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LQ control of coupled hyperbolic PDEs and ODEs: Application to a CSTR-PFR system ⋆

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Abstract: In this paper an infinite-dimensional LQR control-based design for a system containing linear hyperbolic partial differential equations coupled with linear ordinary differential equations is presented. The design is based on an infinite-dimensional Hilbert state-space representation of the coupled system. The feedback control gain is obtained by solving algebraic and differential matrix Riccati equations that result from an operator Riccati equation solution. The designed LQR control is applied to a system containing a continuous stirred tank reactor (CSTR) and a plug flow reactor (PFR) in series with the recycle-rate from PFR to CSTR as controlled variable. The LQR controller's performance is evaluated by numerical simulation of the original nonlinear system.

Keywords: Distributed parameter system (DPS), Lumped parameter system(LPS), LQR control, Infinite dimensional system, Boundary control system

1. INTRODUCTION

Many chemical engineering processes are modeled by ordinary differential equations (ODEs) as they can be assumed to be lumped parameter systems. On the other hand, there are chemical processes which take place in unit operations such as packed bed and tubular reactors, which are distributed in nature and described by partial differential equations (PDEs). Frequently, more complex unit operations involve both lumped parameter system (LPS) and distributed parameter system (DPS) model description. These systems are modeled by a set of coupled partial differential and ordinary differential equations. For example, in a fluidized bed reactor, mass and energy balances are described by PDEs while variations of void fraction is represented by an ODE. Frequently, the models of distributed and lumped parameter systems are coupled through their boundaries. For instance, in a jacket-cooled fixed-bed reactor, the reactor is modeled by a set of PDEs, while the jacket may be described by an ordinary differential equation.

The majority of control research has focused on lumped parameter systems and numerous control techniques are available for these systems. On the other hand, in distributed parameter systems most research is motivated by the system containing pure PDEs (Ray (1980), Christofides (2001)). The most interesting approaches within these research activities are those that directly account for the infinite-dimensional properties of the distributed system in the controller synthesis, e.g., linear quadratic methods (see Curtain and Zwart (1995)) and sliding mode control approach (see Orlov and Utkin (1987)). Research on controlling mixed distributed and lumped parameter systems is scarce. Most research in this area attempts to solve the optimal control problem by using calculus of variations (see Hiratsuka and Ichikawa (1969) and Tzafestas (1970)) or by using dynamic programming (Thowsen and Perkins (1973) and Thowsen and Perkins (1975)).

A classical method in the optimal feedback controller synthesis is the well known Linear Quadratic Regulator (LQR). The objective of a LQR controller is to drive a linear system to a desired state by optimizing a quadratic performance index. Solution of the infinite-horizon LQR control problem for finite-dimensional (lumped parameter) systems involves solving an *algebraic matrix Riccati equation.* For infinite-dimensional (distributed parameter) systems there are two approaches. In the first method, which is called *spectral factorization*, the control law is obtained via solving an *operator Diophantine equation* (Callier and Winkin (1990)). This approach is used by Aksikas et al. (2007) to control the temperature and the concentration in a plug flow reactor. In the second approach, an *algebraic operator Riccati equation* is solved for a given state-space model (Curtain and Zwart (1995)). This approach was used for a particular class of hyperbolic PDEs (Aksikas et al. (2008)). This work was then extended to a more general class of hyperbolic systems by using an infinite-dimensional Hilbert state-space setting with distributed input and output (Aksikas et al. (2009)).

In this paper, the aforementioned work is extended to a system of first-order hyperbolic PDEs coupled with ODEs. In such systems, the input variable affects the distributed system through the lumped parameter system. The control objective is to drive the states of both lumped

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and distributed parameter systems to the equilibrium point in an optimal way.

This paper is organized as follows. In section 2, general formulation for a system containing a set of coupled linear first-order hyperbolic PDEs and linear ODEs is described. The system is then transformed into the Hilbert space and state transformation is used to make homogenous boundary condition. Section 3 focuses on designing an optimal feedback control. To this end, the *operator Riccati equation* is computed. This results in four *matrix Riccati equations*, which should be solved to obtain state feedback gain. In order to evaluate the performance of the proposed method, in section 4, the method is applied to a system containing a CSTR and a PFR in series with the recycle-rate as a control variable. First, the system is linearized around the equilibrium point. Then, the feedback control gain is obtained by solving the related *matrix Riccati equations*. Finally, the designed control policy is applied to the nonlinear system and simulation results are discussed.

2. FORMULATION OF THE PROBLEM

This paper addresses a control synthesis applied to the distributed parameter system which is coupled with the lumped parameter system through the boundaries. In these systems, the control variable affects the boundaries of the distributed system indirectly trough the lumped system. For example in a jacket-cooled fixed-bed reactor, the flow rate of the coolant (control variable) affects the boundary of the reactor (distributed system) through the jacket (lumped system). Mathematical model of these processes involve a set of coupled PDEs and ODEs. When diffusion process can be neglected or it is small in comparison to convection process, the distributed system is stated by a set of hyperbolic PDEs. Other important instances for these kinds of systems are lumped parameter systems followed by a transportation lag in which the pure delay is modeled by PDEs and the lumped system is modeled by ODEs (Hiratsuka and Ichikawa (1969)). The general mathematical model for these systems is given as follows:

$$\frac{\partial x_d}{\partial t}(z,t) = V\frac{\partial x_d}{\partial z}(z,t) + Mx_d(z,t) \tag{1}$$

$$\frac{dx_l}{dt}(t) = Ax_l(t) + Bu(t) \tag{2}$$

$$y(z,t) = C_0[x_d(z,t), x_l(t)]^T \tag{3}$$

with the following boundary and initial conditions:

$$x_d(0,t) = x_l(t) \tag{4}$$

$$x_d(z,0) = x_{d,0}(z) \tag{5}$$

$$x_l(0) = x_{l,0} \tag{6}$$

where, $x_d(.,t) \in L_2(0,1)^n$ and $x_l(t) \in \mathbb{R}^n$ denote the state variables for the distributed and the lumped parameter systems, respectively, $y(z,t) = [y_d(z,t), y_l(t)]^T$, $y_d(.,t) \in \mathscr{Y} := L_2(0,1)^p$ is the output variable for the distributed system, $y_l(t) \in \mathbb{R}^{p\times p}$ is the output variable for the lumped system, $z \in [0,1]$ is the spatial coordinate, $t \in [0,\infty]$ is the time, $u(t) \in \mathbb{R}^m$ is the input variable, $V = -\upsilon I \in \mathbb{R}^{n\times n}$ with $\upsilon > 0$ is a symmetric matrix, M is a real continuous space varying matrix, $B \in \mathbb{R}^{n\times m}$ is a real matrix, $C_0 = \begin{bmatrix} S_0 & 0 \\ 0 & S_0 \end{bmatrix}$ with $S_0 \in \mathbb{R}^{p*n}$, $x_{d,0}$ is a real continuous space varying vector, and $x_{l,0}$ is a constant vector.

The above system can be stated as an infinite-dimensional state-space system in the Hilbert space $\mathscr{H} = L_2(0,1)^n$ (Curtain and Zwart (1995)):

$$\dot{x}_d(t) = \mathscr{A}x_d(t) \tag{7}$$

$$\dot{x}_l(t) = Ax_l(t) + Bu(t) \tag{8}$$

$$y(t) = \bar{C}[x_d(t), x_l(t)]^T \tag{9}$$

$$\mathscr{B}x_d(t) = x_l(t) \tag{10}$$

Here $\mathscr{A}$ is a linear operator defined as:

$$\mathscr{A}h(z) = V\frac{dh}{dz} + Mh \tag{11}$$

where $h(z)$ is a smooth function on $[0,1]$, with the following domain:

$$D(\mathscr{A}) = \{h(z) \in \mathscr{H} : h(z) \text{and} \frac{dh(z)}{dz} \text{ are abs. cont.}, \frac{dh(z)}{dz} \in \mathscr{H}\} \tag{12}$$

$\mathscr{B}$ is a linear boundary operator defined as:

$$\mathscr{B}h(z) = h(0) \tag{13}$$

$$D(\mathscr{B}) = \{h(z) \in \mathscr{H} : h(z) \text{ is abs. cont.}\} \tag{14}$$

$\bar{C}$ is given by $\bar{C} = C_0 I$, where I is the identity operator.

The boundary condition defined in (10) is inhomogeneous. In order to produce a homogenous boundary condition, we apply *boundary control transformation* (see Curtain and Zwart (1995) and Fattorini (1968)). We assume that there is a function $\mathfrak{B}(z)$ such that for all $x_l(t)$, $\mathfrak{B}x_l(t) \in D(\mathscr{A})$ and:

$$\mathscr{B}\mathfrak{B}x_l(t) = x_l(t) \tag{15}$$

By assuming that $x_l(t) \in L_2(0,\infty)^n$ is sufficiently smooth and using the state transformation $\omega(t) = x_d(t) - \mathfrak{B}x_l(t)$ (Curtain and Zwart (1995)), we have:

$$\dot{\omega}(t) = \dot{x}_d - \mathfrak{B}\dot{x}_l$$

Then:

$$\begin{aligned} \dot{\omega}(t) &= \mathscr{F}\omega(t) + \mathscr{A}\mathfrak{B}x_l(t) - \mathfrak{B}\dot{x}_l \\ \omega(0) &= \omega_0 \end{aligned} \tag{16}$$

where $\omega_0 = x_{d,0} - \mathfrak{B}x_{l,0} \in D(\mathscr{F})$ and:

$$\mathscr{F}h(z) = \mathscr{A}h(z)$$

The domain of $\mathscr{F}$ is defined as:

$$D(\mathscr{F}) = D(\mathscr{A}) \cap ker(\mathscr{B}) = \{h(z) \in \mathscr{H} : h(z) \text{ and} \frac{dh(z)}{dz} \text{ are abs. cont.}, \frac{dh(z)}{dz} \in \mathscr{H}, \text{ and } \quad h(0) = 0\} \tag{17}$$

By combining (8) and (16) we obtain infinite-dimensional Hilbert state-space representation of the DPS-LPS as:

$$\begin{aligned} \begin{bmatrix} \dot{\omega}(t) \\ \dot{x}_l(t) \end{bmatrix} &= \begin{bmatrix} \mathscr{F} & \mathscr{A}\mathfrak{B} - \mathfrak{B}A \\ 0 & A \end{bmatrix} \begin{bmatrix} \omega(t) \\ x_l(t) \end{bmatrix} + \begin{bmatrix} -\mathfrak{B}B \\ B \end{bmatrix} u \\ y(t) &= C[\omega(t), x_l(t)]^T \\ \omega(0) &= \omega_0, x_l(0) = x_{l,0} \end{aligned} \tag{18}$$

where $C = \bar{C}\begin{bmatrix} I & \mathfrak{B} \\ 0 & I \end{bmatrix}$. We define state variables of the above system as $x(t) = [\omega(t), x_l(t)]^T$.

Remark 1. In the case of state LQR control, the outputs are the same as the states and therefore $S_0 = I$.

Remark 2. In Aksikas et al. (2009), it is proven that given $V < 0$, operator $\mathscr{F}$ generates an exponentially stable

C_0-semigroup. Therefore, If matrix A is stable, operator $\begin{bmatrix} \mathscr{F} & \mathscr{A}\mathfrak{B} - \mathfrak{B}A \\ 0 & A \end{bmatrix}$ provides a stable C_0-semigroup.

3. OPTIMAL CONTROL DESIGN

In this section we are interested in LQR control design for the DPS-LPS system according to the infinite-dimensional state-space representation of (18). The design is based on the minimization of an infinite-horizon quadratic objective function that requires the solution of an *operator Riccati equation* (Curtain and Zwart (1995); Bensoussan et al. (2007)). Solution of the *operator Riccati equation* of the DPS-LPS results in a set of *algebraic and differential matrix Riccati equations.* The optimal feedback gain can then be found by solving the equivalent *matrix Riccati equations.*

Let us consider the following objective function:

$$J(x_0, u) = \int_0^\infty (\langle Cx(t), PCx(t)\rangle + \langle u(t), Ru(t)\rangle)dt \quad (19)$$

where $x_0 \in \mathscr{H}$ is an initial condition, $P = P_0 I \in \mathcal{L}(\mathscr{Y})$, $P_0 = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \in \mathbb{R}^{2p\times 2p}$ is a positive semi-definite symmetric matrix, and $R \in \mathbb{R}^{m\times m}$ is a positive symmetric matrix. The minimization of the above objective function subject to the system of (18) results in solving the following *operator Riccati equation* (Aksikas et al. (2009) and the references therein):

$$[\mathcal{A}^*Q_0 + Q_0\mathcal{A} + C^*PC - Q_0\mathcal{B}R^{-1}\mathcal{B}^*Q_0]x = 0 \quad (20)$$

where $\mathcal{A} = \begin{bmatrix} \mathscr{F} & \mathscr{A}\mathfrak{B} - \mathfrak{B}A \\ 0 & A \end{bmatrix}$, $\mathcal{B} = \begin{bmatrix} -\mathfrak{B}B \\ B \end{bmatrix}$ and $Q_0 \in \mathcal{L}(\mathscr{H})$ is nonnegative self-adjoint operator. The above *operator Riccati equation* has a unique solution Q_0. The minimum cost function is given by $J(x_0, u_{opt}) = \langle x_0, Q_0x_0\rangle$ (see Curtain and Zwart (1995); Bensoussan et al. (2007)). For any initial condition $x_0 \in \mathscr{H}$ the unique optimal control variable u_{opt}, which minimizes the objective function of (19), is obtained on $t \geq 0$ as:

$$u_{opt} = Kx(t) \quad (21)$$

where

$$K = -R^{-1}\mathcal{B}^*Q_0 \quad (22)$$

Under this condition, $\mathcal{A} + \mathcal{B}K$ generates an exponentially stable C_0-semigroup (Curtain and Zwart (1995)).

Based on the form of operator $\mathcal{A}$ in (18), we consider the following solution:

$$Q_0 := \begin{bmatrix} \Phi(z)I & 0 \\ 0 & \Psi I \end{bmatrix} \quad (23)$$

where $\Phi(z), \Psi \in \mathbb{R}^{n\times n}$ are positive self-adjoint matrices. By substituting for $\mathcal{A}$, $\mathcal{B}$, C, and Q_0 in (20), we have:

$$\mathscr{F}^*\Phi + \Phi\mathscr{F} + S_0^*P_{11}S_0 - \Phi\mathfrak{B}BR^{-1}B^*\mathfrak{B}^*\Phi = 0 \quad (24)$$

$$\Phi(\mathscr{A}\mathfrak{B} - \mathfrak{B}A) + S_0^*P_{12}S_0 + \Phi\mathfrak{B}BR^{-1}B^*\Psi = 0 \quad (25)$$

$$(\mathscr{A}\mathfrak{B} - \mathfrak{B}A)^*\Phi + S_0^*P_{21}S_0 + \Psi BR^{-1}B^*\mathfrak{B}^*\Phi = 0 \quad (26)$$

$$A^*\Psi + \Psi A + S_0^*P_{22}S_0 - \Psi BR^{-1}B\Psi = 0 \quad (27)$$

Equation (24) is a *differential matrix Riccati equation.* We assume that the matrix $V = -vI, v > 0$ is diagonal with general diagonal elements. In this condition, (24) can be solved by the following set of ODEs (Aksikas et al. (2009)):

$$V\frac{d\Phi}{dz} = M^*\Phi + \Phi M + S_0^*P_{11}S_0 - \Phi\mathfrak{B}BR^{-1}B^*\mathfrak{B}^*\Phi$$
$$\Phi(1) = 0 \quad (28)$$

Equation (27) is an *algebraic matrix Riccati equation* which can be easily solved for finding Ψ. Equation (26) is adjoint of (25) and therefore these two equations are the same. Equation (25) can be satisfied by using elements of matrix P_{12} such that matrix P_0 remains positive semi-definite. We can derive the following equation from (25):

$$S_0^*P_{12}S_0 = -\Phi V - \Phi M\mathfrak{B} + \Phi\mathfrak{B}A - \Phi\mathfrak{B}BR^{-1}B^*\Psi \quad (29)$$

Proof. $\mathfrak{B}$ can be found from (15) as:

$$\mathscr{B}\mathfrak{B} = I \quad (30)$$

Then:

$$[\mathfrak{B}(z)]_{z=0} = I, \mathfrak{B}(z) = I + zI \in D(\mathscr{A}) \quad (31)$$

By using (11) we have:

$$\mathscr{A}\mathfrak{B} = V\frac{d\mathfrak{B}}{dz} + M\mathfrak{B} \quad (32)$$

Let us substitute expression for $\mathfrak{B}$ into (32), which yields:

$$\mathscr{A}\mathfrak{B} = V + M\mathfrak{B} \quad (33)$$

By substituting for $\mathscr{A}\mathfrak{B}$ in (25), we obtain (29). □

Remark 3. In the case of state LQR control where $S_0 = I$, the left-hand side of (29) reduces to P_{12}.

The solution procedure for the LQR problem is:

- Choose weighting matrices P_{11}, P_{22}, and R
- Solve (27) and (28) (*algebraic and differential matrix Riccati equations*) for finding Ψ and Φ
- Find P_{12} from (29) and we check whether matrix P_0 is positive semi-definite or not
- In the case that P_0 is not positive semi-definite we choose another P_{11} and P_{22} and resolve (27) and (28)
- Calculate the feedback gain from (22)

It should be noticed that since matrix P_0 is symmetric, $P_{12} = P_{21}$.

Remark 4. P_0 can be ensured to be positive semi-definite by always selecting $P_{22} \gg P_{11}$.

4. CASE STUDY

For the purposes of illustrating the results derived in previous sections, we consider a CSTR-PFR configuration shown in Fig. 1. This system includes a PFR as a distributed parameter system and a CSTR as a lumped parameter system. The combination of CSTR and PFR are used as an optimal reactor network for some complex chemical reactions (e.g. Chitra and Govind (1984)). It is also applied for some polymerization processes (e.g. Chen (1994)).

The following reaction takes place in both CSTR and PFR:

$$A + B \longrightarrow 2C, \qquad -r_A = kC_AC_B$$

The control objective is to control concentrations of all components in CSTR and PFR by using recycle-rate as the control variable.

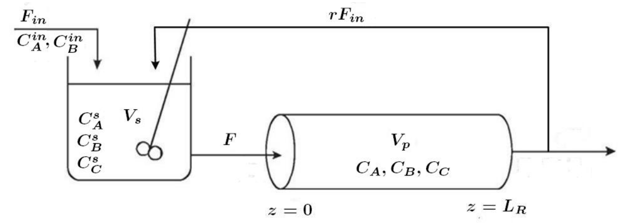

Fig. 1. CSTR-PFR system

Table 1. Dimensionless groups used in the case study

Constant	Expression	Value
K_2	$\frac{kC_0L_R}{v}$	0.3
K_3	$\frac{L_RF_{in}}{vV_s}$	7.67

In order to model the above process, we make the following assumptions:

- The reaction is isothermal
- CSTR volume is constant
- Inlet flow (F_{in}) is constant
- Diffusion is negligible in the PFR
- There are no transportation lags in the connecting lines
- Flow velocity in the PFR is constant with respect to spatial coordinate

In this condition the dimensionless mass balance for the system would be:

$$\frac{\partial x_{d,i}(\bar{z},\bar{t})}{\partial \bar{t}} = -\frac{\partial x_{d,i}(\bar{z},\bar{t})}{\partial \bar{z}} + \nu_i K_2 x_{d,1}(\bar{z},\bar{t}) x_{d,2}(\bar{z},\bar{t}) \quad (34)$$

$$\frac{dx_{l,i}(\bar{t})}{d\bar{t}} = K_3[x_{in,i} + r x_{d,i}(1,\bar{t}) - (1+r)x_{l,i}] + \nu_i K_2 x_{l,1} x_{l,2} \quad (35)$$

With the following boundary and initial conditions:

$$x_{d,i}(0,\bar{t}) = x_{l,i} \quad (36)$$

$$x_{d,i}(\bar{z},0) = x_{d,i,e}(\bar{z}) \quad (37)$$

$$x_{l,i}(0) = x_{l,i,e} \quad (38)$$

where subscripts $i = 1,2,3$ denotes components A,B, and C, respectively, $x_{d,i}(\bar{z},\bar{t}) = \frac{C_i(z,t)}{C_0}$ is the dimensionless concentration of the components in PFR, $x_{l,i}(\bar{t}) = \frac{C_i^s(t)}{C_0}$ is the dimensionless concentration of the components in PFR, $\bar{z} = \frac{z}{L_R} \in [0,1]$ is the dimensionless spatial coordinate, $\bar{t} = \frac{vt}{L_R} \in [0,\infty]$ is the dimensionless time, v is the fluid velocity in the PFR, r is the recycle-ratio, ν is the stoichiometric coefficient, subscribe e denotes the equilibrium point, and K_2 and K_3 are dimensionless groups which are defined in table 1.

We specify the desired concentration of the components at the end of the PFR to obtain desired equilibrium concentration profiles through the PFR and also equilibrium concentrations in the CSTR. Under this condition the inlet dimensionless concentrations of components A ($x_{in,A}$), B ($x_{in,B}$), and C ($x_{in,C}$) are 4, 3, and 0, respectively. The steady-state concentration profiles in the PFR is shown in Fig. 2. The steady-state concentration of each component in the CSTR is equal to the concentration of the corresponding component at the inlet of the PFR (see Fig. 1 and 2).

Now, the system can be linearized around the equilibrium point to obtain the system of (1) and (2). The linearized system can then be transformed into the system of (18).

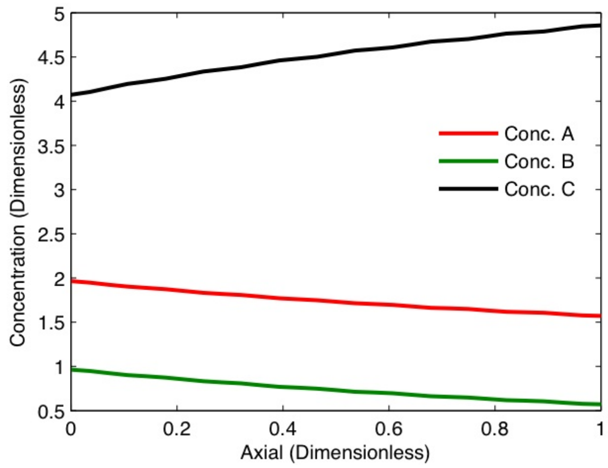

Fig. 2. Steady-state concentration profiles in the PFR

4.1 LQR Design

In this case study the control objective is to control the concentrations of all components and therefore, $S_0 = I_3$. In order to design LQR control for this system, first, we choose $P_{11} = I$ and $R = 1$ and we find Φ by solving the set of ODEs in (28) (*differential matrix Riccati equation*). Then by choosing $P_{22} = I$, we obtain matrix Ψ from (27) (*algebraic matrix Riccati equation*). We use MATLAB for solving (27) and (28). We obtain P_{12} from (29) and we check whether matrix P_0 is positive semi-definite or not. After reselecting matrices $P_{11} = 20I$ and $P_{22} = 100I$ we obtain P_{12} such that matrix P_0 is positive semi-definite. Then we find the feedback gain from (22) as:

$$K = B^*\mathfrak{B}^*\Phi(z) - B^*\Psi \quad (39)$$

4.2 Simulation Results

In this work gPROMS has been used to solve (34) to (38). *Orthogonal collocation on finite element* method is used to solve the coupled PDEs-ODEs system. In order to evaluate the performance of the designed LQR, we used an arbitrary initial conditions $[x_{l,A}(\bar{t}), x_{l,B}(\bar{t}), x_{l,C}(\bar{t})] = 0$ and $[x_{d,A}(\bar{z},\bar{t}), x_{d,B}(\bar{z},\bar{t}), x_{d,C}(\bar{z},\bar{t})] = 0.2\bar{z}^2$. We implemented the designed LQR controller to the original non-linear DPS-LPS. Fig. 3 to 5 show the simulation results for the closed-loop concentrations profiles in the PFR. It can be observed that the distributed states converge quickly from the arbitrary initial condition to the chosen equilibrium profile shown in Fig. 2. Simulation results for the closed-loop concentration changes in the CSTR is shown in Fig. 6. As it can be seen, the lumped states also converge quickly to the chosen equilibrium points from the selected initial condition. Finally, the variation of the control input is shown in Fig. 7.

5. CONCLUSION

In this work, LQR control problem for a class of coupled distributed and lumped parameter system was solved.

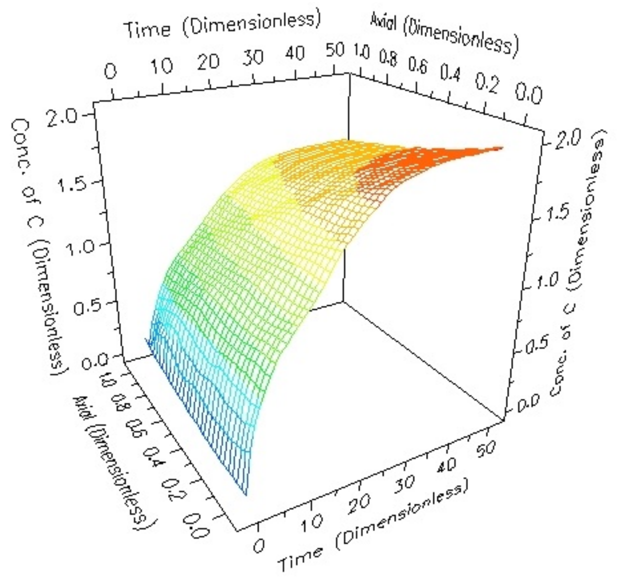

Fig. 3. Closed-loop concentration distribution for component A in the PFR

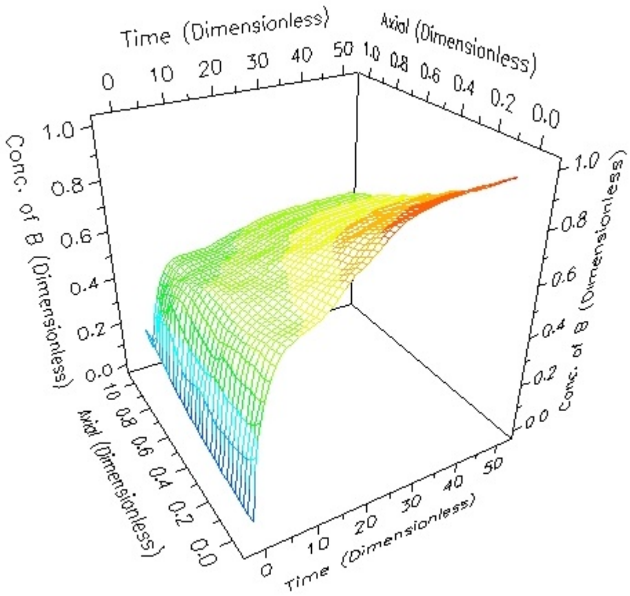

Fig. 4. Closed-loop concentration distribution for component B in the PFR

The system includes a set of hyperbolic PDEs coupled with a set of ODEs at the boundary condition. First, the system stated in a state-space form in the Hilbert space. Then, by introducing a new state, the system was transformed to a new state-space form with a homogenous boundary condition. The LQR control problem formulated and solved by converting the *operator Riccati equation* into the equivalent *algebraic and differential matrix Riccati equations*. The designed LQR was applied to a CSTR-PFR configuration and numerical simulation was performed by implementing the control system on the original non-linear process.

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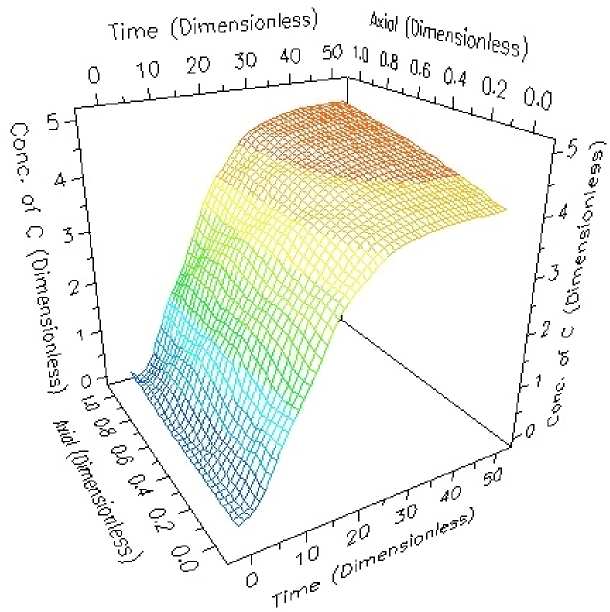

Fig. 5. Closed-loop concentration distribution for component C in the PFR

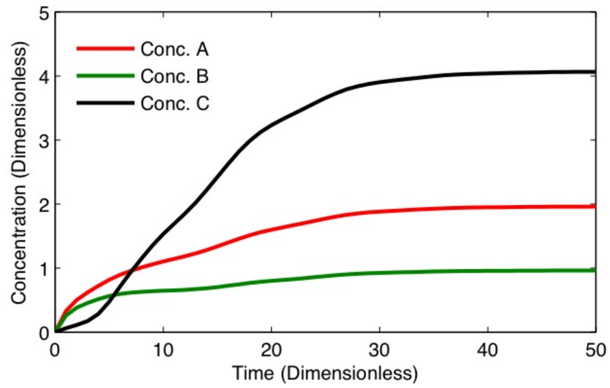

Fig. 6. Closed-loop concentrations in the CSTR

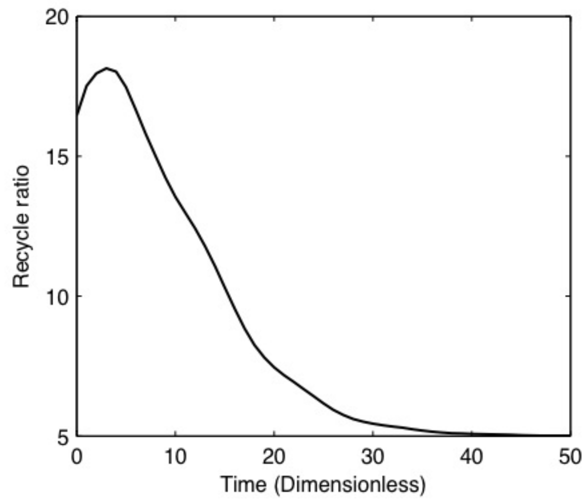

Fig. 7. Control input

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