

Suboptimal Control Strategies Applied to Nonlinear Batch Reactor with Constraints

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Abstract— This work studies the control of a batch reactor for the production of penicillin. For this purpose, it is proposed an initial design of two control strategies which result simple for their implementation. These strategies are developed inside the optimal control framework applied to non-linear systems. The first one, based on finite horizon optimal control theory, minimizes a quadratic cost derived from the linear approximation of the costates from the Hamiltonian associated to the system. The resulting suboptimal control is a feedback proportional law.

The second strategy use linear matrix inequalities (LMIs) for incorporating restrictions which were not considered in the value function of the optimal control problem. The new restrictions are boundaries for the states and the manipulated variable. However, the design of this strategy is restricted to an infinite horizon optimal control problem and, the proportional-integral (PI) modes resulting have constant gains. Finally, the goodness of the two proposed strategies is showed through numerical simulations.

Keywords— nonlinear processes, optimal control, linear matrix inequalities, input and state constraints.

1. INTRODUCTION

The efficient design of simple controllers to implement in an industrial process has been one of the biggest challenges in control engineering.

The proportional-integral-derivative (PID) controller, because of its simplicity, remains the most widely used in the industry. However, other control techniques have made inroad in the industry, as the model predictive control (MPC), in order to improve the performance of the controlled variable. In spite of many advantages of MPC, some disadvantages as, the high computational cost, the necessity to dispose control engineers highly specialized in plant, and the not good MPC performance with processes with fast

dynamic, i.e. with short sampling time ([12]), among other, had made of MPC a not very popular technique in the industry.

The optimal control paradigm based on the Hamiltonian formalism gives answer to many industrial control requirements. When the problem is regular, there exists an explicit form for the control strategy. For linear systems, it has shown that this control strategy is in fact a proportional feedback law $u(t) = Kx(t)$ (see [13] and [5] for details) with K evaluated from the solution of algebraic Riccati equation (ARE) for infinite horizon problem or from differential Riccati equation (DRE) for finite horizon problem.

In general, for nonlinear systems, the resulting control strategy is not a feedback control law such as linear case, in contrast, is an open-loop strategy relies depending on non-physical costate of Hamiltonian system associated to the process (see [6], [7], for instance). However, with adequate mathematical manipulation, assumptions on nonlinear costates and, approximations on nonlinear dynamics, this control strategy could become in a feedback form. Because of this, the optimality is lost but it is possible to design robust controller with easy implementation, which also be able meet certain performance criteria and satisfy constraints.

This article proposes an initial design for suboptimal industrial controllers. The first strategy is based on nonlinear optimal control with finite horizon time, where the costates of the system ($\lambda(t)$) are approximated to a linear form.

The Hamiltonian formalism incorporates some restrictions and, these are expressed in the functional cost of the problem. The considered restrictions are boundaries in the states and the control law inside the optimization horizon as is detailed in [9]). In addition, it is possible to impose restrictions at the end of states. Other kind of restrictions as maximum or minimum values allowed, both for the states and the control action, are not considered.

The utilization of the LMI allows adding boundaries as restrictions to the optimal control problem, as is shown by [10]. But, despite considering those re-

restrictions, the disadvantage of this formulation is that forces the design to be developed as infinite horizon control problem, where the resulting controller gain (K) is constant during the operation of the process.

The paper has the following structure: After de Introduction, in Section 2, a brief description of the 4-dimensional chemical process model and its constraints are presented. Then, in Section 3 the optimal nonlinear control problem is introduced and the explicit form of the control strategy is shown. Section 4 develops an strategy to generate a suboptimal control law in finite horizon. In Section 5 the second strategy based on infinite horizon optimal linear control with LMIs is proposed. For this last case, constraints are included in the optimization problem. After, the control strategies are reviewed by means of numerical simulation. Finally, in Section 6 the conclusions and perspectives are presented.

2. DESCRIPTION OF MODEL PROCESS

In this section a fed-batch fermentor for penicillin production like a case study is considered (see [8] and [1]). The nonlinear process model is given by the following equations:

$$\begin{aligned}\dot{x}_1(t) &= h_1 x_1 - u \left(\frac{x_1}{500 x_4} \right), \quad x_1(0) = 1.5, \\ \dot{x}_2(t) &= h_2 x_1 - 0.01 x_2 - u \left(\frac{x_2}{500 x_4} \right), \quad x_2(0) = 0, \\ \dot{x}_3(t) &= -\frac{h_1 x_1}{0.47} - x_1 \left(\frac{0.029 x_3}{0.0001 + x_3} \right) - \dots \quad (1) \\ &\quad h_2 \frac{x_1}{1.2} + \frac{u}{x_4} \left(1 - \frac{x_3}{500} \right), \quad x_3(0) = 0, \\ \dot{x}_4(t) &= \frac{u}{500}, \quad x_4(0) = 7.\end{aligned}$$

$$\begin{aligned}h_1 &= 0.11 \left(\frac{x_3}{0.006 x_1 + x_3} \right), \\ h_2 &= 0.0055 \left(\frac{x_3}{0.0001 + x_3(1 + 10 x_3)} \right).\end{aligned} \quad (2)$$

$$y = Cx = x_2. \quad (3)$$

In this model x_1 , x_2 , x_3 and x_4 are the biomass, penicillin concentration, substrate concentrations (g/L), and the reactor volume (L) respectively. The output system is the penicillin concentration, i.e. $C = (0 \ 1 \ 0 \ 0)$. The objectives of the optimization problem are:

(i) To reach in 132 hours ($t_f = 132$ is the time horizon) a final penicillin concentration of 8 g/L, i.e. the desired output is $\bar{y} = \bar{x}_2 = 8$. All numerical values like t_f and \bar{x}_2 were extracted from [1].

(ii) In addition the nonlinear model includes several constraints, which must be satisfied during the operation process. These are upper and lower bounds in the state variables:

$$\begin{aligned}0 &\leq x_1 \leq 40 \\ 0 &\leq x_3 \leq 25 \\ 0 &\leq x_4 \leq 10\end{aligned} \quad (4)$$

and an upper and lower bounds on the only control variable (feed rate of substrate),

$$0 \leq u \leq 50. \quad (5)$$

3. NONLINEAR OPTIMAL CONTROL SETUP

Consider the initialized autonomous nonlinear control affine system

$$\dot{x} = f(x) + g(x)u, \quad x(0) = x_0 \quad (6)$$

with a cost general functional written as

$$\mathcal{J}(T, 0, x_0, u(\cdot)) = \int_0^T L(x(\tau), u(\tau)) d\tau + x'(T) S x(T), \quad (7)$$

where a quadratic Lagrangian L and symmetric constant coefficient matrices are given by

$$L(x, u) = x' Q x + R u^2, \quad (8)$$

$$Q, S \geq 0, \quad R > 0, \quad T < \infty. \quad (9)$$

The value function \mathcal{V} can always be defined for such problem, namely

$$\mathcal{V}(t, x) \triangleq \inf_{u(\cdot)} \mathcal{J}(T, t, x, u(\cdot)), \quad t \in [0, T] \quad (10)$$

and, if the problem has a unique solution, then this solution is called the optimal control strategy u^* ,

$$u^*(\cdot) \triangleq \arg \inf_{u(\cdot)} \mathcal{J}(T, t, x, u(\cdot)). \quad (11)$$

The optimal control solution for this problem can be expressed as

$$u^*(t) = -\frac{1}{2} R^{-1} g'(t) \lambda(t). \quad (12)$$

where λ is called the costate and $\lambda \in \mathbb{R}^n$, (x, λ) ranging in $2n$ -dimensional phase-space. The Hamiltonian \mathcal{H} of such problem is defined as,

$$\mathcal{H}(x, \lambda, u) \triangleq L(x, u) + \lambda' f(x, u). \quad (13)$$

Since \mathcal{H} is assumed regular, then there exists a unique H -optimal control u^0 , namely

$$u^0(x, \lambda) \triangleq \arg \min_u \mathcal{H}(x, \lambda, u), \quad (14)$$

and the derivative of \mathcal{H} with respect to u vanishes at $(x, \lambda, u^0(x, \lambda))$.

A regular Hamiltonian explicitly means that the function $u^0(x, \lambda)$ is known (not only its existence but also its explicit form) and that it is sufficiently smooth on its variables. The control-Hamiltonian,

$$\mathcal{H}^0(x, \lambda) \triangleq \mathcal{H}(x, \lambda, u^0(x, \lambda)), \quad (15)$$

gives rise to the Hamiltonian canonical equations (HCEs) ([13])

$$\dot{x} = \left(\frac{\partial \mathcal{H}^0}{\partial \lambda} \right)'; \quad x(0) = x_0, \quad (16)$$

$$\dot{\lambda} = - \left(\frac{\partial \mathcal{H}^0}{\partial x} \right)'; \quad \lambda(T) = 2Sx(T), \quad (17)$$

and then the optimal costate variable λ^* results in

$$\lambda^*(t) = \left[\frac{\partial \mathcal{V}}{\partial x} \right]'(t, x^*(t)). \quad (18)$$

4. FINITE-HORIZON SUBOPTIMAL CONTROL STRATEGY

In the present Section, the first control strategy is devised. In order to convert the control expressed in (12) to a linear feedback law, the following assumptions are made:

(i) Costates expressed in Eq. (18) are linear, i.e.

$$\lambda \triangleq 2P(t)(x(t) - \bar{x}), \quad (19)$$

where \bar{x} is the equilibrium state or the desired state. In the regulation problem \bar{x} takes the 0 value. On the contrary, in the change of set-point problem, \bar{x} may be different from zero.

(ii) Only when the control law is calculated, the system considered will be a linear approximation of system mentioned in (1)-(3) that is,

$$f(x) \approx A(t)x(t); \quad g(x) \approx B(t), \quad (20)$$

$$\dot{x} \approx A(t)x(t) + B(t)\tilde{u}(t), \quad x(0) = x_0, \quad (21)$$

where A and B are the resulting matrices of a standard linearization of the nonlinear system around a given trajectory.

Therefore, the optimal control law expressed in Eq. (12) is turned to a suboptimal control law in feedback form ¹

$$u \approx \tilde{u} = -R^{-1}B'(t)P(t)(x(t) - \bar{x}) \quad (22)$$

with $P(t)$ a solution of the differential Riccati equation (DRE):

$$\dot{P}(t) = PB(t)R^{-1}B'(t)P - PA(t) - A(t)'P - Q; \quad P(T) = S \quad (23)$$

¹Notice that, in this article, u is the manipulated variable corresponding to nonlinear problem and \tilde{u} is the implemented linear control law.

where $Q = I_{4 \times 4}$, $R = 3$ and $S = sI_{4 \times 4}$ ($s = 20$ for numerical evaluations).

The main difficult here is to solve the Eq. (23). This could be solved:

(i) Off-line with a backward integration with $t_f = 132$ and $s = 20$.

(ii) Transforming the boundary-value into a final-value problem related to the differential Riccati equation (DRE) as is shown in [13]. The disadvantages of this approach are that the linearization must be done around a fixed point, for instance $t = 0$, and that this method would be solved only for a pair (t_f, s) .

(iii) Through the recently discovered partial differential equations (PDEs) for the initial coestates and final states described by [4] for nonlinear systems and [5] for linear systems. Here, this implementation is adopted since it allows keeping in memory $P(t)$ solutions for a range of t_f and s . However, the standard linearization must be made around a fixed point too. For the case study, A and B read

$$A = \begin{pmatrix} 0 & 0 & 18.3 & 0 \\ 0 & -0.01 & 82.5 & 0 \\ 0 & 0 & -542.7 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} -0.0004 \\ 0 \\ \frac{1}{500} \\ \frac{1}{500} \end{pmatrix}. \quad (24)$$

The control law (22) was applied to the system (1) and in Fig. 1 the evolution of the states for the finite horizon optimization and control problem are depicted. The process has a typical response (see [1]), but there exists a final error between the desired state $\bar{x}_2 = 8$ and the real state reached, $x_2 = 6.47$ at the end of the operation time of the batch reactor. In other words, this final error is presented due to the implemented proportional feedback law. The others states are close to their targets (which are detailed in [1]).

As it is known, the principal problem with the proportional mode is the final error (i.e., when there exist an error between the set-point or target and the real states at the end, see [3]). A common practice for reducing the final error is to include an integral mode associated to the error between the controlled variable and the set-point ($\bar{x} - x$), and to redefine an extended control problem including a fictitious state. This point will be studied in the next section.

4.1. A Suboptimal PI Controller

Following the classical control theory ([11]), to reduce the error in the output at the end of the operation, a new fictitious state ξ is added to a linear system expressed in (20) (but keeping the linearization around a fixed point) and, an augmented linear system can be defined as,

$$\begin{pmatrix} \dot{x} \\ \dot{\xi} \end{pmatrix} = \begin{pmatrix} A & 0 \\ -C & 0 \end{pmatrix} \begin{pmatrix} x(t) \\ \xi(t) \end{pmatrix} + \begin{pmatrix} B \\ 0 \end{pmatrix} \tilde{u}(t) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} r(t), \quad (25)$$

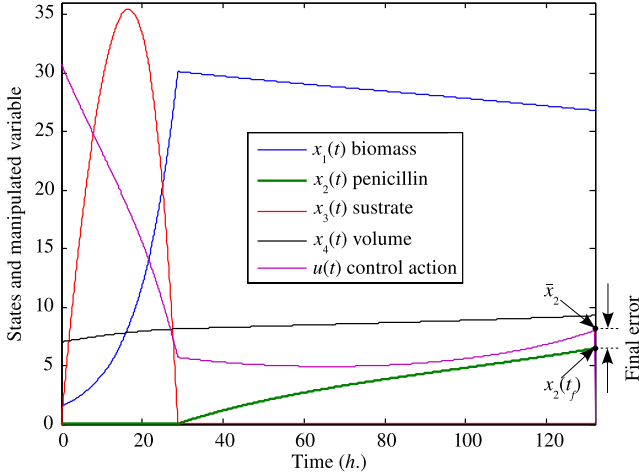


Figure 1: States and control trajectories for finite horizon set-up. $T = 132$ and $s = 20$

$$\dot{\xi} = r(t) - y(t) = r(t) - Cx(t). \quad (26)$$

For this system and holding the cost function (7), the resulting PI control law is

$$\tilde{u} = -\hat{K}\tilde{x} = -k_p(t)x(t) + k_i(t)\xi(t) \quad (27)$$

where $\hat{K} = R^{-1}\tilde{B}'\tilde{P}(t) = [K(t) \ k_i(t)]$, $K(t) = k_p(t)$, $\tilde{x} = \begin{pmatrix} x(t) - \bar{x} \\ \xi(t) \end{pmatrix}$, with states $x(t)$ coming from the real process and $\tilde{P}(t)$ a solution of the Eq. (23) with $Q = 2.2I_{5 \times 5}$, $R = 0.21$, $s = 0.1$ and

$$\hat{A} = \begin{pmatrix} A & 0 \\ -C & 0 \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} B \\ 0 \end{pmatrix}.$$

Notice that, the PI control law has time variant modes as a result of solving a finite-horizon optimal control problem.

Figure 2 shows that the control system severely reduce the final error. The new control law is calculated through Eq. (27) and, the state value x_2 at the end of the operation is 8.02, that is approximately 0.25% over the target, which is tolerable. However, state x_1 is almost in its saturation level and state x_4 is out of its upper bound.

5. INFINITE-HORIZON SUBOPTIMAL CONTROL STRATEGY

At this point, the main challenge is to design a controller such that an acceptable final error can be reached, and the constraints imposed to the batch reactor can be satisfied. Thus, because of the acceptable results obtained in previous section, a PI controller is designed by solving the ARE (as it is shown in classical text books, [11], among others) but, in order to include the restrictions in the design, the asymptotic

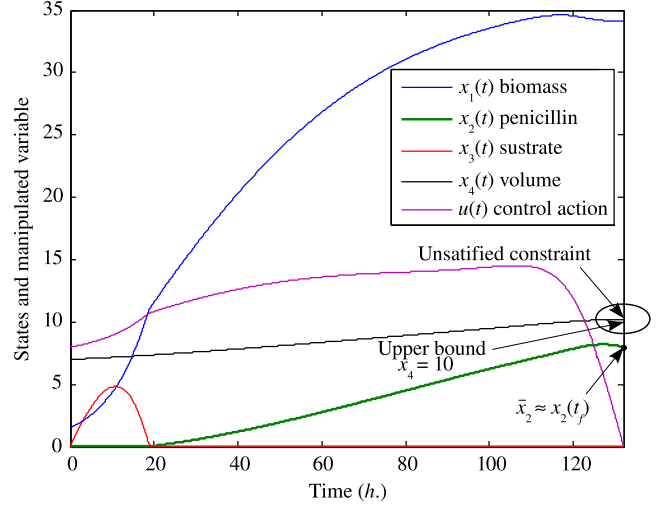


Figure 2: States and control trajectories for PI control law.

stability condition and the constraint in the manipulated variable are written as two LMIs.

5.1. Input and State Constraints via LMI

For understanding this point, a brief introduction to LMI and some optimization problems based on LMI is done. For more details, it is suggested to see [2] and [10].

A linear matrix inequality or LMI is a matrix of the form

$$\mathcal{F}(\pi) \triangleq \mathcal{F}_0 + \sum_{i=1}^m \pi_i \mathcal{F}_i > 0 \quad (28)$$

where $\pi \in \mathbb{R}^m$ and π_i are the optimization variables, and the positive and symmetric matrices $\mathcal{F}_i = \mathcal{F}_i' \in \mathbb{R}^{m \times m}$, $i = 1, \dots, m$, are given. The LMI (28) is a convex constraint on π , i.e., the set $\{\pi \mid \mathcal{F}(\pi) > 0\}$ is convex. In particular, linear and quadratic inequalities, matrix norm inequalities, and constraints that arise in control problems, such as Riccati Eq. (28) and control and state bounds, can be all cast in the form of an LMI.

One important advantage with the LMI is that the problem with multiple constraints can be expressed with multiple LMIs $\mathcal{F}^1(\pi), \dots, \mathcal{F}^n(\pi) > 0$ and then these LMI can be written as a single LMI given by

$$\text{diag}(\mathcal{F}^1(\pi), \dots, \mathcal{F}^n(\pi)) > 0. \quad (29)$$

A common procedure to convert convex nonlinear (matrix norm, quadratic, etc.) inequalities to a LMI form is through the well-know Schur complements. The basic idea is as follows

$$\begin{pmatrix} Z(\pi) & D(\pi) \\ D'(\pi) & W(\pi) \end{pmatrix} > 0 \quad (30)$$

where $Z(\pi) = Z'(\pi)$ and $W(\pi) = W'(\pi)$, and $D(\pi)$ depend affinely on π , is equivalent to

$$W(\pi) > 0, \quad Z(\pi) - D(\pi)W(\pi)^{-1}D'(\pi) > 0 \quad (31)$$

or

$$Z(\pi) > 0, \quad W(\pi) - D'(\pi)Z(\pi)^{-1}D(\pi) > 0 \quad (32)$$

i.e., the set of nonlinear inequalities (31 or 32) can be represented as the LMI (30). The main observation in this LMI-based optimization problem is that the LMI is tractable, in other words, the optimization problem can be solved easily with low computational effort.

In this paper, the following control problems will be treated as a single LMI optimization problem:

1. If a infinite horizon is considered, it is well known that when the control weighting matrix R in the cost functional is positive definite and the state weighting matrix Q is nonnegative definite, the LQR problem is well posed and can be solved via the classical algebraic Riccati equation (ARE) (see [13] for more details). When constraints are included, the optimization problem becomes

$$\Pi\hat{A} + \hat{A}'\Pi + Q - \Pi\hat{B}R^{-1}\hat{B}'\Pi > 0, \quad (33)$$

with $\Pi > 0$ solution of the last inequality and it is defined as $\Pi \in \mathbb{R}^{n+1 \times n+1}$ a symmetric matrix. Since $R > 0$, and using Eq. (31), the algebraic Riccati inequality on LMI form can be written as,

$$\mathcal{F}^1(\Pi) = \begin{pmatrix} \Pi\hat{A} + \hat{A}'\Pi + Q & \Pi\hat{B} \\ \hat{B}'\Pi & R \end{pmatrix} > 0 \quad (34)$$

2. Physical limitations inherent in process equipment invariably impose hard constraints on the manipulated variable $u(t)$. These constraints are incorporated to control problem (1) as a LMI optimization problem. Considering that the linear system (21) (when $u(t)$ is a stabilizing control law) is inside of an invariant ellipsoid as is shown in [10], a LMI for input constraint can be incorporated.

Remark. The following LMI

$$\mathcal{F}^2(\Pi) = \begin{pmatrix} u_{\max}^2 \gamma I & \Pi\hat{B}R^{-1} \\ R^{-1}\hat{B}'\Pi & I \end{pmatrix} > 0. \quad (35)$$

is equivalent to

$$\|u(t)\|_2 < u_{\max}, \quad t \geq 0. \quad (36)$$

Proof. Consider that,

$$\begin{aligned} \max_{t \geq 0} \|u(t)\|_2^2 &= \max_{t \geq 0} \left\| R^{-1}\hat{B}\Pi x(t) \right\|_2^2 \\ &\leq \lambda_{\max}^2(R^{-1}\hat{B}'\Pi\Pi\hat{B}R^{-1}) \quad (37) \\ &= v(R^{-1}B'\Pi\Pi BR^{-1}) < u_{\max}^2 \end{aligned}$$

with $\gamma = \frac{1}{v}$ a real positive constant that satisfies $x'(t)\Pi x(t) < \gamma$ (see [2] and [10] for instance) for any t time. Then, the Eq. (35) can be written.

■

Using the property (29), it is possible to write only one LMI as

$$\mathcal{F}(\Pi) = \begin{pmatrix} \Pi\hat{A} + \hat{A}'\Pi + Q & \Pi B & 0 & 0 \\ \hat{B}'\Pi & R & 0 & 0 \\ 0 & 0 & u_{\max}^2 \gamma I & \Pi\hat{B}R^{-1} \\ 0 & 0 & R^{-1}\hat{B}'\Pi & I \end{pmatrix} > 0 \quad (38)$$

Thus, the optimization problem is solved by traditional numerical methods ([2]) and implemented with standard software as Matlab or Octave. The LMI $\mathcal{F}(\Pi)$, for the studied case was solved using Matlab where $Q = 5I_{5 \times 5}$, $R = 1$, and $u_{\max} = 7.3$.

γ value is a constant which should ensure the system remains inside the designed ellipsoid. However, doing this involves a complex optimization problem further. For practical purposes, this γ value can be determined at trial and error. For the dissipative system to open loop, the adopted initial value was $v = \|x(0)\|_2^2$ as suggested in [3].

Although, the initial restriction on the manipulated variable u described by Eq. (5) is 50, for the optimization problem is imposed the value of 7.3, since it seeks to ensure that both states (especially the level of the reactor) and the manipulated variable do not exceed the restrictions imposed. However, Fig. 2 shows that the state $x_4(t)$ is above the constraint and, as the dynamics are directly related to the manipulated variable u , then, to help the convergence of the optimization algorithm is limited to $x_4(t)$ by changing the saturation value of u . Nevertheless, this does not affect the control law too much, since the different simulations carried out showed that it tends to take lower values.

Regarding the typical behaviors of the fed-batch processes ([1]), at this point, it is possible to improve the strategy devised if the linear system given by Eq. (25) is taken as an observer of the nonlinear process, i.e. if the linear system is seen as a time-variant system. Therefore, an update of the Riccati gain (\hat{K}) could be made at each sampling time. In some way a $\hat{K}(t)$ would be available to send to the system. The procedure to implement this strategy is:

i) To identify the system using some well known method. In this paper it will be performed by the standard linearization evaluated at each sampling time.

ii) To calculate at $t = 0$ the first LMI using the matrices $\hat{A}(0)$ and $\hat{B}(0)$ and the initial data $\hat{x}(0)$, $u(0)$. For computing these matrices, the initial control may be taken as the equilibrium control at $t = 0$.

iii) The first calculation of the LMI provide us the first Riccati matrix. The \hat{K} control gain could be computed.

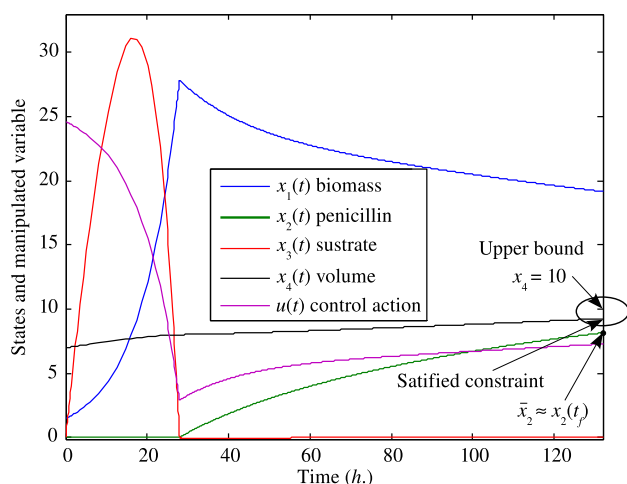


Figure 3: States and control trajectories for P+I control law.

iv) To run in parallel the process and the control system. At each sampling time the LMI should be updated using the matrices $\hat{A}(t)$ and $\hat{B}(t)$.

The improved strategy for the infinite horizon devised above was implemented, and in Fig. 3 the results were depicted. The reader can notice that the objectives fixed for the problem are satisfied, i.e., the output x_2 is close to desired value and the manipulated variable satisfies the constraint. Likewise, other states do not exceed maximum levels set in the problem.

6. CONCLUSIONS

It was presented two strategies for tuning PI controllers, which are able to generate suboptimal trajectories such that, in the second case, different constraints are satisfied. Both strategies were developed under the optimal control theory framework. The first one was developed using finite horizon optimal control theory with the restrictions that supports the definition of the objective function. Since the control action written in co-state terms and, assuming linearity in the co-states, the resulting control law has time-varying gains. The second strategy is presented under infinite horizon optimal control framework and allows the inclusion of new restrictions as for example, maximum and minimum constraints in the states and control variable. Maintaining the linearity in the co-states, it is possible to find a PI feedback law, but with feedback gains constant. The numerical results show a good performance in the controlled variables with the PI control strategies, and especially, in the second strategy where a constraint for the reactor volume is satisfied. In general, all variables have a good performance inside the operation time fixed for the batch reactor.

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