NONLINEAR FED-BATCH REACTOR PI CONTROL WITH CONSTRAINTS

Eduardo J. Adam ∗∗ Pablo S. Rivadeneira ∗

∗ Grupo de Sistemas No Lineales, INTEC, CONICET-UNL, Santa Fe, Argentina - psrivade@santafe-conicet.gov.ar
∗∗ Grupo de Control de Procesos, INTEC, CONICET-UNL, Gemes 3450, Santa Fe, Argentina - eadam@santafe-conicet.gov.ar

Abstract: This work studies the control of a fed-batch reactor for the production of penicillin and the design of suboptimal control strategies which result simple for their implementation. These strategies are able to (i) generate a suboptimal control that lead to the batch process towards its desired outputs, (ii) attenuate perturbations and noises always present in the operation of the process and, (iii) handle constraints upon the manipulated or control variable $u(t)$. The control strategy always result a linear feedback, since proper assumptions on the costates of the nonlinear and Hamiltonian system are made, besides it is shown that this feedback law is a simple PI that actualize its suboptimal parameters ‘on-line’. Inside this scheme, basically, two strategies are designed. The former minimizes a quadratic cost plus a final (also quadratic) penalty on the states in a finite horizon fashion. The latter use linear matrix inequalities (LMIs) for incorporating constraints which were not considered in the value function of the first optimal control problem. Finally, the goodness of the proposed strategies is showed through numerical simulations.

Keywords: nonlinear systems, optimal control, linear matrix inequalities, input constraints, optimal noise attenuation.

1. INTRODUCTION

Batch processes have received important attention during the past two decades due to incipient chemical and pharmaceutical products, new polymers, and recent bio-technological processes.

In a batch processes, the control problem is usually given as a tracking problem for a time-variant reference trajectories defined in a finite interval. Usually, the engineers talk about that a batch process has three operative stages clearly different, startup, batch run and, shutdown. While these three stages are widely studied by the engineers for each particular batch process, it is important to remark that in a widely number of cases, the most industries have managed to successfully operate these processes, but this operation is clearly far from optimal. Only with the experience of operators and engineers and, the repeated runs can be improved the operation control and the product quality.

The efficient design of simple control action algorithms to implement a processes into an industrial environment has been one of the biggest challenges in control engineering. The proportional-integral-derivative (PID) controller, because of its simplicity, remains the most used in the industry. However, other control techniques have made inroad in the industry in order to improve the performance of the controlled variable.

The optimal control paradigm, where the Hamiltonian formalism plays a major role, is in active development and it should give answer to the many industrial control requirements, for example, for handling restrictions on batch processes. If the optimal control problem is regular, i.e. a
In this paper, an initial design of control strategies based on the scheme in Fig. 1 adapted to the optimal control framework is presented. This scheme integrates feedforward and feedback characteristics in a technique called ‘two-degree-of-freedom design’, which is preferred when both the construction of a reference trajectory, and its tracking or disturbance attenuation are required (see Murray (2009), Costanza and Rivadeneira (2008b), Costanza and Rivadeneira (2009), for instance).

In this section a fed-batch fermentor for penicillin production like a case study is considered (see Cuthrell and Biegler (1989) and Banga et al. (2005)). The nonlinear process model is given by the following ordinary differential equations (ODEs):

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

\[
\begin{align*}
h_1 &= 0.11 \left( \frac{x_1}{0.006x_1 + x_3} \right), \\
h_2 &= 0.0055 \left( \frac{x_3}{0.0001 + x_3(1 + 10x_3)} \right). \\
y &= Cx = x_2.
\end{align*}
\]

In this model, \(x_1, x_2, x_3\) and \(x_4\) are the biomass, penicillin concentration, substrate concentration (g/L), and the reactor volume (L) respectively. The output system is the penicillin concentration, i.e. \(C = (0 \ 1 \ 0 \ 0)\), in consequence, it is assumed that this variable is monitored on-line. 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 \(y_{sp} = x_{sp2} = 8\). These operative conditions were extracted from Banga et al. (2005).

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

\[
\begin{align*}
0 \leq x_1 \leq 40 \\
0 \leq x_3 \leq 25 \\
0 \leq x_4 \leq 10
\end{align*}
\]

as well as, in the control variable (feed rate of substrate),

\[
0 \leq u \leq 50.
\]
3. FED-BATCH TRAJECTORY GENERATION

In this section, basically the Hamiltonian formalism for nonlinear process is introduced. Many of these ideas are well-documented and developed by Costanza and coworkers (see Costanza and Rivadeneira (2009, 2008a,b, 2010) for instance).

3.1 Nonlinear Hamiltonian formalism

Consider the initialized autonomous nonlinear control affine system

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

with a general cost functional written as

\[ J(T, 0, x_0, u(\cdot)) = \int_0^T L(x(\tau), u(\tau))d\tau + x'(T)Sx(T), \]  

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

\[ L(x, u) = x'Qx + Ru^2, \]  

\[ Q, \ S \geq 0, \ R > 0, \ T < \infty. \]  

Now, consider the value function \( V \) which can always be defined for such problem, namely

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

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

\[ u^*(\cdot) \triangleq \arg \inf_{u(\cdot)} J(T, t, x, u(\cdot)). \]  

The optimal control solution for this problem can be expressed as

\[ u^*(t) = -\frac{1}{2}R^{-1}g'(t)\lambda^*(t), \]  

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

\[ H(x, \lambda, u) \triangleq L(x, u) + \lambda'f(x, u). \]  

Since \( H \) is assumed regular, then there exists a unique \( H \)-optimal control \( u^0 \), namely

\[ u^0(x, \lambda) \triangleq \arg \min_u H(x, \lambda, u), \]  

and the derivative of \( H \) 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,

\[ H^0(x, \lambda, u) \triangleq H(x, \lambda, u^0(x, \lambda)), \]  

gives rise to the Hamiltonian canonical equations (HCEs) (Sontag (1998))

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

\[ \dot{\lambda} = -\left( \frac{\partial H^0}{\partial x} \right); \quad \lambda(T) = 2Sx(T), \]  

and then the optimal costate variable \( \lambda^* \) results in

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

3.2 A linear-feedback control law

In the present Section, the necessary assumptions are devised in order to convert the feedforward control action expressed in (12) to a linear feedback law (which will only depend on the real states of the system). These assumptions read

(i) The costates expressed in Eq. (18) will be approximately linear, i.e.

\[ \lambda \triangleq 2P(t)(x(t) - x_{sp}), \]  

where \( x_{sp} \) is the desired state (which is not necessarily an equilibrium state since this paper is proposed for fed-batch reactors) normally designed by the process engineer and \( P(t) \) is the gain adaptive matrix of the controller.

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

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

where \( A(t) \) and \( B(t) \) are the resulting matrices of a standard linearization of the nonlinear system around a given trajectory. For this reason, the linear problem results in a linear time variant (LTV) problem. These matrices may be identified along with the process. Several identification and observers algorithms are available in the control theory literature. We will use a standard linearization of the model process for obtaining the \( A(t), B(t) \) matrices since the scope of this paper is not the identification system.

Taking into account the assumptions above, the optimal control law expressed in Eq. (12) is turned to a suboptimal control law in feedback form

\[ u \approx \tilde{u} = -R^{-1}B'(t)P(t)(x(t) - x_{sp}) \]  

3.3 The First control strategy: Finite-time horizon fashion

The subsequent optimization problem is a linear one with the same cost function (Eq. (7)) but

---

1. Notice that, in this article, \( u \) is the manipulated variable corresponding to nonlinear problem and \( \tilde{u} \) is the calculated linear control law.
using the linear dynamics (36). It is well-known that the solution a that problem is the differential Riccati equation (DRE):
\[
P'(t) = PB(t)R^{-1}B(t)P - PA(t) - A(t)'P - Q ;
\]
with a final boundary condition
\[
P(T) = S ,
\]
where \( Q = I_{4 \times 4}, R = 3 \) and \( S = sI_{4 \times 4} \) for the case-study.

To solve the DRE may be a really difficult task. However, this could be done by:

(i) A off-line backward integration with \( T_f = 132 \) and \( s = 20 \). But, This option precludes the on-line implementation of the control law, so it will be discarded.

(ii) Transforming the boundary-value into a final-value problem related to the differential Riccati equation (DRE) as is shown in Sontag (1998). The disadvantages of this approach are that the linearization must be done around a fixed point, for instance \( t = 0 \), besides, 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 estates described by Costanza (2008b) for nonlinear systems and Costanza and Rivadeneira (2008a) 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 matrices \( A \) and \( B \) must be constant, as a result, the standard linearization must be made around a fixed point too. An adaptive scheme can be designed to update the controller gain as matrices \( A \) and \( B \) are being updated.

For the case study, \( A \) and \( B \) are initially calculated at \( t = 0 \), namely
\[
A = \begin{pmatrix} 0 & 0 & 18.3 & 0 \\ 0 & 0.01 & 82.5 & 0 \\ 0 & 0 & 5427 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 500 \end{pmatrix}.
\]

The control law (21) was applied to the system (1) and in Fig. 2 the evolution of the states for the finite horizon optimization and control problem are depicted. The batch process has a typical response (see Banga et al. (2005)), but there exits a final error between the desired state \( x_{sp2} = 8 \) 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 Banga et al. (2005)).

\[\begin{align}
\dot{q} & = \left( \begin{array}{c} A \ 0 \\ -C \ 0 \end{array} \right) \left( \begin{array}{c} x(t) \\ \xi(t) \end{array} \right) + \left( \begin{array}{c} B \\ \hat{0} \end{array} \right) \tilde{u}(t) + \left( \begin{array}{c} 0 \\ 1 \end{array} \right) r(t), \\
\dot{\xi} & = r(t) - y(t) = r(t) - Cx(t).
\end{align}\]

For this system and holding the cost function (7), a PI control law can be written as,
\[
\hat{u} = -\hat{K}\tilde{x} = -k_p x(t) + k_i \xi(t)
\]
where \( \hat{K} = R^{-1} \hat{B}' \hat{P}(t) = [K(t) \ k_i(t)] \), \( K(t) = k_p(t), \tilde{x} = \left( x(t) - x_{sp} \right) \xi(t) \), with states \( x(t) \) coming from the real process and \( \hat{P}(t) \) a solution of the Eq. (22) with
\[
\hat{A} = \begin{pmatrix} A & 0 \\ -C & 0 \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} B \\ 0 \end{pmatrix}.
\]
and for this case-study \( Q = 2.2I_{5 \times 5}, R = 0.21, \quad s = 0.1 \). Notice that, the PI control law has time variant modes as a result of solving a finite-horizon optimal control problem.

Figure 3 shows that the control system severely reduce the final error at the end of the batch operation. 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 over its upper bound.

\[\begin{align}
\dot{x} & = \hat{A} x + \hat{B} u, \\
\end{align}\]

\footnote{Some interesting results in this topic are presented by González et al. (2008) and Maeder et al. (2009)}
LMI given by and then these LMIs can be written as a single LMI optimization problem. In this paper, the following control problems will be treated as a single LMI optimization problem: One important advantage with the LMI is that the algebraic Riccati inequality can be written as a LMI, \( F^1(\Pi) = \begin{pmatrix} \Pi A + \dot{A}' \Pi + Q - \Pi B R^{-1} B' \Pi & 0 \\ B' \Pi & R \end{pmatrix} > 0 \). \( F^2(\Pi) = \begin{pmatrix} R^{-1} B' \Pi & I \\ B' \Pi & R \end{pmatrix} > 0 \). These constraints are incorporated to system (1) as a LMI optimization problem. Considering that the linear system (20) (when \( u(t) \) is a stabilizing control law) is inside of an invariant ellipsoid as is shown in Khotare et al. (1996), a LMI for input constraint can be incorporated. Remark. The following LMI \( F^2(\Pi) = \begin{pmatrix} \Pi A + \dot{A}' \Pi + Q - \Pi B R^{-1} B' \Pi & 0 \\ B' \Pi & R \end{pmatrix} > 0 \) is equivalent to \( \|u(t)\|_2 < u_{\text{max}}, \ t \geq 0. \) Using the property (29), it is possible to write only one LMI as \( F(\Pi) = \begin{pmatrix} \Pi A + \dot{A}' \Pi + Q & \Pi B \\ B' \Pi & R \end{pmatrix} > 0 \). Thus, the optimization problem is solved by traditional numerical methods (Boyd et al. (1994)) and implemented with standard software as Matlab. The LMI \( F(\Pi) \), for the studied case was solved using Matlab where \( Q = 5I_{5 \times 5}, \ R = 1, \) and \( u_{\text{max}} = 7.3. \)
will be performed by the standard linearization In particular for the batch model considered, it is a well-known method described in the literature. To identify the system we will use some way a ˆ\(x\) could be made at each sampling time. In some processes (Banga et al. 2005), at this point, an update of the Riccati gain ( ˆ\(K\)) would be available to send to the control law.

Likewise, other states do not exceed maximum saturation value of \(u\) directly related to the manipulated variable do not exceed the restrictions imposed. 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. 3 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 (Banga et al. 2005), 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 ( ˆ\(K\)) could be made at each sampling time. In some way a ˆ\(K(t)\) would be available to send to the system. To identify the system we will use some well-known method described in the literature. In particular for the batch model considered, it will be performed by the standard linearization evaluated at each sampling time.

The improved strategy for the infinite horizon devised above was simulated, and in Fig. 4 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.

![Figure 4. States and control trajectories for P+I control law.](image)

The state solution \(x(t)\) coming from the linearized system integration and the identification stage provides a desired state-trajectory, but at some time \(t\) the states \(x(t)\) of the real system may differ from \(x(t)\) due to perturbations in the signals. To cancel the effect of these perturbations a corrected control \(u(\cdot)\) may be necessary. To construct the control deviation \(U\), we assume that these differences are relatively small, then the deviation variables \(x(t) = x(t) - x^*(t), U(t) = u(t) - u^*(t), \ t \in [0, T]\)

must approximately follow a linear dynamics (see Sontag (1998) for details)

\[ \dot{X}(t) = \dot{x}(t) - \dot{x}^*(t) = f(x(t), u(t)) - f(x^*(t), u^*(t)) \approx f_x(x^*(t), u^*(t))X(t) + f_u(x^*(t), u^*(t))U(t) = A(t)X(t) + B(t)U(t) . \]  

The control deviation \(U\) may then be designed, either in a finite-horizon context (typically with the same duration \(T_f < \infty\) of the original problem), or in an asymptotic tracking fashion as it was shown in the previous sections.

### 4.2 Noise in I/O signals. Optimal compensation.

Disturbances will be reinterpreted as signal noises in this subsection. In other words, the linear system given by (36) will model the deviation system, but since \(x(t)\) is now a stochastic process, an estimation of \(\dot{x}\) will be needed. In short, the dynamics of the deviation \(\dot{x}\) from output measurements \(y\) will be

\[ \dot{\dot{x}} = \dot{A}(t)\dot{x}(t) - \frac{1}{2} \dot{W}(t)\dot{x}(t) + r_1 , \]  

\[ \dot{y} = C\dot{x} + r_2 = y - C\dot{x}^* , \]  

where, as usual, \(r_1\) and \(r_2\) are stochastic differentials of Brownian motions (i.e. the \(r_1\) may be considered as zero-mean Gaussian white noises) with covariance matrices \(r_1\) and \(r_2\) respectively. For the batch reactor proposed, \(C = (0 \ 1 \ 0 \ 0)\).

According to Eqns. (36, 19), the stochastic deviation process will be rewritten as

\[ \dot{\dot{x}} = \ddot{A}(t)\dot{x}(t) + r_1 , \]  

with

\[ \ddot{A}(t) \triangleq \dot{A}(t) - \dot{W}(t)\dot{P}(t) . \]  

In this context, a Kalman-Bucy filter for the approximated model is optimal, and can be implemented through (see Costanza and Rivadeneira (2010), Sontag (1998))

\[ \dot{\dot{x}}(t) = \ddot{A}(t)\dot{x}(t) + G(t)[\dot{y} - C\dot{x}]; \ \dot{x}(0) = \mathbb{E}(x_0) = x_0 , \]  

(41)
where the notation \( \hat{x} \) is also used for the estimation of the stochastic deviation for simplicity, and where \( G(t) \) and \( \Pi(t) \) is the solution to another Riccati-type ODE, namely,

\[
\dot{\Pi}(t) = \hat{A}(t)\Pi + \Pi \hat{A}(t)' - \Pi C'C^{-1}C\Pi + C_1; \quad (42)
\]

with an initial value

\[
\Pi(0) = \text{Cov}(x_0) \quad (43)
\]

The entire 2DOF strategy was applied to fed-batch process and the requirements imposed are: i) to keep the process close to its set-point; ii) to satisfy the restrictions on the manipulated variable, which is reflected in the fourth state (the reactor volume) and which should not exceed the value of 10; iii) to mitigate the process noise.

The covariances of the white noise were taken as \( \sigma_1 = I_{4 \times 4} \) which directly affects to the process and, \( \sigma_2 = I_{4 \times 4} \) which has an effect on the controlled output. Figure 5 illustrates the application of the control strategy, which successfully meets conditions imposed on the system.

5. CONCLUSIONS

In this paper a complete control scheme has been developed and illustrated. This scheme integrates characteristics of feedback control that allows both the generation of the trajectory to be followed by the batch process to achieve their desired final states or outputs and, to mitigate noise disturbances inherent to the process. This control scheme has been called by traditional control theory as a control of two-degrees-of-freedom.

The innovation in this paper is that besides allowing incorporating restrictions on the manipulated variable in the design of the control system, all tools developed to design the degrees of freedom come from modern optimal control theory, based on the Hamiltonian formalism, which clearly sets out the relationship between state, co-state and control law.

It is important to remark that the entire proposed scheme is implemented on-line, where the controller parameters are updated on-line. This is because the resulting controller is based on the simplifications made of co-state on the system and, in consequence, a simple PI industrial controller can be online tuned. Thus, the two resulting strategies for tuning PI controllers are able to generate suboptimal trajectories such that, in the second case, different constraints can be satisfied.

Also, it is significant to comment that the first strategy 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. On the other hand, the second strategy is presented under infinite horizon optimal control framework and allows the inclusion of new constraints by means of LMI 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 suboptimal PI feedback law, but with feedback gains constant. In this point it is remarkable that the simplifications needed to generate the linear control law produces a losing optimality. The counterpart of this, it is that the reduction in the complexity of the mathematical problem treatment leads to less computational effort.

Finally, 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 inclusive when noises are present.

REFERENCES


