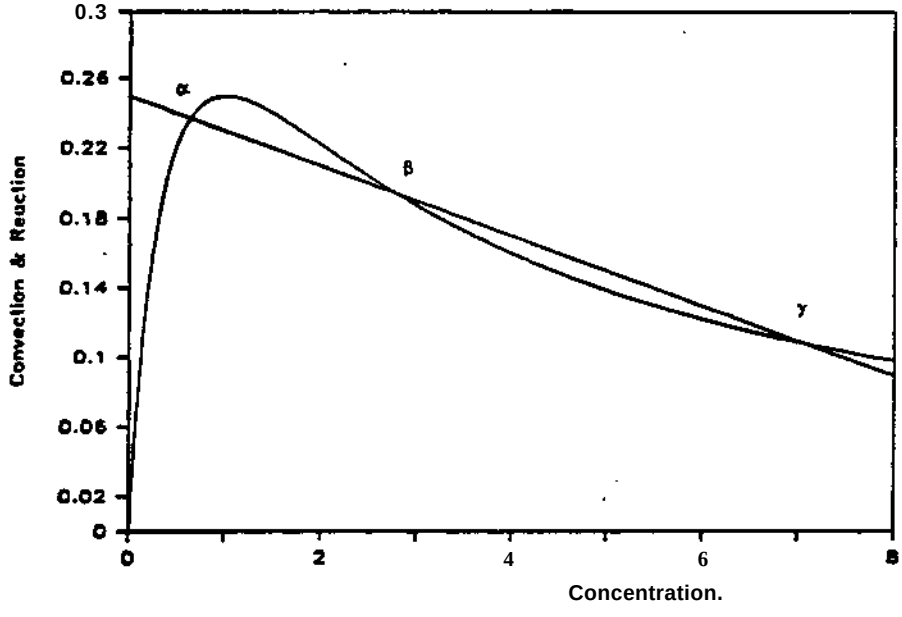


Figure 4: Multiequilibrium points at steady state

From Figure 4 we can observe that the system gain changes sign as the operating point changes from one side of point p to the other. In addition, from this unstable equilibrium point a small disturbance can drive the system to two stable equilibrium points o or 7. depending on increase or decrease of B concentration in the reactor caused by the disturbance.

The control objective Is to minimize the difference between the reactor output and setpoint. All simulation results are presented at the end of the paper. (Figures are numbered by roman numerals *I*, *II*. etc.) Two sets of initial conditions are used. Set (1) is in the region where the system automatically goes to point o without any control. Set (2). on the other hand, is in the region where the system goes to point

Y without any control. Table 2 shows the numerical values of these initial conditions.

We simulate and control this example problem with various control variable constraints and without putting any constraints on the state variable. The u, and u_2 have same tower and upper bounds. The tower bounds of u, and u_2 are zero. The upper bounds varied from 5.10 to infinity. Footnotes In Figures *I* through *IV* indicate the various upper bounds on the u, and u_2. Figures *I* and *II* are y, and y_2 vs. time, respectively, using set (1) initial conditions. Figures *III* and *IV* are similar plots with set (2) initial conditions. The simulation results show that the algorithm efficiently drives the system to the set point without violating constraints.

In Figure *I*. increasing the upper bound from 5.0 to 10.0 on u, and u_2. the overshoot of y, decreases. When the upper bounds of u, and u_2 are removed, the overshoot of y, is totally eliminated. In Figure *III* the best performance of outputs is the one with no upper bound on the control variables. In Figures *II* and *IV,* the rise time decreases with increasing the upper bound on u, and u_2.

Intuitively, one would think that the higher the upper bound on u, and u_2. the better the performance, since the feasible regton of control profile is increased. This is what we actually observe in all plots of this example. However, it is not always true. Consider the simulation results of the next example. Here, as will be explained later, the best performance of some outputs is not from the most relaxed bounds on the control profile.

To control and simulate this example problem for 50 sampling times, required roughly 30 CPU seconds on a MicroVax II.

Example 2: A Stirred Tank Reactor (2)

The first order reversible exothermic reaction

$$A \underset{k^*}{\overset{k_1}{\rightleftharpoons}} B$$

Is carried out in a Ideal stirred tank shown in Figure 5.

We assume that the combined concentration of A and B is constant. The tank is wen stirred with liquid outlet determined by the liquid height in the tank h. I.e.. $F(h) = 2.5h^{\circ\bullet*}$. The nonlinear differential-algebraic equations that models the dynamics of the reactor can be found In Appendix C. They are derived from differential mass and energy balances. The values of various parameters can be found in Table 3. After substituting numerical values tor all the parameters, the model can be simplified as follows:

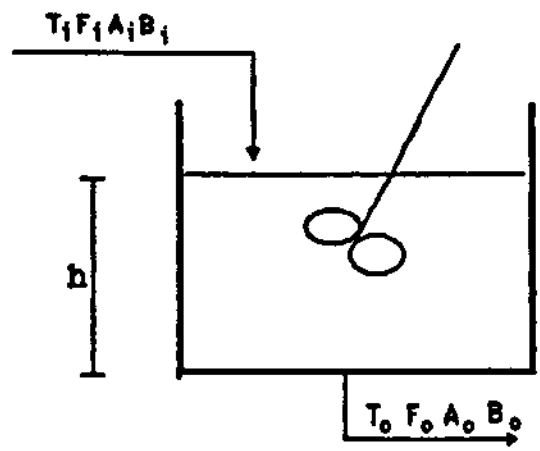


Figure 5: A stirred tank reactor (2)

$$\frac{dx_1}{dt} = f_1(x, u) = -0.16x_1x_3^{-1.0}u_1 + K_1(1.0 - x_1) - K_2x_1$$

$$\frac{dx_2}{dt} = f_2(x, u) = 0.16u_1u_2x_3^{-1.0} - 0.16x_2x_3^{-1.0}u_1 + 5.0\times[K_1(1.0 - x_1) - K_2x_1]$$

$$\frac{dx_3}{dt} = f_3(x, u) = 0.16u_1 - 0.4x_3^{0.5} \qquad (39)$$

$$y_1 = x_1$$

$$y_2 = x_3$$

The control objective is to operate the reactor output as close as possible to the setpoint subject to the process constraints. Figure 6 shows the equilibrium vs. reactor temperature (x_2) when the height of liquid level (y_1) Is at the set point (y_1=0.16). Two sets of initial conditions were used. One is at the lefthand side of maximum point of the equilibrium reactor curve; another one is on the righthand side. Since the height of liquid level is not initially at the set point the actual initial point can only be presented in a three-dimensional plot. The reason we used two sets of initial conditions is because the linear IMC controller is unstable at set(2) initial conditions with fixed height of liquid level (Economou, Morari 1985). Table 4 shows the details of the two sets of initial conditions.

Using the algorithm developed previously, we first simulate this example problem with various control variable constraints and without putting any constraints on the state variable. We varied the u_2 upper bound with a fixed tower bound at 300. u_1 is not bounded. Figures V and VI are y_1, y_2 vs. time .

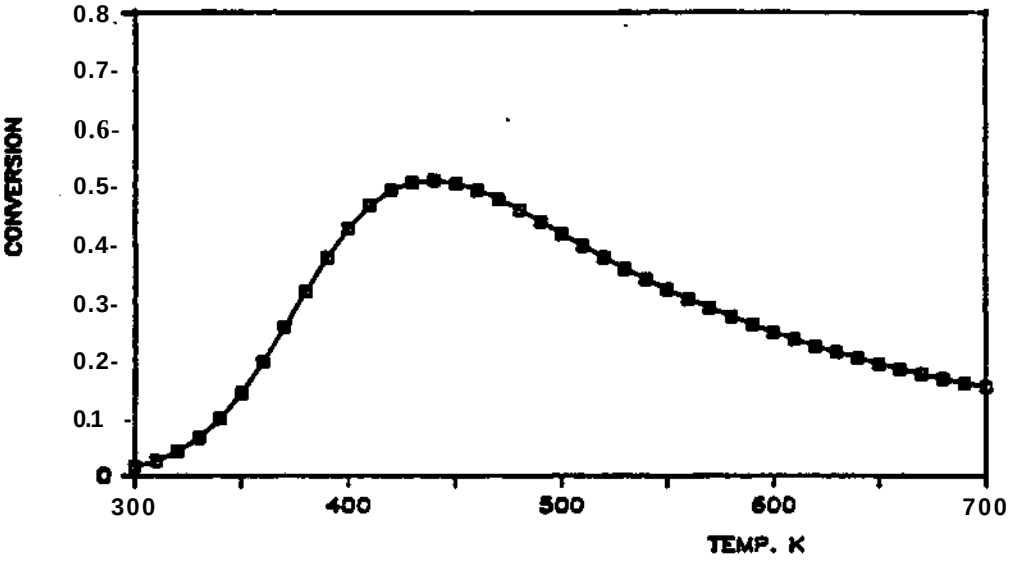


Figure 6: Equilibrium diagram

respectively, using set (1) initial conditions. Figures *VII* and *VIII* are similar plots with set (2) initial conditions. Footnotes in the figures indicate the various upper bounds on the u_2 corresponding to various curves. In Figure Wwe observe that the best performance is obtained when there is no upper bound on u_2. However, Figure *Vis* different; that is, the best performance is obtained when the upper bound on u_2 is 490. One possible explanation for this is that in MIM0 systems, it is often possible to trade off good performance of one output against poor performance of another. Here, even though one output has the best performance with no upper bound on u_2 • another output is relatively poor in performance. This observation tells us that although the overall performance of a MIM0 system in terms of achieving the lowest values in the optimal objective function may be improved by relaxing control variable bounds, the improvement of individual outputs is not guaranteed.

In order to demonstrate the effectiveness of state variable constraints, we simulated this example problem with both control variable and state variable constraints. The results were compared with the output which had no state variable constraints. Figures /Xand Xshow y_t and y_2 vs. time, respectively, with set(1) initial condition. Three curves were plotted in each figure. Curve 1 has no state variable constraints; Curve 2 has a loose constraint on x_t; Curve 3 has a tight constraint on x_t. Figures *XI* and *XII* are similar plots with set (2) initial conditions. The Table 5 shows the details of these constraints.

Figures /Xand X/show that the controller with state variable constraints performs better than one without constraints. The reason may be that when a Newton-type control law is derived, the second or higher order terms are truncated and some system information related to these higher order terms is lost. Then a full Newton step will be taken which may be oversized and the new control variable u^{**1} may not yield a good value. By including the state variable constraints with our iteration algorithm, we also use an Armijo line search to control the stepsize and iterate until the optimal point has been found. This improves the performance of the controller.

In problem (23), the hard constraints of control variables are always satisfied during the iterations due to the structure of the problem. In addition, the hard constraints of state variables are also guaranteed to be satisfied at the end of iterations. This can be shown as follows. When convergence criterion is satisfied, $(du)^T(du)$ s e, which implies du -> 0, $x_{n4i}(t_l)$ must then be equal to zero. In other words, the state variable constraints are not violated in the one step time horizon. Our simulation results also support this claim.

From Figures /Xand X/, Curve 3 avoids the oscillation which occurs in both Curve 1 and Curve 2. The rise time in Curve-3 is similar or shorter than Curve 1 and Curve 2. The price to be paid for having better control on x_1 is that one has to tolerate sluggish response on x_3. In other words, one can manipulate the state variable constraints to change the response speed of the individual state variable.

The optimal solutions for this example problem usually require 3 to 4 iterations except at the first sampling interval, where more iterations are required to find an optimal solution. To simulate and control 10 sampling times (T - 1.0 min.) in this example required roughly 1.5 to 2.0 CPU minutes on a MicroVax II. Of course problems without state variable constraints require much less computation since only one QP solution is required for a time step.

7. STABILITY ANALYSIS

In the IMC structure, a filter is introduced to reduce the loop gain and to achieve the desired degree of robustness. If a perfect IMC controller has process constraints, the robustness of the system can be achieved by adjusting the constraints. In this case a filter is not needed

Before we prove the similarity between a filter and use of process constraints, let us briefly introduce the nonlinear IMC structure for an autonomous lumped parameter MIMO system (Economou and Morari, 1986). The block diagram of this structure is shown in Figure 7.

In the Figure 7 the nonlinear operator F, C, P, and M denote the filter, controller, plant, and model, respectively. Blocks with double lines are used to emphasize that the operators are nonlinear and that the linear block diagram manipulations cannot be used.

We also introduce some mathematical concepts which are needed in the proof. A more detailed treatment of these concepts can be found in the work of Kolmogorov and Fomin (1954), Rail (1969).

Norm

A linear space R is said to be normed if to each element x e R there corresponds a nonnegatrve number |W| , called the norm of x_t such that:

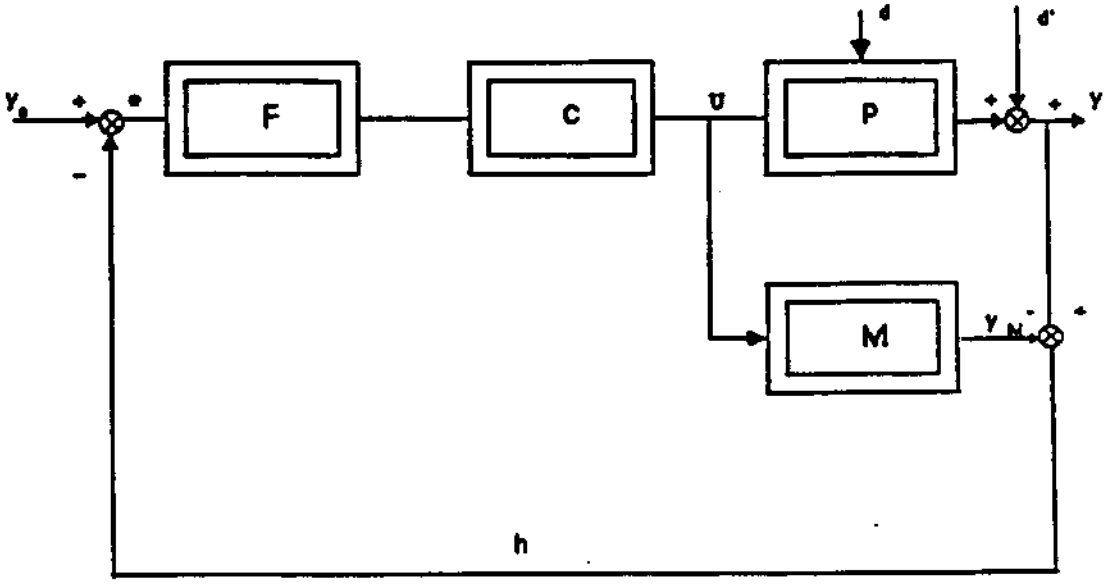


Figure 7: A complete nonlinear IMC structure

1). IWI-0, Iffx-0

2). llotxll « (a| llxll

a is an arbitrary constant.

3). llx+yll £ IWI • ltvll

A complete normed space is said to be a Banach space.

Linear Operator

Let D and R be two Banach spaces, whose elements are denoted respectively as u and y. Let a rule be given according to which to each u in some set U c D there is assigned some element y in the space R. Then an operator y • Mu with range of values in R can be defined on the set U. An operator M is said to be linear if the equality

$$M(\alpha_1 u_1+\alpha_2 u_2)=\alpha_1 Mu_1+\alpha_2 Mu_2 \qquad (40)$$

is satisfied for any two elements $u_v u_2$ € 1/. a, and o^ are arbitrary real numbers. An operator M is considered when it does not possess the above property.

Operator Gain

Let us consider a nonlinear operator M which transforms the input subspace D to the output subspace R

$$y=Mu \qquad u \in D; \qquad y \in R \qquad (41)$$

Define the.gain of M, denoted by o(M), be

$$g(M) = \sup \frac{\|(Mu)\|}{\|u\|} \qquad (42)$$

where the supremum is taken over all u € D.

Zames' (1966) **small** gain theorem:

If the open loop gain is less than one, then the closed loop is bounded.

For the IMC structure, It is equivalent to (Economou and Morari, 1986)

$$g[(P_d-M)C] \leq g(C)g(P_d-M) < 1 \qquad (43)$$

P_d denotes the plant operator with the effect of disturbance. When $P_d = M$, the perfect model case, IMC controller C is open loop stable, and then the inequality is trivially satisfied. When the process is poorly modeled, which means $g(P_d * M)$ is large, the control gain g(C) has to be small. Usually, the perfect controller $C = M^r$ cannot be used because the condition of (43) may not be satisfied. In order to satisfy the stability condition, an adjustable filter F is introduced such that $C = M^rF$. Then the stability condition of (43) becomes:

$$g(M^rF)g(P_d-M) \leq g(F)g(M^r)g(P_d-M) < 1 \qquad (44)$$

Notation:

u — the inputs determined by an IMC controller without the constraints on u
C — the IMC perfect controller , $C = M^r$
u_r — the inputs determined by an IMC controller with the constraints on u
C_r — IMC controller with constraints on u

If the constrained SQP controller is used, the stability analysis of the closed bop system is straightforward. Without loss of generality let us assume u is scaled and constrained as follows:

$$-\delta \le u_r \le \delta \tag{45}$$

Then the constrainted controller maps the error e to the constrained control variable u_r.

$$u_r = C_r e \tag{46}$$

where e is defined as $e = y - y^*$

We assume the process is open loop stable, i.e. any bounded input gives a bounded and continuous output. Then since all inputs are bounded, the closed loop process with the constrained controller will remain input-output stable. Using Zames small gain theory, one can verify this as follows.

To simplify the proof we assume the plant operator P_d maps zero into itself, i.e.

$$y = P_d u = 0 \; ; \qquad for \; u = 0 \tag{47}$$

Consider a scaled and constrained QP so that

$$\begin{aligned} \underset{\Delta u}{Min} \quad & C^T \Delta u^s + \frac{1}{2}(\Delta u^s)^T H \Delta u^s \\ s.t \quad & -\delta \le u_r \le \delta \end{aligned} \tag{48}$$

where δ is greater or equal to 0. We can partition u_r into components at bounds u_d and unconstrained components, u_u, with $\|u_b\|_\infty = \delta$; $\|u_u\|_\infty < \delta$. Then controller gain with constraints becomes:

$$g(C_r) = sup \; \frac{\|(C_r e)\|}{\|e\|} = sup \; \frac{\|u_r\|}{\|e\|} \tag{49}$$

The gain of the IMC controller is

$$g(C) = sup \; \frac{\|(Ce)\|}{\|e\|} = sup \; \frac{\|u\|}{\|e\|} \tag{50}$$

Combining Eq.(49) and Eq.(50), we have

$$g(C_r) = \frac{\|u_r\|}{\|u\|} g(C) \le \frac{\delta}{\|u\|} g(C) \tag{51}$$

To express the sufficient condition of closed loop stability, the inequality (51) can be written as follows.

$$8(C_r)g(P_rM) \quad £ \quad \pm\hat{}Qg(P_rAf) \quad < \quad 1 \qquad (52)$$

To satisfy condition (52) consider two cases:

a). If Ml - 0, the plant operator maps zero into itself. The output y is zero and the controller is stable.

b). UNI * 0 and by making S small enough |K|| >> 6 and the sufficient condition (52) can be made to hold.

Comparing stability condition (52) with (44), we can see that putting constraints on u has a similar function as the filter in the nonlinear IMC structure. Both of them make the process more robust.

8. CONCLUSION

An extension of the nonlinear IMC design procedure to a special form of successive quadratic programming strategy to handle process constraints was presented. This strategy can efficiently handle both soft and hard constraints. Simulation results for two nonlinear reactor control problems show the effectiveness of this strategy. Finally, since all of the control variables can be bounded, the stability of the constrained controller is guaranteed as long as the process is open loop stable. This can be proved by the small gain theory of Zames.

The algorithm developed in this work is a single step method, which means that the algorithm only predicts one step ahead. It assumes that the process will reach the setpoint at the end of the first step. If a process to be controlled possesses time delay that is longer than one sampling time interval, or if the time delay associated with different pairs of inputs and outputs is not the same, the single step algorithm is not capable of handling it. Moreover, H a batch process needs to be controlled, an optimal control profile in the entire time horizon rather than a single step should be calculated. Therefore, a multistep predictive algorithm needs to be developed. In addition, even V a process does not possess time delay, the controller performance may also benefit from the long time prediction.

In addition, most chemical processes are difficult to model precisely since there unavoidably exist parameter and disturbance uncertainties. The structure of the model can usually be derived from a mathematical description of fundamental physicochemical phenomena taking place in the process. If on-Ine computer control is used, the process measurements can be used to estimate the uncertain parameters and disturbances. Then the updated model can be used to calculate the optimal control profile in future time horizon. A reliable algorithm of parameter estimation needs to be developed in the future.

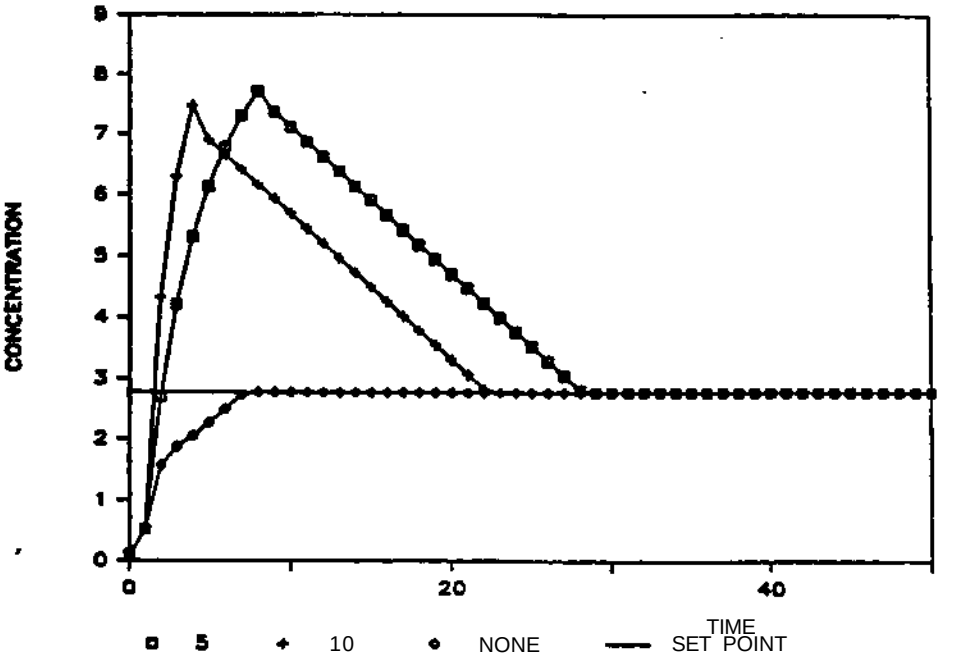
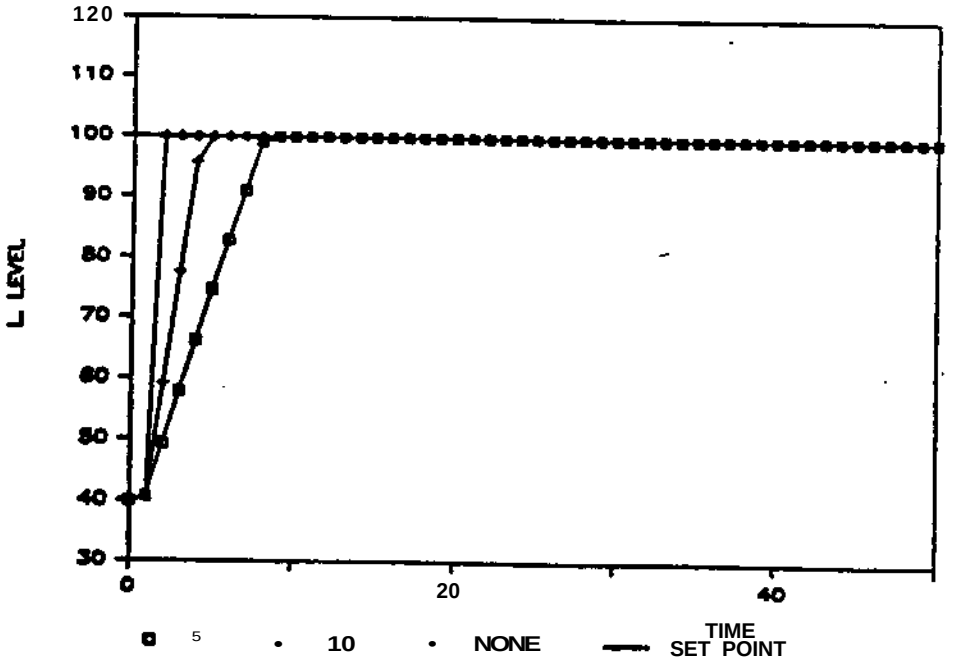


Figure /: Concentration vs. time



ngure//: Liquid level vs. time

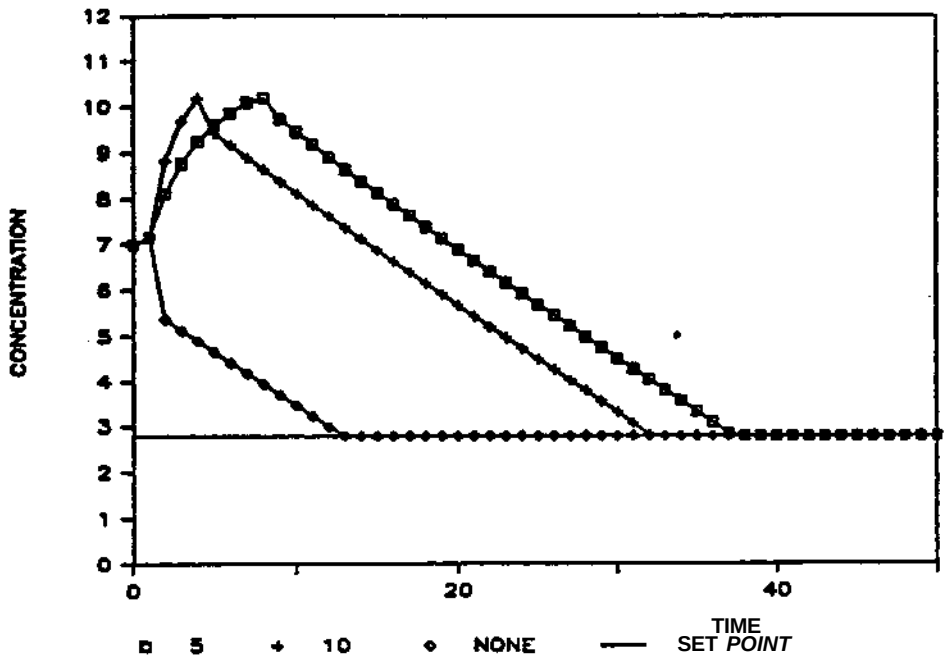


Figure ///: Concentration vs. time

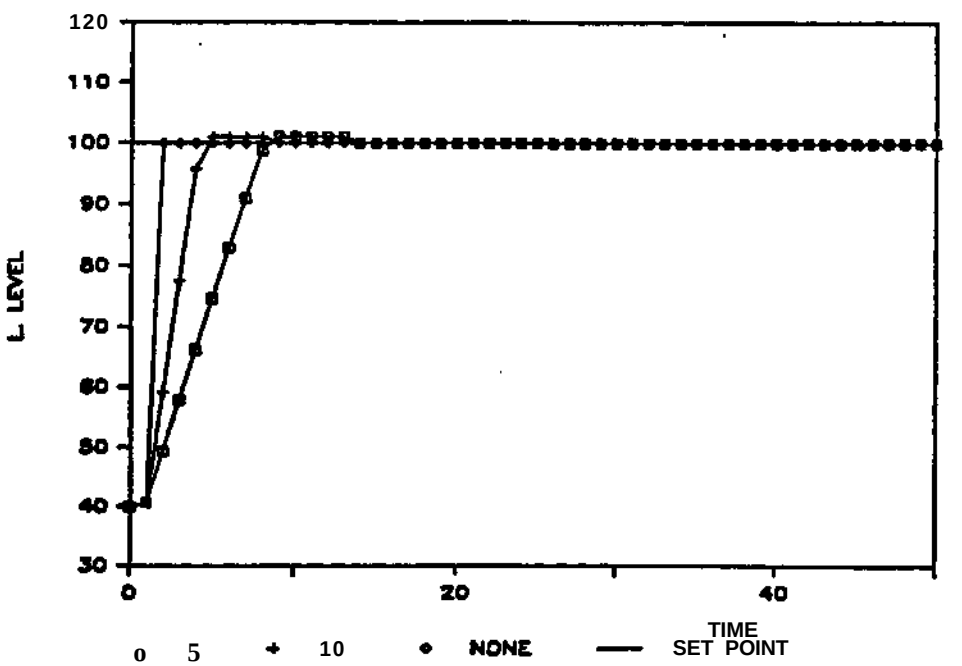


Figure *IV:* Uquid **level** vs. time

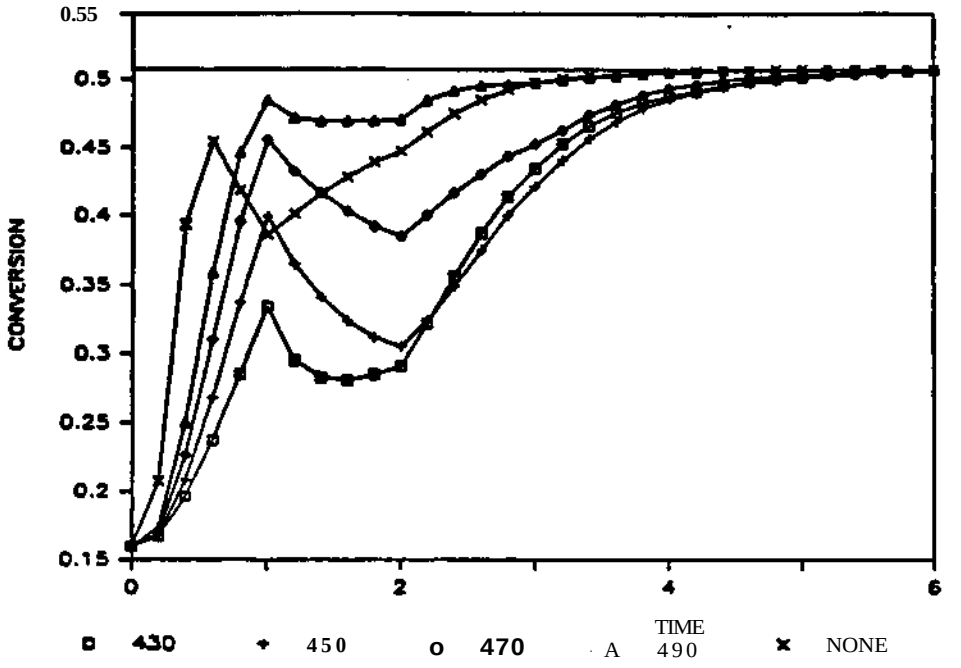


Figure *V:* Conversion vs. time (without state constraints)

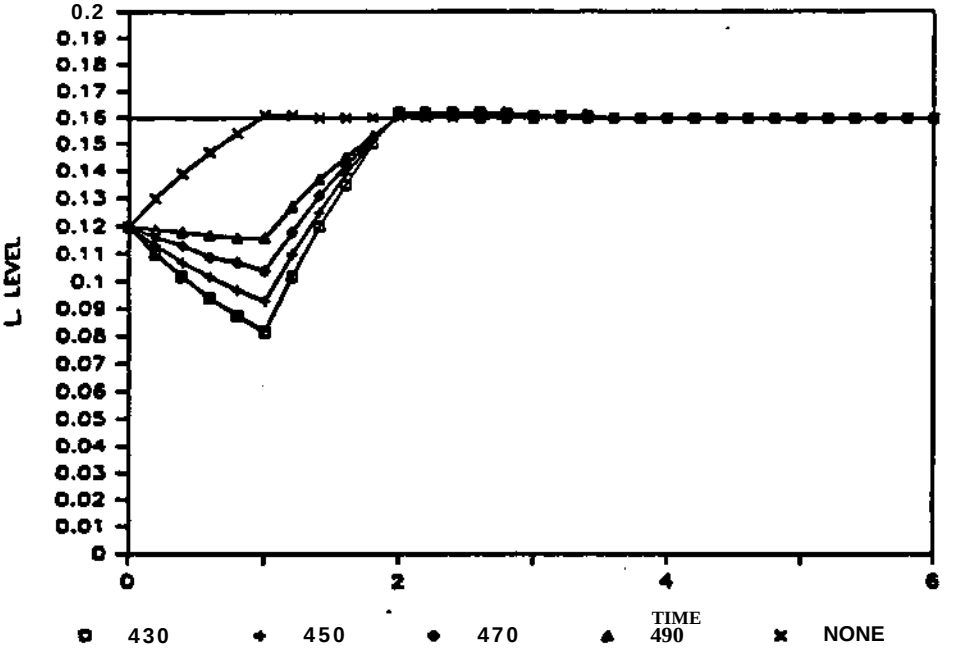


Figure *Vk* Uquid level vs. time(without state constraints)

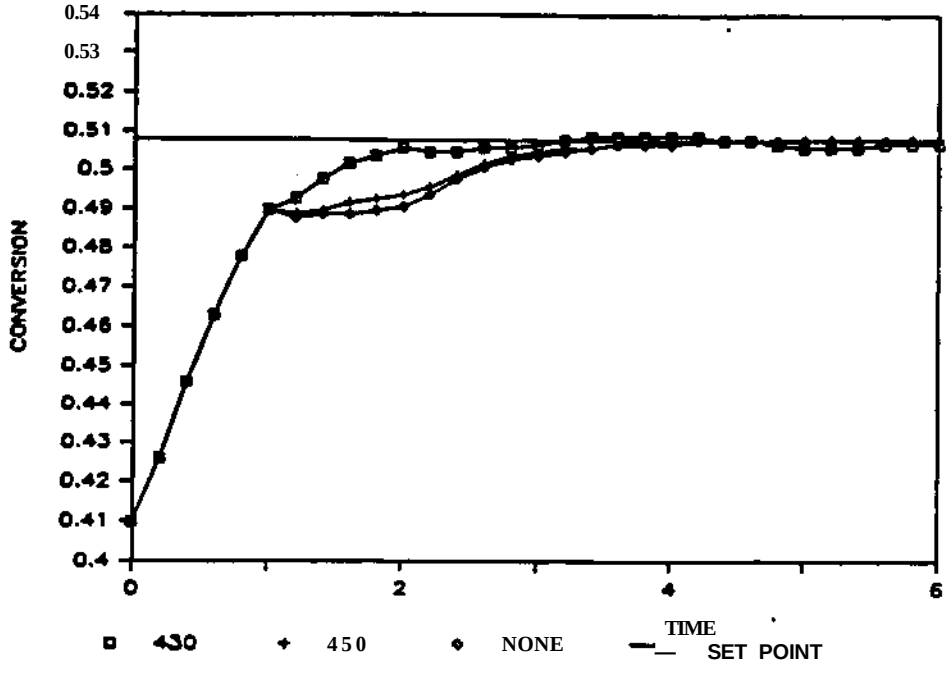


Figure *VII:* Conversion vs. time (without state constraints)

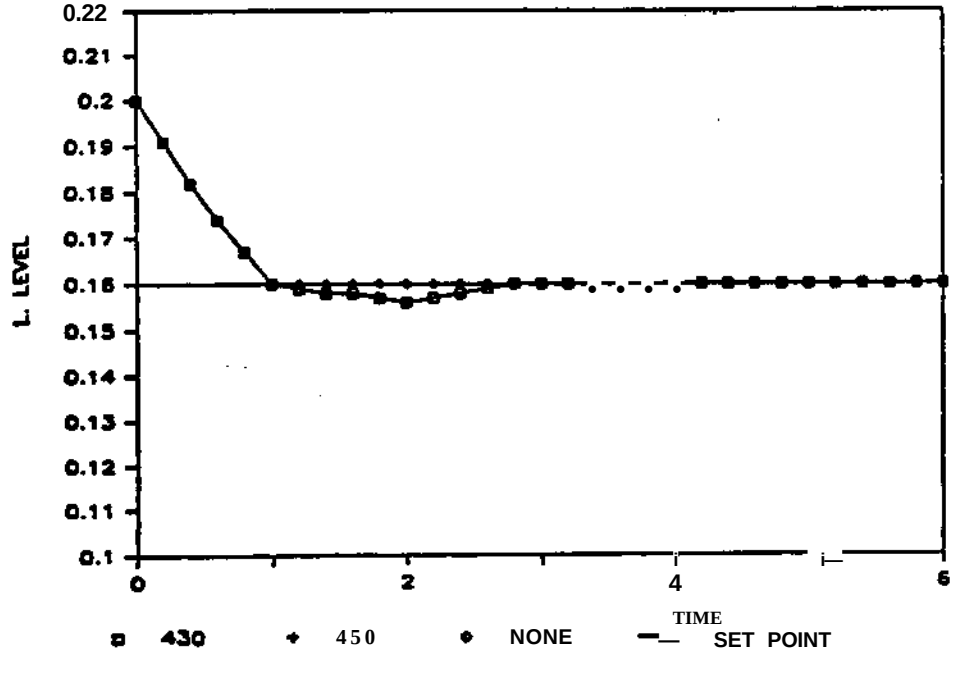


Figure *Vllh* Liquid level vs. time(without state constraints)

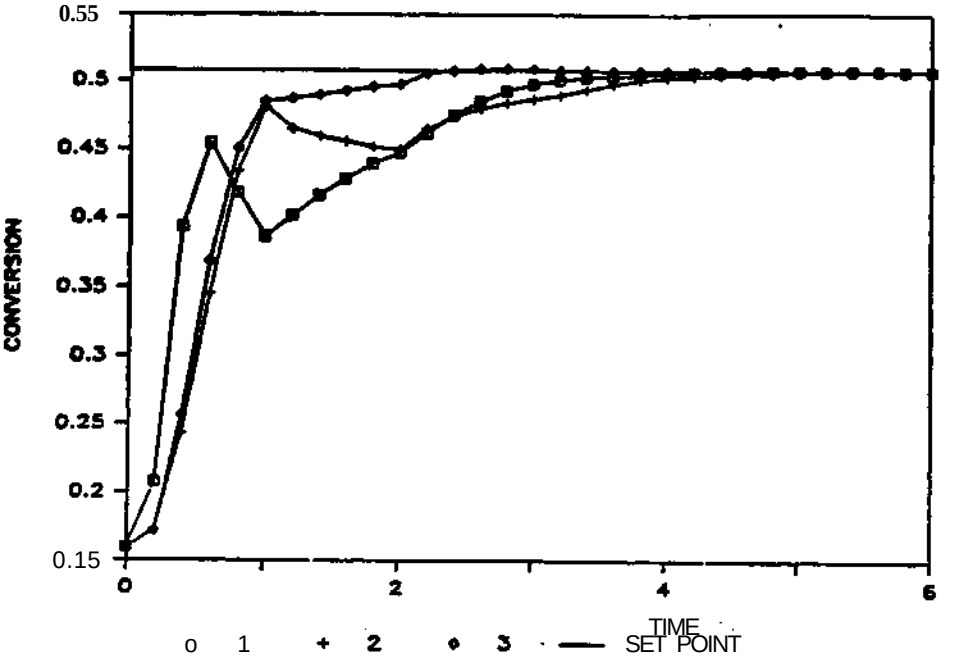


Figure *IX:* Conversion vs. time (with & without state constraints)

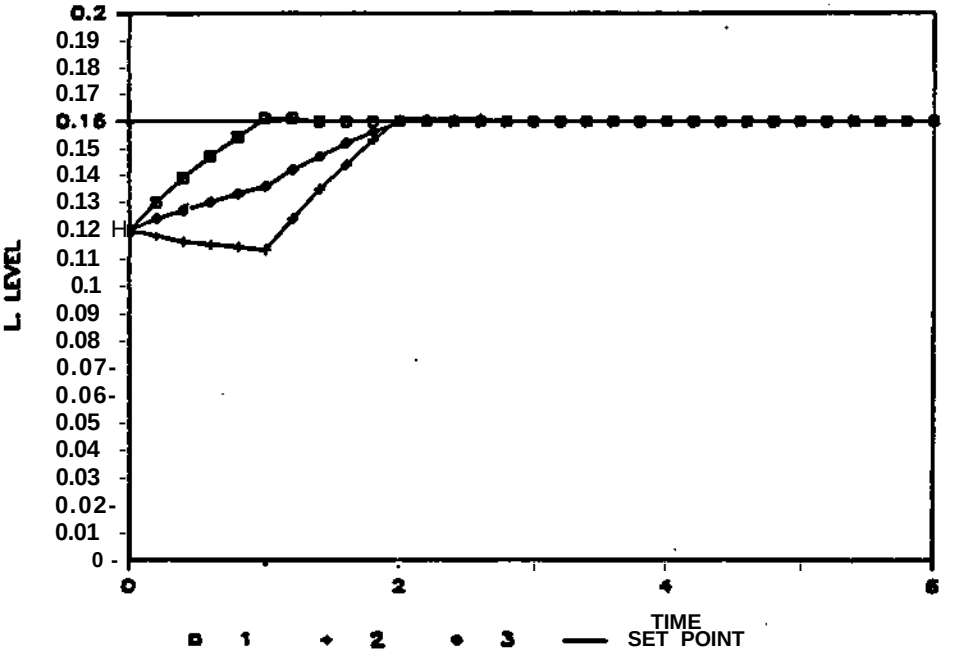


Figure *X:* Liquid level vs. time(with & without state constraints)

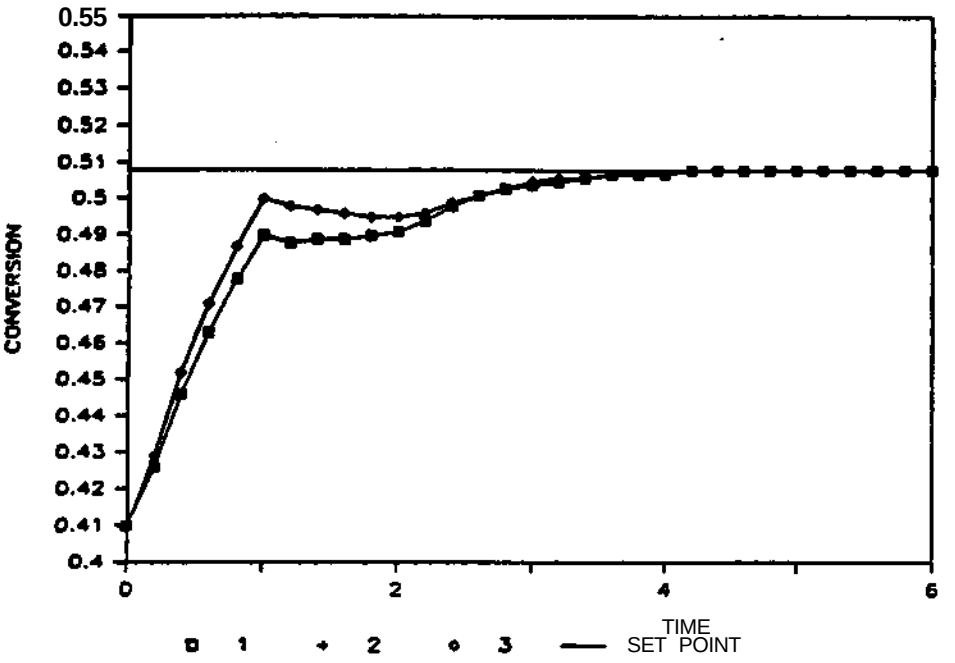


Figure X: Conversion vs. time (with & without state constraints)

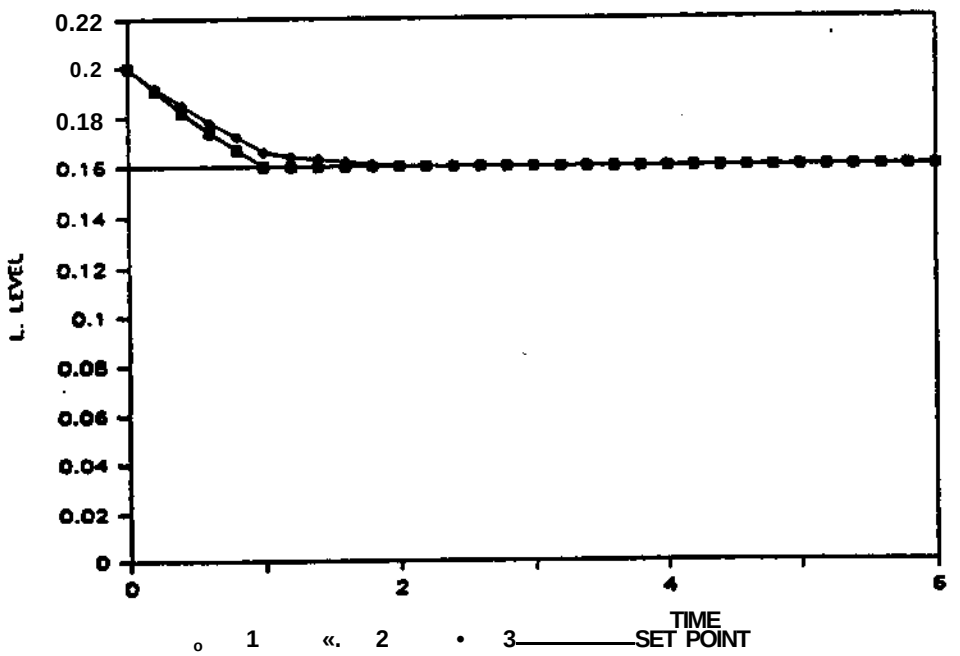


Figure *XII:* Liquid level vs. time(with & without state oonstraints)

APPENDIX A

Referring to Eq.(12), let

$$\mathbf{T} = -C^{s+1}\Gamma^{s} \tag{i.a}$$

$$\Omega = C^{s+1}\Phi^{s+1}(x^{s}-\chi^{s}) + (y^{s}-y^{s+1}) \tag{i.b}$$

Now Eq.(12) becomes

$$\Omega + \mathbf{T}\Delta u = 0 \tag{ii}$$

Equation (ii) is equivalent to the following problem

$$\underset{\Delta u}{Min}\ \Omega^{T}\mathbf{T}\Delta u+0.5\Delta u^{T}\mathbf{T}^{T}\mathbf{T}\Delta u \tag{iii}$$

Proof: Let

$$\begin{aligned} F &= 0.5(\Omega+\mathbf{T}\Delta u)^{T}(\Omega+\mathbf{T}\Delta u) \\ &= 0.5(\Omega^{T}\Omega+\Delta u^{T}\mathbf{T}^{T}\Omega+\Omega^{T}\mathbf{T}\Delta u+\Delta u^{T}\mathbf{T}^{T}\mathbf{T}\Delta u) \\ &= 0.5(2.0\Omega^{T}\mathbf{T}\Delta u+\Delta u^{T}\mathbf{T}^{T}\mathbf{T}\Delta u+\Omega^{T}\Omega) \end{aligned} \tag{iv}$$

When the optimal condition is satisfied, we have

$$\frac{\partial F}{\partial \Delta u} = 0.5(2.0\ \Omega^{T}\mathbf{T} + 2.0\ \Delta u^{T}\mathbf{T}^{T}\mathbf{T}) = 0 \tag{v}$$

Then we have

$$(\Omega^{T}+\Delta u^{T}\mathbf{T}^{T})\mathbf{T} = 0 \tag{vi}$$

which is equivalent to the following

$$\Omega + \mathbf{T}\Delta u = 0 \tag{vii}$$

Then Eq(i4) and (15) become

$$C^T \text{ « } G^T T \qquad \{viiLa)$$

$$H \text{ « } T^T T \qquad (yûi.b)$$

Here T needs ID be square and nonsingular or must have

$$dim(y) * dim(u) \qquad (ix)$$

APPENDIX B

When differentiating Eq(20)in respect to t we have

$$\frac{\partial K_1^{s+1}}{\partial t} = \frac{\partial}{di}\frac{\partial x_{n+1}}{Bu}$$

$$= \frac{\partial}{du}\frac{\partial x_{n+1}}{dt}$$

$$= 2.0\sum_{i=1}^{n}\{num\ (0.\ x^{*"\wedge})\} - \min(0.\ x\wedge\langle t)\}\frac{\partial x_i}{\partial u}\Big|_{u=u_{j-1}}^{s+1}$$

$$K_1(t') = 0$$

Similarly, **the** differential of Kf^{+1} can be written

$$\frac{\partial K_i^{s+1}}{dt} = \frac{\partial}{dt}\frac{\partial x_{n+i}}{du}$$

$$\bullet\ 2.0\{\min\ (0,\ x\hat{}O\text{-}\dot{x}))\} - min(0,\ \ddot{x}_i'' - x/(t))\}\frac{dx_i}{\partial u}\Big|_{u=u_{j-1}}^{s+1}$$

$$Kff) - 0.$$

APPENDIX C

The following nonlinear differential-algebraic equations model the dynamics of the second example. They are derived from differential mass and energy balances. The meaning of variables can be found from the nomenclature at the end of this appendix. The values of various parameters can be found in Table 3.

$$\frac{d(VA_0)}{dt} = A_iF_i - A_oF_o - V(K_1A_o - K_2B_o)$$

$$\frac{d(VB_0)}{dt} = B_iF_i - BJF. + V\{K_XA_O - K_2B_o)$$

$$\frac{d(VT_0)}{dt} = T_iF_i - T_oF_o + DH\times V(K_1A_o - K_2B_o)$$

$$A_c\frac{dh}{dt} = F_i - F_o$$

$$K_i = C_i\exp\left(-\frac{E_i}{RT_o}\right) \qquad \text{I - 1. 2}$$

$$A_{(} \cdot Bi \ll A_0 + B_e \ll 1.0$$

$$DH \ll -$$

V « v!eJi

We define:

X, - B_o £/, - F;
X_2 - r_0 $t/_2$ - ^
X_3 « A

NOMENCLATURE

^	the cross area of the tank
Aj	the concentration of A in inflow
AQ	the concentration of A in outflow
Bj	the concentration of B in inflow
B_o	the concentration of B in outflow
C_p	heat capacity of the liquid
Cj	Arrhenius's constant (i • 1.2)
Ej	activation energy (I • 1,2)
h	the height of the liquid level in trie tank
Kj	reaction constant (i • 1,2)
Fj	Inlet flow rate
F_o	outlet flow rate
H_B.	heat of reaction

R universal gas constant
V volume of the tank
P density of the liquid in the tank

PARAMETER	PARAMETER	SET POINT
$K_1 = 1.0$	C_{Bi}-24.9	y,*-2.787
K_2«1.0	$C_{B2} = 0.10$	y_2*-100.0

Table 1: Parameter values of example 1.

SET(1)	SET(2)
x_{10}-0.10	x_{10} - 7.00
*z> - 40.0	Xao - 40.0

Table 2: Initial conditions of example 1.

PARAMETER	PARAMETER	SET POINT
Aj-LOmol/l	E,-IC^cal/mol	y/ • ,508mol/l
Ag-6.25m^2	E_2-1.5x10^4cal/mol	y_2*«.16m
B, *m* 0.0mol/l	H_R - 5000cal/mol	
$C_1 = 5x10^3$/s	R-1.987 cal/l	
C_2-1x10^6/$	p-1.0kg/l	
C_p-1000cal/mol		

Table 3: Parameter values of example 2.

SET(1)	SET(2)
x,-0.16	X, . 0.41
X_2-351.	x_2-503.
X3-0.12	Xg-0.20
u,-0.866	u,«1.12
u_2-352.	U_2-5O4.

Table 4: Initial conditions of example 2.

Figure *IX &X*	x_1^l	$x_1^{w\,u}$	X_2	x_2
Curve 1.	/	/	/	/
Curve 2.	.16	.51	300.	550.
Curve 3.	.40	.51	300.	550.
Figure *XI & XII*	x_1^l	x_1	«t'	X_2
Curve 1.	/	/	/	/
Curve 2.	.41	.51	300.	550.
Curve 3.	.49	51	300.	550.

Note: no constraints on u_v u_2, and x_3

Table 5: Process constraints **of** example **2.**

References

1. Cutler, C.R., and B.L Remaker, -Dynamic Matrix Controt-A Computer Control Algorithm",, AIChE National Mtg., Houston.TX., 1979.

2. Eoonomou, C.G., and M. Morari, -Newton Control Laws For Nonlinear Controller Design",, IEEE Conference On Decision and Control, Fort Lauderdate, FL, December 1985.

3. Eoonomou, C.G., and M. Morari, "Internal Model Control. 5. Extension to Nonlinear systems'*, *Ind. Eng. Chem. Process Des.Dev.yol* 251986, pp. 403.

4. Garcia, G.E., M. Morari, -Internal Model Control. 1. A unifying Review and some New Results*', *Ind. Eng. Chem. Process Des.* Oev.,Vol. 211982. pp. 308.

5. Garcia, G.E., M.Morari, "Internal Model Control. 2. Design Procedure for Multivariable Systems", *Ind. Eng. chem. Process Des.* 0ev.,Vol. 241985a, pp. 472.

6. Garcia, G.E., and M. Morari, "Internal Model Control. 3. Multivariable Control Law Computation and Tuning Guidelines'*, *Ind. Eng. Chem. Process Des. Dev.yol* 241985b, pp. 485.

7. Jang, S.S, B. Joseph, and H. Mukal, "On-Line Optimization of Constrained Multivariable Chemical Processes", *Journal of the American Institute of Chemical Engineers,* Vol. 33No. 1 1987, pp. 26.

8. Morari, M, "Robust Stability of System With Integral Control",, Proc. 22nd IEEE Conference on Decision and Control, San Antonio, Tex, December 1983.

9. Kolmogorov, A.N., and S.V. Fomin, *Elements of the Theory of Functions and Fucntional Analysis,* Graylock Press., Rochester, 1957.

10. Prett, D.M., and R.D. Gillette, "Optimization and Constrained Multivariable Control of a Catalytic Cracking Unit",, AIChE National Mtg., Houston TX., 1979.

11. Rail, L.B., *Computational Solution of Nonlinear Operator Equations,* John, Wiley & Sons, Inc., New York, 1969.

12. Sargent .R.W.H., and G.R. Sullivan, The development of an Efficient Optimal Control Package",, 1977.

13. Matsuura.T and M. Kato, "Concentration Stability of the Isothermal Reactor", *Chemical Engineering* Science,Vol. 221967, pp. 171-184.

14. Zames, G., "On the Input-Output Stability of Time-Varying Nonlinear Feedback Systems. Part I: Conditions Derived Using Concepts of Loop Gain, Conicity, and Positivity", *IEEE Trans, Autom. Controt.Vol* AC-11 1966, pp. 228.