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# Use of the Riccati Equation On-Line for Adaptively Controlling a CSTR Chemical Reactor

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# Use of the Riccati Equation On-Line for Adaptively Controlling a CSTR Chemical Reactor

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**Abstract**

*An idealised nonlinear model of an isothermal continuous stirred-tank reactor (CSTR) is analysed and simulated for optimal control based on the continuous on-line recomputation of a Riccati Controller as proposed by Banks[1]. The controller and resulting behaviour are derived analytically and confirmed to be optimal by derivation also via Dynamic Programming. For comparison purposes, the behaviour of the same model under linear proportional control (with feedforward compensation) is derived also and the predicted behavioural patterns confirmed by SIMULINK simulation in both cases.*

*The Banks controller is shown to outperform the linear version not only in terms of the pre-formulated quadratic cost function but also in terms of response time for systems of equal maximum input excursion. It is shown to tolerate non-negative flow constraints omitted from the pre-formulated cost function.*

## 1. Introduction

Banks[1] has proved that, under a wide range of circumstances, a nonlinear processes that can be described by

$$\underline{\dot{x}} = \underline{A}(\underline{x})\ \underline{x} + \underline{B}(\underline{x})\ \underline{u} \tag{1}$$

are optimally controlled to minimise cost

$$V = \int_0^{\infty} \{\ \underline{x}^T \underline{Q}\ \underline{x}\ + \underline{u}^T \underline{Ru}\ \}\ dt \tag{2}$$

by using the control law

$$\underline{u} = -\underline{D}(\underline{x})\ \underline{x} \tag{3}$$

where $$\underline{D}(\underline{x}) = \underline{PBR}^{-1} \tag{4}$$

$\underline{P}$ being the solution of the Riccati Equation

$$\underline{Q} + \underline{A}^T \underline{P} + \underline{PA} - \underline{PBR}^{-1} \underline{B}^T \underline{P}\ = 0 \tag{5}$$

For a linear time invariant process (i.e for $\underline{A}$ and $\underline{B}$ constant), the result is well known of course. In such a case, $\underline{P}$ and hence feedback coefficient matrix $\underline{D}$ is computed off-line from known matrices $\underline{A}$, $\underline{B}$, $\underline{Q}$, and $\underline{R}$ beforehand. On-line control then involves merely utilising $\underline{D}$ as a constant feedback coefficient for calculating the optimal control $\underline{u}$ from measurements of process state $\underline{x}$. What is novel in Banks' findings is that, if $\underline{A}$ and $\underline{B}$ are state dependent and the functions $\underline{A}(\underline{x})$ and $\underline{B}(\underline{x})$ are known, then $\underline{D}$ can be calculated via exactly the same equations (4) and (5) but now in an on-line manner using continously updated values of $\underline{A}(\underline{x})$ and $\underline{B}(\underline{x})$ in Riccati Eqn. (5). Banks demonstrates much improved and robust control for aircraft and inverted pendulum examples when compared to controllers based on locally linearised models. In particular, the range of state-space from which his controller can bring the process to a chosen reference point is greatly expanded compared to the range of conventional methods.

This report examines the performance of the on-line Riccati controller for an idealised continous stirred tank reactor (CSTR). This exercise is a useful preliminary to the application to a binary distillation column planned and formulated in a previous Research Report(2) in this series. The reactor is much simpler (amenable to analytic solution) yet shares some essential features of the column model.

## 2. Modelling The Reactor

Figure 1 illustrates the reactor in which reagents A and B enter in equal proportions at a total molar flowrate F. Model derivation follows Nicholson(3), Chapter 3. The forward reaction involves one mol of A reacting with one mol of B to form two mols of C, i.e the so-called stoichiometric equation of the reaction is :

$$A + B \rightleftharpoons 2C \qquad (1)$$

As indicated, for generality, we allow the reverse reaction also to occur. For linear reactions, we assume the following forms for the law of mass action pertaining to the two directions :

$$r_1 = 2k_1 [A]^{0.5} [B]^{0.5} \qquad (2)$$

$$r_2 = k_2 [C] \qquad (3)$$

where $r_1$ is the rate of generation of C in mols p.u volume p.u time and $r_2$ is the rate of disintegration of C back into reagents of A and B expressed in the same units. The square brackets denote concentrations of A, B and C expressed in mols (of each chemical) p.u volume V of the reacting mixture. $k_1$ and $k_2$ are reaction velocity coefficients that ideally depend only on temperature which is here kept constant (i.e the reactor is assumed to be isothermal). Assuming ideal fluids (i.e one mol of any component A, B or C occupies the same volume) then the molar density $\rho$ of the reacting mixture will remain constant. We assume the reactor level is kept constant so that V is constant and the molar inflow and outflow are therefore equal at F(t). Flowrate F(t) is therefore best considered as a throughput that is adjustable by, say, the outflow valve as shown in Fig. 1, leaving the level controller to maintain V at the desired value by rapid manipulation of the inflow (also as shown).

Now $$[A] + [B] + [C] = \rho \tag{4}$$

and since A and B enter and react in equal proportions

$$[A] = [B] \tag{5}$$

so that $$[A] = \frac{\{\rho - [C]\}}{2} \tag{6}$$

Rather than working in concentrations, it will be more convenient finally to work in so-called mol/fractions. If X is the fraction of C-mols of all those (i.e of A, B <u>and</u> C) in the reactor then, clearly :

$$X = \frac{[C]}{\rho} \tag{7}$$

We now form the dynamic balance equation for the generation, disintegration, outflow and accumulation of C in the reactor. Clearly generation-minus disintegration-rate must equal outflow-plus accumulation-rate so that, in mols p.u time :

$$r_1 V + r_2 V = FX + V\frac{d[C]}{dt} \tag{8}$$

Hence $$k_1 \{\rho - [C]\} V - k_2 [C] V = FX + V\frac{d[C]}{dt} \tag{9}$$

If F = 0, i.e as in a so-called batch reactor, then, in steady state :

$$[C] = [C_e] = \frac{\rho k_1}{k_1 + k_2} \tag{10}$$

or $$X = X_e = \frac{k_1}{k_1 + k_2} \tag{11}$$

where suffix e denotes the so-called 'equilibrium' value. $X_e$ would be unity only in the absence of a reverse reaction (i.e if $k_2 = 0$). The process equation may therefore be written :

$$X_e - X = T_b \left\{\frac{F}{\rho V} X + \frac{dX}{dt}\right\} \tag{12}$$

where $T_b$ is the batch reactor time constant given by

$$T_b = \frac{1}{(k_1 + k_2)} \tag{13}$$

Thus setting control U as

$$U = F\left(\frac{T_b}{\rho V}\right) \tag{14}$$

the process equation reduces to the simple bilinear form:

$$X_e - X = UX + \dot{X} \qquad (15)$$

where $$\dot{X} = \frac{dX}{d\tau} \qquad (16)$$

and t is normalised time wrt $T_b$, i.e

$$\tau = \frac{t}{T_b} \qquad (17)$$

Clearly, in steady state, with constant U

$$X = \frac{X_e}{1 + U} \qquad (18)$$

or $$U = \frac{X_e - X}{X} \qquad (19)$$

i.e so-called equllibrium conditions can be achieved only for $U = 0$ as expected. Otherwise, $X < X_e$, in steady state and, again as would be expected, the greater the normalised throughput U, the greater the shortfall $X_e - X$ in product purity.

## 3. Optimal Control Derivation by Continuous, Nonlinear Dynamic Programming

Before considering use of the Banks, On-line Riccati method, we first derive the truly optimal control law by means of the continuous version of Dynamic Programming[(4)]. Time constant $T_b$ is set to 1.0 so making $\tau = t$ in all following analysis. The cost function is:

$$V = \int_0^T L(\underline{x}, \underline{u})\, dt = \int_0^T \left\{ (X_r - X)^2 + \lambda (U_r - U)^2 \right\} dt \qquad (20)$$

where $X_r$ and $U_r$ are desired reference values for product purity X(t) and normalised throughput U(t). These are chosen to be steady-state consistent according to eqns. (18) and (19) i.e

$$X_r = \frac{X_e}{1 + U_r} \qquad (21)$$

and $$U_r = \frac{X_e - X_r}{X_r} \qquad (22)$$

These constraints ensure that in steady state, the integral terms $(X_r - X)^2$ and $(U_r - U)^2$ can be simultaneously zero so that :

$$\lim_{t \to \infty} \frac{\partial V}{\partial t} = 0 \qquad (23)$$

This ensures that there is no residual cost-rate once steady state is achieved and that the entire cost rate can be controlled to zero by optimal choice of U(t). Certain complications in the optimal control design are thus avoided as will be demonstrated. In particular, if $V^*(\underline{x}, t)$ denotes the optimal cost of the process in state $\underline{x}$ at time t, then the law of continuous dynamic programming :

$$\frac{\partial V^*}{\partial t} = \min_{\underline{u}} \left[ \dot{\underline{x}} \frac{\partial V^*}{\partial x} + L(\underline{x}, \underline{u}) \right] \quad (24)$$

can be written simply

$$\min_{\underline{u}} \left[ \dot{\underline{x}} \frac{\partial V^*}{\partial x} + L(\underline{x}, \underline{u}) \right] = 0 \quad (25)$$

to generate a converged optimal control law

$$\underline{u}^* = \underline{u}^* (\underline{x}) \quad (26)$$

that will apply for most of the process time T provided of course T >> 1.0.

In this application, eqn (25) may be written

$$\min_{U} \left[ \{X_e - (1+U)X\} \frac{\partial V^*}{\partial X} + (X_r - X)^2 + \lambda(U_r - U)^2 \right] = 0 \quad (27)$$

so that for the minimum [ ... ] in eqn.(27)

$$-X \frac{\partial V^*}{\partial X} - 2\lambda (U_r - U) = 0$$

$$\therefore \quad \frac{\partial V^*}{\partial X} = -\frac{2\lambda (U_r - U)}{X} \quad (28)$$

The optimal control law is attained by using eqn.(28) to eliminate $\frac{\partial V^*}{\partial X}$ from eqn.(27), giving

$$\{X_e - (1+U)X\} \left\{ \frac{-2\lambda (U_r - U)}{X} \right\} + (X_r - X)^2 + \lambda (U_r - U)^2 = 0 \quad (29)$$

Recalling from eqns. (21) and (22) that

$$X_r = \frac{X_e}{1 + U_r} \quad \text{and} \quad U_r = \frac{X_e - X_r}{X_r}$$

eqn. (29) can be written as a quadratic in $U_r$ - U thus :

$$\lambda(U_r - U)^2 + (U_r - U)\, 2\lambda \left( U - U_r + \frac{X_e}{X_r} - \frac{X_e}{X} \right) + (X_r - X)^2 = 0 \quad (30)$$

Hence, setting

$$\Delta U = U_r - U \quad (31)$$

and

$$\Delta X = X_r - X \quad (32)$$

we obtain the following quadratic in ΔU and ΔX :

$$\Delta U^2 + \frac{2X_e \Delta X}{X X_r} \Delta U - \frac{\Delta X^2}{\lambda} = 0 \quad (33)$$

the solution of which is

$$\Delta U = -\frac{X_e \Delta X}{X X_r}\left[1 \pm \sqrt{1 + \frac{X^2 X_r^2}{\lambda X_e^2}}\right] \tag{34}$$

Now for stability the overall feedback from ΔX to ΔU must be positive (since the process gain from U to $\dot{X}$ is negative as inspection of process eqn. (15) reveals). Hence we must take the bottom sign of the square root ($\sqrt{\ }$) term in eqn. (34) to give the control law :

$$U = U_r + \left[\frac{(X_r - X)X_e}{X X_r}\right]\left[1 - \sqrt{1 + \left(\frac{X X_r}{X_e}\right)^2 \frac{1}{\lambda}}\right] \tag{35}$$

Comments on this control strategy and demonstration of its use are postponed until Sections 5 and 6. Before that we show that the identical result emerges from the application of the on-line Riccati Equation.

## 4. On-Line Riccati Solution : Analytic Derivation

Starting with process eqn. (15) written in the form

$$\dot{X} = -X(1 + U) + X_e \tag{36}$$

and specifying constant state and input reference values $X_r$ and $U_r$ where for steady state consistency

$$\dot{X}_r = 0 = -X_r(1 + U_r) + X_e \tag{37}$$

we can write the process equation thus :

$$\Delta\dot{X} = A\,\Delta X + B\,\Delta U \tag{38}$$

in term of deviations :

$$\Delta U = U_r - U \tag{39}$$

and $$\Delta X = X_r - X \tag{40}$$

where $A = -(1 + U_r)$.

(41)

and $$B = (\Delta X - X_r) \tag{42}$$

i.e eqn. (39) takes the form :

$$\Delta\dot{X} = -(1 + U_r)\Delta X + (\Delta X - X_r)\Delta U \tag{43}$$

Now if again the cost function to be minimised is :

$$V = \int_0^\infty \left(\Delta X^2 + \lambda \Delta U^2\right) dt \tag{44}$$

we recall again that $\frac{dV}{dt} = 0$ in steady state so that we may use the converged Riccati eqn.

$$\underline{\dot{P}} = \underline{Q} + \underline{A}^T\underline{P} + \underline{PA} - \underline{PBR}^{-1}\underline{B}^T\underline{P} = 0 \qquad (45)$$

where, in this first order application the $\underline{P}$, $\underline{Q}$, $\underline{R}$, $\underline{A}$ and $\underline{B}$ matrices are all scalar, viz

$$\underline{Q} = 1.0 \qquad (46)$$
$$\underline{R} = \lambda \qquad (47)$$
$$\underline{A} = A = -(1 + U_r) \qquad (48)$$
$$\underline{B} = B = \Delta X - X_r \qquad (49)$$

Thus the cost and process coefficient matrices are constant apart from $\underline{B}$ which is state dependent (as allowed by the Banks' method).

Setting $\underline{P}$ = scalar p (50)
in the Riccati eqn.(45) we readily obtain the following quadratic for p, i.e.

$$p^2X^2\lambda^{-1} + 2(1 + U_r)p - 1 = 0 \qquad (51)$$

which solves to give :

$$p = -\frac{(1+U_r) \pm \sqrt{(1+U_r)^2 + X^2\lambda^{-1}}}{X^2\lambda^{-1}} \qquad (52)$$

Now the optimal control law is :

$$\Delta U = D\,\Delta X$$

where feedback coefficient D is given by :

$$D = R^{-1}B^T p = \frac{1}{\lambda}(\Delta X - X_r)p \qquad (53)$$

so that $$D = -\frac{Xp}{\lambda} \qquad (54)$$

Hence substituting solution (52) for p in Eqn. (54) we get :

$$\Delta U = -\left[\frac{1 + U_r \pm \sqrt{(1+U_r)^2 + X^2\lambda^{-1}}}{X}\right]\Delta X \qquad (55)$$

Now from eqns. (21) and (22) relating $U_r$ and $X_r$ we note that

$$1 + U_r = 1 + \frac{X_e - X_r}{X_r} = \frac{X_e}{X_r} \qquad (56)$$

so that, in term of U and X (rather than deviations $\Delta U$ and $\Delta X$), control law eqn.(55) becomes :

$$U = U_r + \left[\frac{X_r - X}{X}\right]\left[\frac{X_e}{X_r} \pm \sqrt{\left(\frac{X_e}{X_r}\right)^2 + \frac{X^2}{\lambda}}\right] \qquad (57)$$

Again we should take the lower sign of the $\sqrt{\ }$ term to obtain positive feedback of X to U and thus achieve stable control of our -ve gain process (eqn. (36)), yielding the control law :

$$U = U_r + \left[\frac{(X_r - X)}{X X_r}\right] X_e \left[1 - \sqrt{1 + \frac{X^2 X_r^2}{X_e^2 \lambda}}\right] \tag{58}$$

which is identical to law (35) derived from General Dynamic Programming in section 3. This demonstrates the true (long-term) optimality of the Banks' solution despite the state dependent nature of matrix **B**.

## 5. Analytic Derivation of Process Response under Optimal Control

As well as the optimal control law being derivable analytically in this application (as already shown in Sections 3 and 4 of this report) it is also possible to proceed to an analytic solution for the time response $X(\tau)$ of the optimally controlled system from disturbed initial condition $X(0)$. This is achieved by eleminating control $U(\tau)$ between process equation (36) and control law (58) as follows :

Combining the two equations as indicated yields the result :

$$\dot{X} = -X\left[1 + U_r + \frac{(X_r - X)}{X X_r} X_e \left\{1 - \sqrt{1 + \left(\frac{X X_r}{X_e}\right)^2 \frac{1}{\lambda}}\right\}\right] + X_e \tag{59}$$

which readily reduces to simpler form :

$$\dot{X} = \frac{X_e}{X_r}(X_r - X)\sqrt{1 + \left(\frac{X X_r}{X_e}\right)^2 \frac{1}{\lambda}} \tag{60}$$

Differential equation (60) can be integrated analytically with the aid of various substitutions of variables as now shown :

From (60), starting from initial condition $X(0) = 0.0$, we deduce that :

$$\tau = \int_0^X \left\{\frac{X_e}{X_r}(X_r - X)\sqrt{1 + \left(\frac{X X_r}{X_e}\right)^2 \frac{1}{\lambda}}\right\}^{-1} dX \tag{61}$$

and, in terms of normalised variables

$$\tau' = \tau \frac{X_e}{X_r} \tag{62}$$

$$Y = \frac{X}{C} \tag{63}$$

and

$$Y_r = \frac{X_r}{C} \tag{64}$$

where $$C = X_e \frac{\sqrt{\lambda}}{X_r} \tag{65}$$

we obtain simply :

$$\tau' = \int_0^Y \frac{dY}{(Y_r - Y)\sqrt{1+Y^2}} \tag{66}$$

The first substitution towards integration of eqn. (66) is :

$$Y = \sinh\theta \tag{67}$$

so that $$dY = \cosh\theta\, d\theta \tag{68}$$

and $$\sqrt{1+Y^2} = \cosh\theta \tag{69}$$

so that $$\tau' = \int_0^\theta \frac{d\theta}{Y_r \sinh\theta} \tag{70}$$

or $$\tau' = \int_0^\theta \frac{2d\theta}{2Y_r - e^\theta + e^{-\theta}} \tag{71}$$

The second substitution needed is :

$$\zeta = e^\theta \tag{72}$$

so that $$d\zeta = e^\theta\, d\theta, \quad \text{or} \quad d\theta = \frac{d\zeta}{\zeta} \tag{73}$$

giving in term of $\zeta$ rather than $\theta$,

$$\tau' = 2\int_1^\zeta \frac{d\zeta}{-\zeta^2 + 2Y_r\zeta + 1} \tag{74}$$

the integrand of which factorises and partial fractions to yield

$$\tau' = \frac{1}{\sqrt{1+Y_r}} \int_1^\zeta \left[\frac{1}{\zeta - Y_r + \sqrt{\ }} - \frac{1}{\zeta - Y_r - \sqrt{\ }}\right] d\zeta \tag{75}$$

in which $$\sqrt{\ } = \sqrt{1+Y_r^2} \tag{76}$$

Integration of (75) therefore yields

$$\tau' = \frac{1}{\sqrt{1+Y_r^2}} \left[\log\left(\frac{\zeta - Y_r + \sqrt{\ }}{\zeta - Y_r - \sqrt{\ }}\right)\left(\frac{1 - Y_r - \sqrt{\ }}{1 - Y_r + \sqrt{\ }}\right)\right] \tag{77}$$

For simplicity we now introduce another normalised time $\tau''$ given by :

$$\tau'' = \tau'\sqrt{Y_r^2+1} = \tau\frac{X_e}{X_r}\sqrt{\frac{X_r^2}{C^2}+1} = \tau\frac{X_e}{X_r}\sqrt{\frac{X_r^4}{X_e^2\lambda}+1} \tag{78}$$

or,
$$\tau'' = \frac{\tau}{T_{co}} \tag{79}$$

where time constant $T_{co}$ is given by :

$$T_{co} = X_r\sqrt{\frac{\lambda}{X_r^4+\lambda X_e^2}} \tag{80}$$

Thus, taking antilogs of eqn. (77) and extracting variable $\zeta$ $(= e^{\theta})$ gives :

$$\zeta = \frac{(Y_r-1)(1-Y_r-\sqrt{\ })-\exp(\tau'')(Y_r+\sqrt{\ })(1-Y_r+\sqrt{\ })}{(1-Y_r-\sqrt{\ })-\exp(\tau'')(1-Y_r+\sqrt{\ })} = e^{\theta} \tag{81}$$

We now need to convert back from $\zeta$ $(= e^{\theta})$ to our original variable $Y\left(=\frac{X}{C}\right)$.

Now if we denote the numerator function of eqn.(81) as N and its denominator as D, then, since

$$e^{\theta} = \frac{N}{D},\ e^{-\theta} = \frac{D}{N}$$

and hence

$$\sinh\theta\ (= Y) = \frac{(e^{\theta}-e^{-\theta})}{2} = \frac{(N^2-D^2)}{2ND} \tag{82}$$

Now
$$N = Y_r+1-\sqrt{\ } -\exp(\tau'')\left(Y_r+1+\sqrt{\ }\right) \tag{83}$$
$$D = Y_r-1-\sqrt{\ } -\exp(\tau'')\left(1-Y_r+\sqrt{\ }\right) \tag{84}$$

from which we deduce

$$N^2-D^2 = 4Y_r-4Y_r\sqrt{\ }-8\exp(\tau'')Y_r+\exp(2\tau'')\left(4Y_r+4Y_r\sqrt{\ }\right) \tag{85}$$

and
$$ND = 2-2\sqrt{\ }+\exp(\tau'')\,4Y_r^2+\exp(2\tau'')\left(2+2\sqrt{\ }\right) \tag{86}$$

Hence, from eqn. (82), (85) and (86) we get

$$Y(\tau'') = Y_r\left[\frac{1-\sqrt{\ }-2\exp(\tau'')+\exp(2\tau'')\left(1+\sqrt{\ }\right)}{1-\sqrt{\ }+2Y_r^2\exp(\tau'')+\exp(2\tau'')\left(1+\sqrt{\ }\right)}\right] \tag{87}$$

where
$$\sqrt{\ } = \sqrt{1+Y_r^2} \tag{88}$$

$X(\tau)$ is readily obtained from $Y(\tau'')$ by means of equations (63), (64), (65) and (78) (which were used for normalisation merely to simplify manipulations by omission of unnecessary constant $X_e$, $X_r$ and $\lambda$).

It is readily observed that solution (87) is consistent with the assumed initial condition $Y(0) = 0$ and that $\lim_{\tau''\to\infty} Y(\tau'') = Y_r$ as expected. However the transient response is a non-linear combination of exponential terms exp($\tau''$) and exp($2\tau''$) rather than a linear one.

## 6. Response Under Linear Control

### 6.1 Closed Loop Differential Equation

Analytical prediction of the process step-response under linear control is possible also and is included here for behavioural comparison purposes in Section 7.

The incremental proportional control law :

$$\Delta U = K\,\Delta X \tag{89}$$

in which K denotes the controller gain, may be written :

$$U = U_r - K\,(X_r - X) \tag{90}$$

where $U_r$ and $X_r$ again denote constant reference signals for flow and output mol-fraction respectively. If these are chosen to be steady-state consistent (i.e satisfying equations (21) and (22)) then the control law may be expressed thus :

$$U = \frac{(X_e - X_r)}{X_r} + K\,(X - X_r) \tag{91}$$

Combining this with open-loop process equation (15) (to eliminate control flow, U) yields the quadratic closed-loop equation :

$$\dot{X} = X_e + X\left(K\,X_r - \frac{X_e}{X_r}\right) - K\,X^2 \tag{92}$$

or $$\dot{X} = (X_r - X)\left(K\,X + \frac{X_e}{X_r}\right) \tag{93}$$

### 6.2 Solution for Constant Reference and Zero Initial Condition

Clearly, since $\dot{X}$ denotes $\frac{dX}{d\tau}$, if $X(0) = 0$, then equation (93) can be expressed :

$$\tau = \int_0^X \frac{dX}{(X_r - X)\left(K\,X + \frac{X_e}{X_r}\right)} \tag{94}$$

and the integrand partial fractions to give :

$$\tau = \frac{X_r}{(K X_r^2 + X_e)} \int_0^X \left[ \frac{1}{(X_r - X)} + \frac{K}{K X + \frac{X_e}{X_r}} \right] dX \tag{95}$$

The integral is readily evaluated to give :

$$\tau''' = \log \left[ \frac{X_r \left( X + \frac{X_e}{K X_r} \right)}{(X_r - X)\left( \frac{X_e}{K X_r} \right)} \right] \tag{96}$$

where $\tau''' = \dfrac{t}{T_{CL}}$ (97)

and time-constant $T_{CL}$ is given by :

$$T_{CL} = \frac{X_r}{K X_r^2 + X_e} \tag{98}$$

From (96) it follows that :

$$\exp(\tau''') = \frac{(K X_r^2)\left( X + \frac{X_e}{K X_r} \right)}{(X_r - X) X_e} \tag{99}$$

from which the solution for X is found to be :

$$X = \frac{X_r \{\exp(\tau''') - 1\}}{\left\{ \exp(\tau''') + \frac{K X_r^2}{X_e} \right\}} \tag{100}$$

or $$X = \frac{X_r \left\{ 1 - \exp\left( \frac{-\tau}{T_{CL}} \right) \right\}}{\left\{ 1 + \left( \frac{K X_r^2}{X_e} \right) \exp\left( \frac{-\tau}{T_{CL}} \right) \right\}} \tag{101}$$

## 6.3 Predicted Characteristics of the Response

The response is an exponential rise of time-constant $T_{CL}$ (given by eqn. (98)) but modulated by the time-dependent denominator term of eqn. (101). The rate of response is clearly given by :

$$\frac{dX}{d\tau} = \frac{X_r \left\{ \exp\left(\frac{\tau}{T_{CL}}\right) \left(1 + \frac{KX_r^2}{X_e}\right) \right\}}{T_{CL} \left\{ \exp\left(\frac{\tau}{T_{CL}}\right) + \frac{KX_r^2}{X_e} \right\}^2} \qquad (102)$$

so that :

$$\left. \frac{dX}{d\tau} \right|_0 = \frac{X_r}{T_{CL}\left(1 + \frac{KX_r^2}{X_e}\right)} = X_e \qquad (103)$$

The predicted initial response rate (=$X_e$), from initial state X(0)=0.0, is thus independent of K and this is in complete accord with the process equation (15), $\dot{X} = X_e - (1+U)X$ with X = 0.0. Time constant $T_{CL}$ is reduced by increase of K (see eqn. (98)) but this speeds up the response-rate only at a later stage of the response as confirmed by the simulation results of Fig. 2. The responses are all bounded by the lines $X = X_e \tau$ and $X = X_r$, being tangential to these lines at $\tau = 0$ and $\infty$ respectively.

Substitution of response eqn. (101) into control law (91) gives :

$$U(\tau) = \frac{X_e - X_r}{X_r} - \frac{KX_r\left(1 + \frac{KX_r^2}{X_e}\right)}{\exp\left(\frac{\tau}{T_{CL}}\right) + \frac{KX_r^2}{X_e}} \qquad (104)$$

so that :

$$U(0) = \frac{X_e - X_r}{X_r} - K X_r^2 \qquad (105)$$

The gain K must therefore be set such that :

$$K < \frac{X_e - X_r}{X_r^2} \qquad (106)$$

for $\quad U(0) > 0 \qquad (107)$

For setting of K larger than the above limit, the controller must set a zero limit on the flow demand since negative values of U are unfeasible.

input deviation. Like the linear controller of high gain, $K \to \infty$, the performance of the optimal controller approaches that of switched time-optimal control as $\lambda \to 0.0$.

The performance of the isothermal CSTR is constrained by the speed limit of the (zero-flow) batch reactor which in turn is set by the reaction velocity coefficients. Because these are temperature dependent, extension of the research to include adjustable reactor cooling may well allow an even more convincing demonstration of the Banks' controller superiority.

## References


(1) Banks, S. P and Mhana, K. J., 'Optimal Control and Stabilization for Nonlinear Systems', IMA Journal of Mathematical Control and Information, 1992, Vol. 9, pp179-196.

(2) Edwards, J. B and Mohd Noor, S. B., 'Interpretion and Utilisation of Parametric Models of Binary Distillation Columns: Relating Plant and Control Design', University of Sheffield, ACSE Research Report 573, April 1995.

(3) Edwards, J. B., 'Modelling of Chemical Process Plant', Chap. 2 of Modelling of Dynamical Systems, Ed. H. Nicholson, IEE Control Eng. Series 12, Peregrinus, 1980, pp25-61.

(4) Noton, A. R. M., 'Variational Methods in Control Engineering', London, Pergamon Press, 1965



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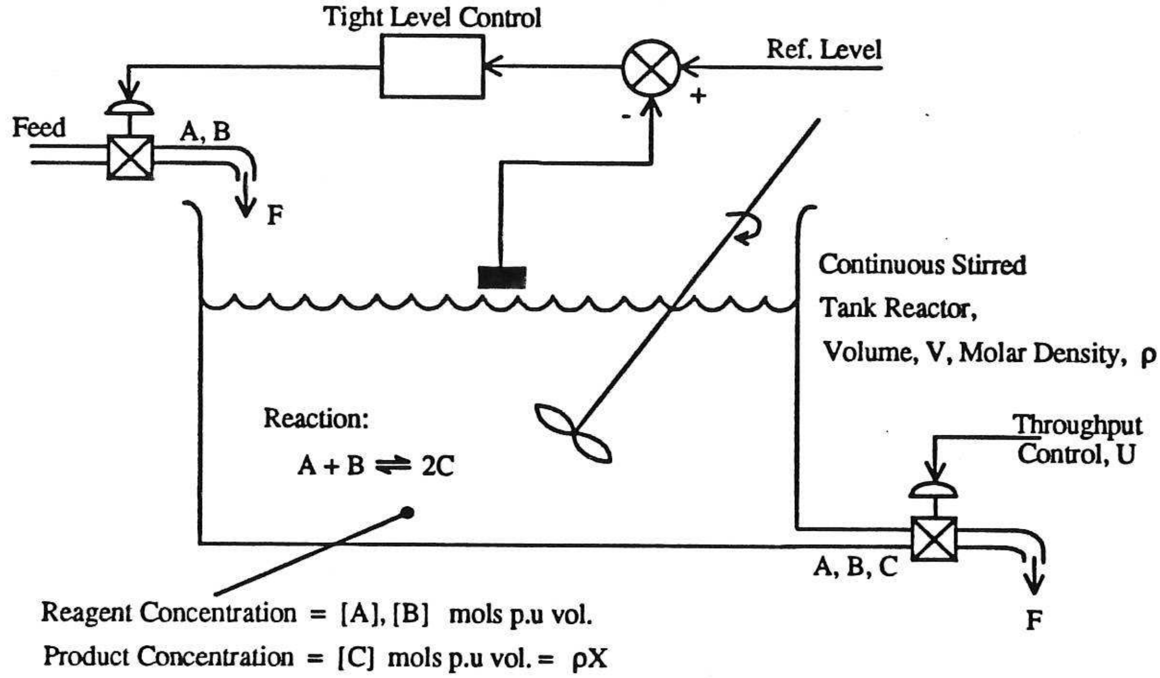


Figure 1. CSTR Reactor

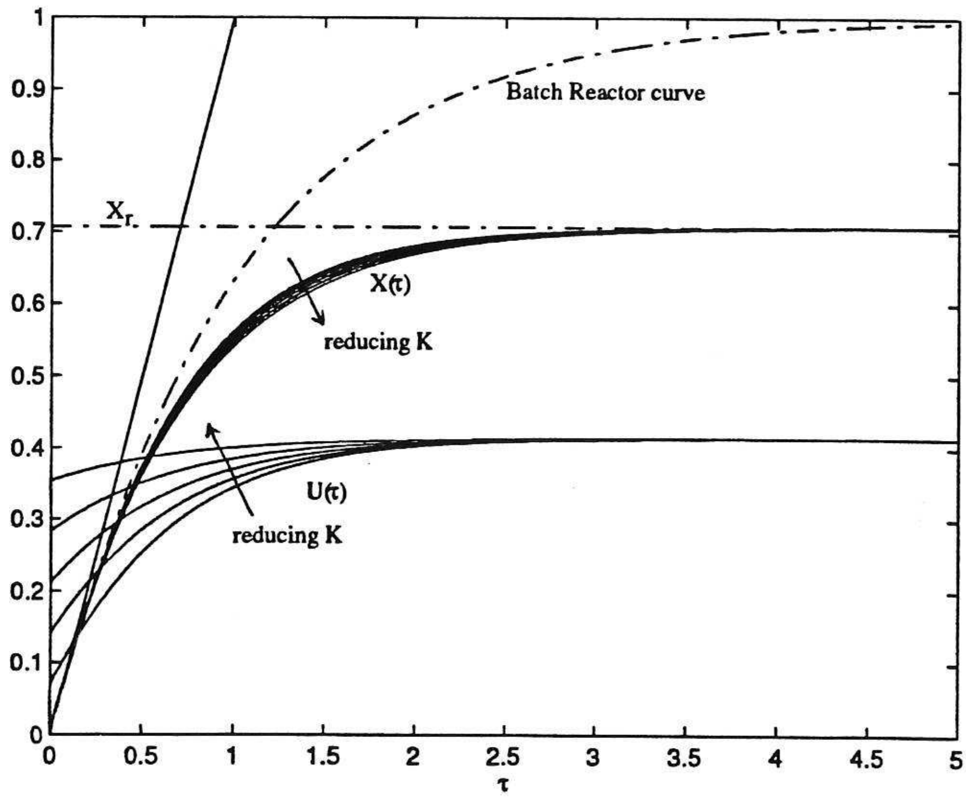


Fig. 2. Responses of CSTR under linear proportional control

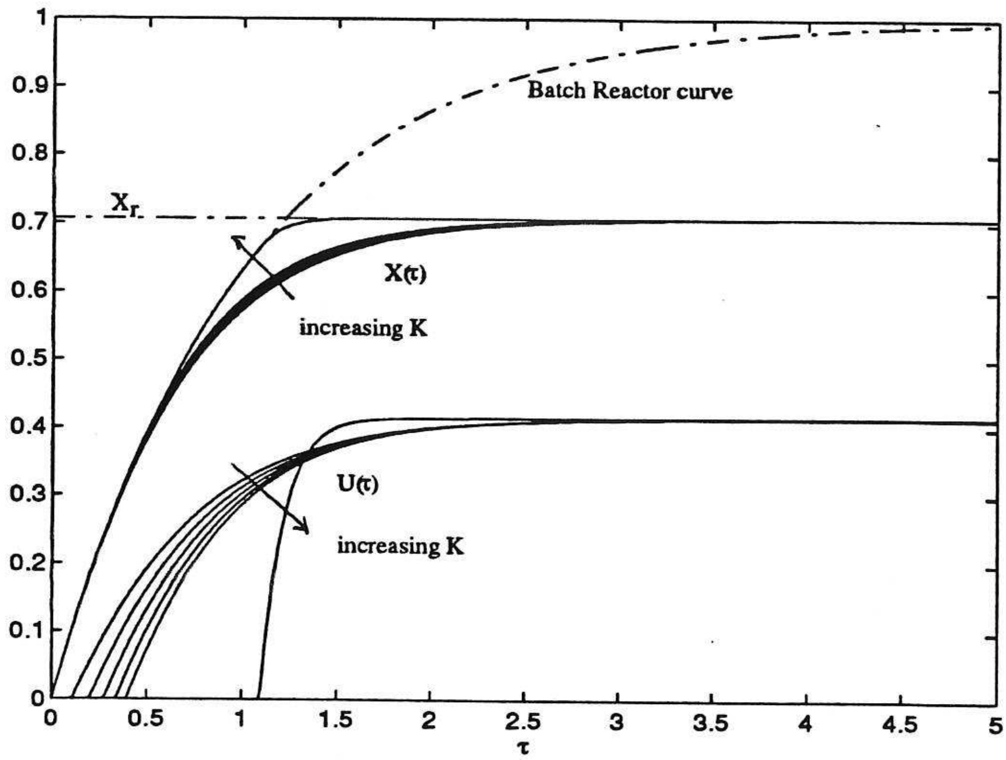


Fig. 3. Higher gain linear control, showing the effect of the non-negative flow constraint.

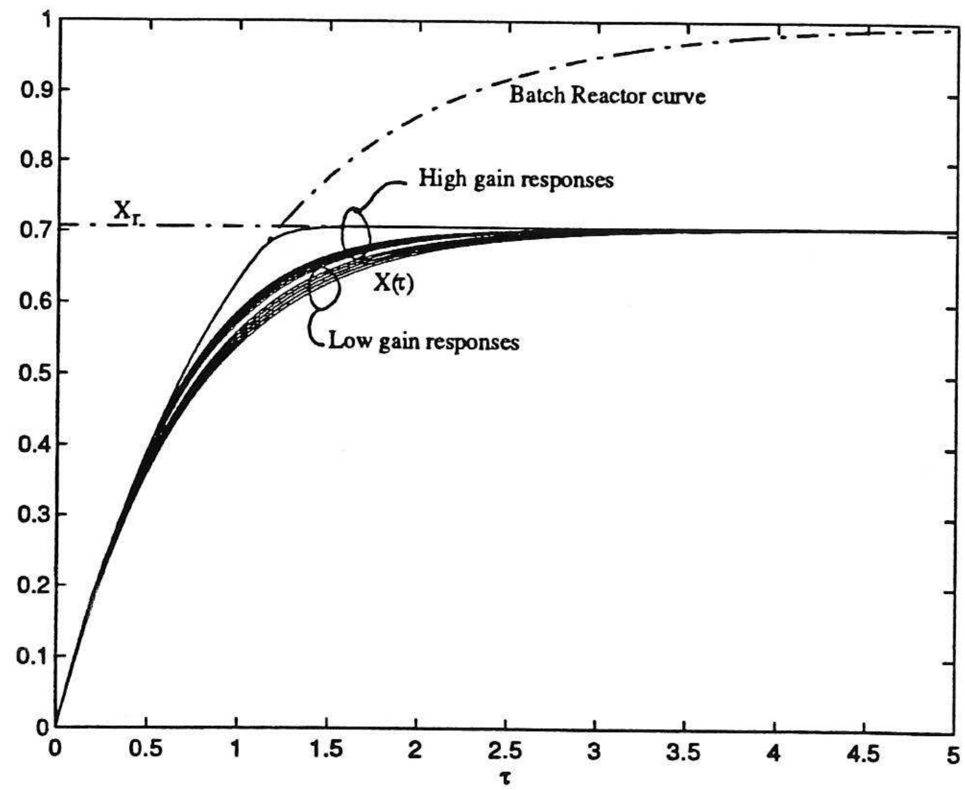


Fig. 4. Comparing high and low gain control responses of X(τ) from Fig. 2 and Fig. 3

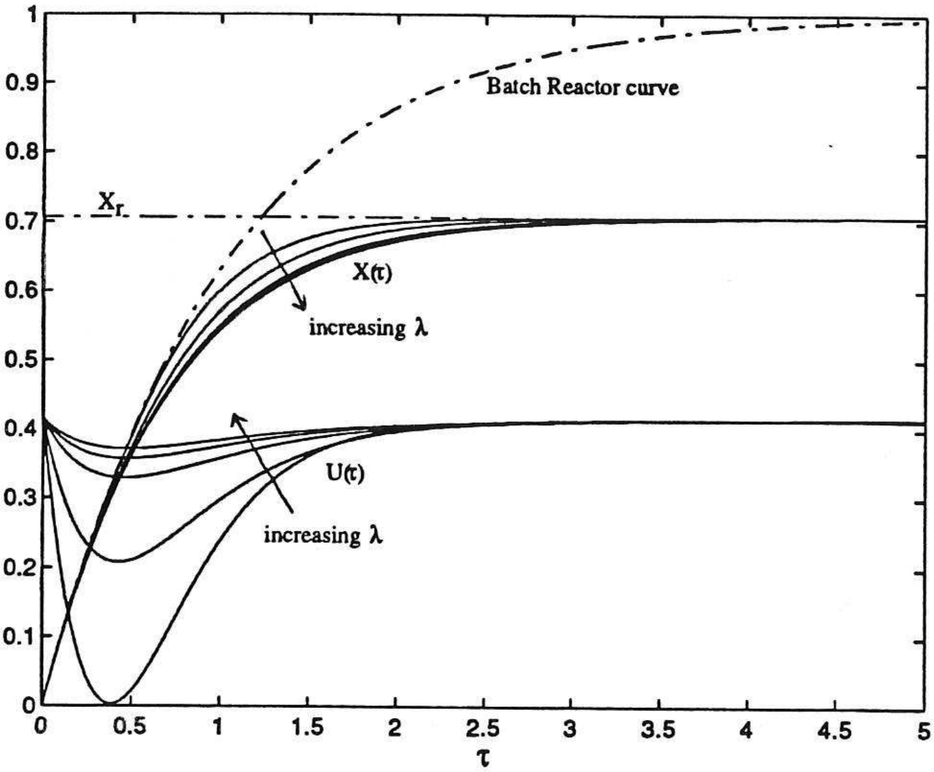


Fig. 5. Showing the effect of varying input deviation cost weighting on the optimally controlled process response.

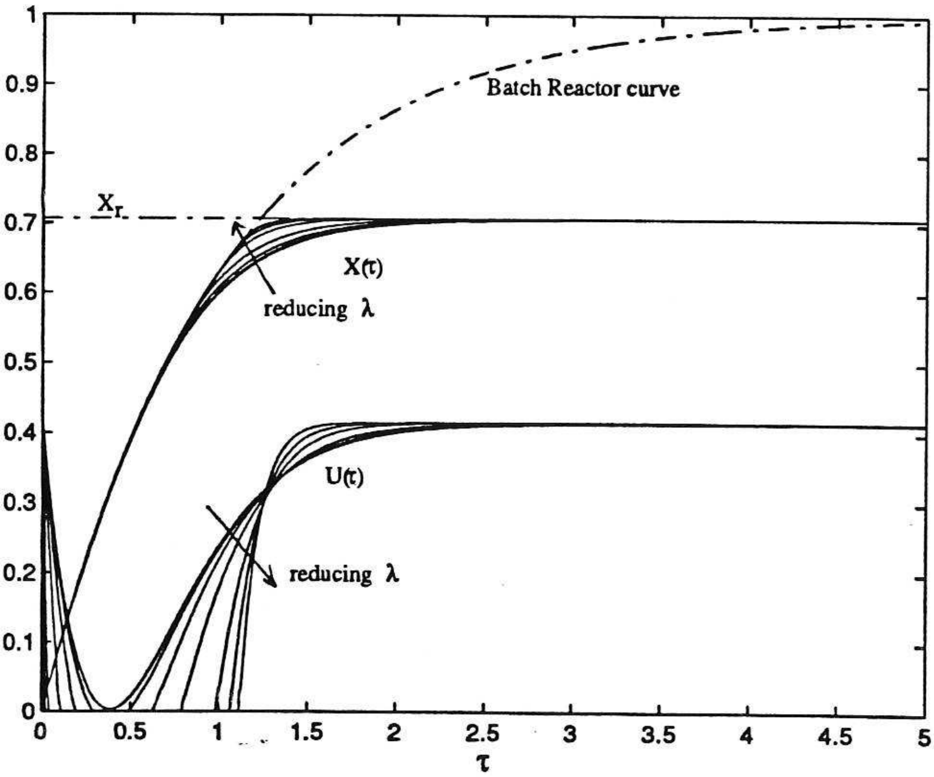


Fig. 6. Showing the effect of the non-negative flow constraint on the optimally controlled process with low input cost weighting.

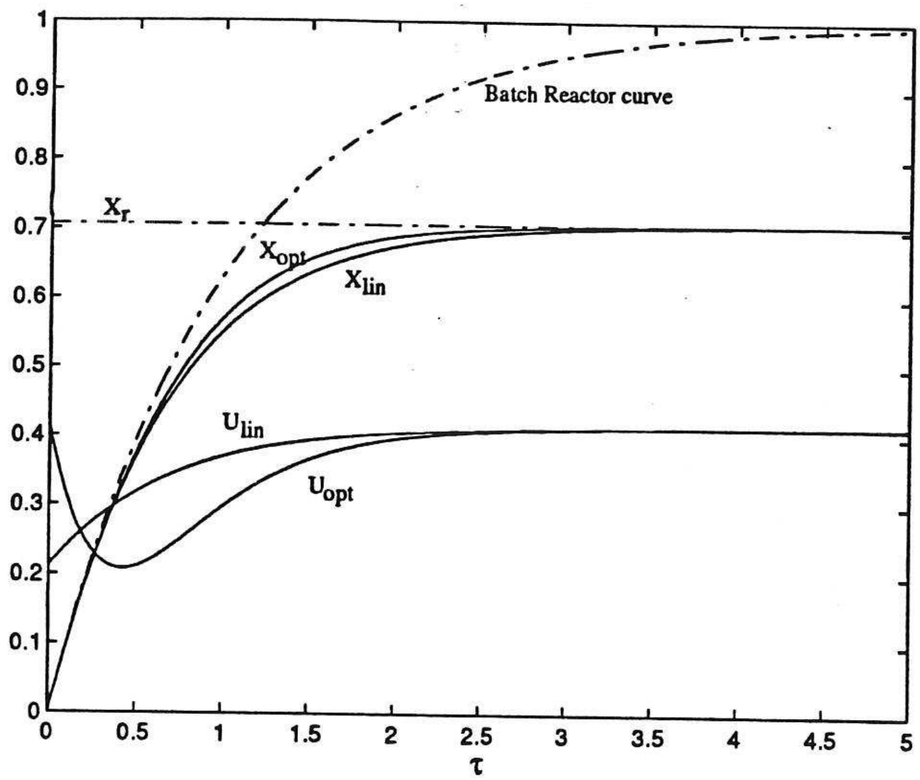


Fig. 7. Comparing the responses of the optimal and linarly controlled process for equal minimum flow conditions.

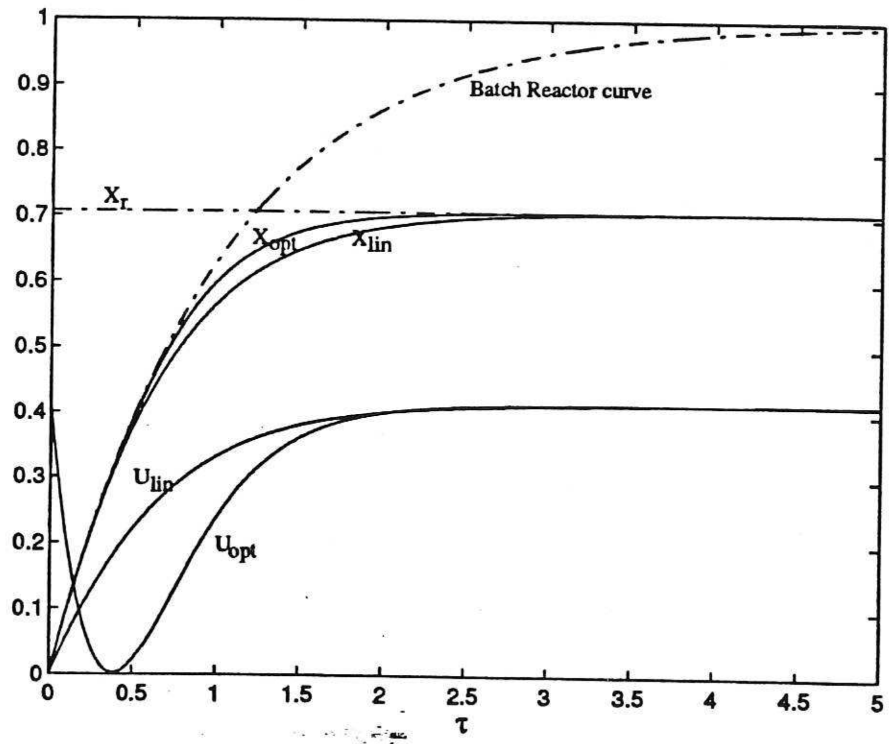


Fig. 8. Comparing the responses of the optimal and linearly controlled process for the maximum possible unconstrained input excursion.

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