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Brief paper

Boundary optimal (LQ) control of coupled hyperbolic PDEs and ODEs*

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ABSTRACT

This contribution addresses the development of a linear quadratic (LQ) regulator for a set of hyperbolic PDEs coupled with a set of ODEs through the boundary. The approach is based on an infinite-dimensional Hilbert state-space description of the system and the well-known operator Riccati equation (ORE). In order to solve the optimal control problem, the ORE is converted to a set of matrix Riccati equations. The feedback operator is found by solving the resulting matrix Riccati equations. The performance of the designed control policy is assessed by applying it to a system of interconnected continuous stirred tank reactor (CSTR) and a plug flow reactor (PFR) through a numerical simulation.

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1. Introduction

Many chemical processes are of a distributed nature. A common approach for modelling such distributed processes involves the use of PDEs. Lumping assumptions are often used to convert the PDEs to sets of ODEs, which allows the use of standard control methods applicable to ODE systems; however, this approximation results in some mismatch in the dynamical properties of the original distributed parameter and the lumped parameter models, which affects the performance of the designed model-based controller. A more rigorous way to deal with distributed parameter processes is to exploit the infinite-dimensional characteristic of the system. This approach was first applied in Harmon Ray (1980) to design controller for PDE systems using modal analysis. Other researchers also investigated the distributed nature of PDE systems in the area of non-linear control (Christofides, 2001; Orlov & Utkin, 1987), optimal control (Bensoussan, Da Prato, Delfour, & Mitter, 2007; Curtain & Zwart, 1995; Dubljevic, Mhaskar, El-Farra, & Christofides,

2005; Shang, Forbes, & Guay, 2004), using backstepping approach (Krstic & Smyshlyaev, 2008b), and Lyapunov methods (Coron, d'Andréa Novel, & Bastin, 2007; Orlov, 2000) to design high-performance controllers.

Occasionally, distributed chemical processes are coupled with lumped parameter processes. Such systems are modelled by a combination of PDEs and ODEs (DPS-LPS), in which the interaction can appear either in the differential equations or in the boundary conditions. For instance, in pressure swing adsorption, the mass balances for the components are modelled by a set of PDEs and the adsorption rates are modelled by a set of ODEs. Another example includes a jacket-equipped fixed-bed reactor, where the reactor (DPS) is interacting with the well-mixed jacket (LPS) via its boundary (see Borsche, Colombo, & Garavello, 2010, Oh & Pantelides, 1996, Tzafestas, 1970a, Wang, 1966 for more examples). Composite PDE-ODE models can also be used to describe transportation delay process accompanied by other chemical processes such as chemical reactions or mixing where differential-difference equations fail to model the system (Hiratsuka & Ichikawa, 1969). In such systems, the transportation delay process can be modelled by hyperbolic PDEs and the other portion of the system can be described by ODEs.

Despite the importance and inherent complexities in the structure of composite lumped and distributed parameter systems, research in the area of feedback control for these systems is relatively scarce. Well-posedness and controllability of coupled PDE-ODE systems were treated in some research work (see e.g. Borsche, Colombo, & Garavello, 2012, Littman & Markus, 1988,

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Weiss & Zhao, 2009). Stability and boundary feedback stabilization of such systems were also addressed (Bekiaris & Krstic, 2011; d'Andréa Novel, Boustany, Conard, & Rao, 1994; Krstic, 2009; Krstic & Smyshlyaev, 2008a; Rasmussen & Michel, 1976; Susto & Krstic, 2010; Tang & Xie, 2011). Most solid studies on optimal control of PDE-ODE systems were made in the 60s and 70s. In Wang (1966) a sufficient condition for stability and asymptotic stability for a scalar parabolic PDE-ODE system was derived by using the maximum principle for parabolic partial differential equations; however, this work assumed a specific type of the elliptical operator to use the weak maximum principle; moreover, the coupling terms were assumed to be uniformly bounded. In Tzafestas (1970b) classical Calculus of Variations was used to solve the optimal control problem for non-linear, mixed lumped and distributed parameter systems, and the associated canonical equations were derived. In addition, the optimal final-value control problem for these systems was solved in Tzafestas (1970a), and necessary optimality conditions were found by applying Green's identity together with functional analysis techniques. In Tzafestas (1970a), the optimal control input was calculated by solving a set of non-linear canonical equations, which involved a large number of coupled PDEs and ODEs. Dynamic programming was used in Thowsen and Perkins (1973) and Thowsen and Perkins (1975) to solve the discrete-time optimal feedback control problem for a class of linear composite systems.

Classical method in the optimal feedback controller synthesis is the well-known linear quadratic (LQ) regulator. The main objective of this control policy is to regulate a linear system by minimizing a quadratic performance index. An important advantage of LQ control is that it uses a state feedback law, in which the state feedback gain is calculated off-line by using LTI system's dynamics and thereby the amount of on-line calculations is reduced, significantly. In solving an LQ problem for an infinitedimensional (distributed) system, two common methods are available in the literature. The first approach is based on frequency domain description and is known as spectral factorization. In this method the control law is obtained via solving an operator Diophantine equation (Callier & Winkin, 1990). This technique was applied in Aksikas, Winkin, and Dochain (2007) to control the temperature and the concentration in a plug flow reactor. The second method involves solving an ORE for a given state-space model (Curtain & Zwart, 1995). This method was used in Aksikas, Winkin, and Dochain (2008) for a particular class of hyperbolic PDEs. The approach was then extended to a more general class of hyperbolic systems by using an infinite-dimensional Hilbert statespace setting with distributed input and output (Aksikas & Forbes, 2010; Aksikas, Fuxman, Forbes, & Winkin, 2009). When a statespace model is available, solving the optimal control problem with the ORE method requires less computational effort in comparison to the spectral factorization approach, which is more convenient for transfer function models.

The present work focuses on the development of an OREbased LQ control strategy for a class of linear hyperbolic distributed parameter systems interacting with a linear lumped parameter system through a Dirichlet boundary condition. In such system, the boundary control actuation involves finitedimensional dynamics, i.e., the manipulated input acts through the lumped system on the boundaries of the distributed system. The paper's main contributions can be summarized as follows: first, the system under study is described as an infinite-dimensional state-space by using the boundary control transformation method. Then, dynamical properties of the system including stability, stabilizability, and detectability are analysed. Subsequently, the infinite-time horizon LQ control problem for the system is formulated, and the related ORE is converted to a set of matrix Riccati equations. Finally, a computational algorithm is proposed for solving the resulting matrix Riccati equations. To demonstrate the theory, an illustrative example is given.

2. Problem statement

The general mathematical formulation for the systems considered is given as follows:

$$\frac{\partial x_d}{\partial t}(t,z) = V \frac{\partial x_d}{\partial z}(t,z) + M(z)x_d(t,z) + B_d(z)u(t)$$
 (1)

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

$$y(t) = C(\cdot)[x_d(t,\cdot), x_l(t)]^T$$
(3)

with the following boundary and initial conditions:

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

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

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

where $x_d(t,\cdot) \in L_2(0,1)^n$ and $x_l(t) \in \mathbb{R}^n$ denote the state variables for the distributed and the lumped parameter systems, respectively; $y(t) = [y_d(t,\cdot), y_l(t)]^T \in L_2(0,1)^p \oplus \mathbb{R}^p$; $y_d(t,\cdot) \in \mathscr{Y} := L_2(0,1)^p$ is the output variable for the distributed system; $y_l(t) \in \mathbb{R}^p$ 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; $V = \operatorname{diag}(v_1,v_2,\ldots,v_n) < 0$ is a symmetric matrix; M(z) and $B_d(z)$ are continuous matrices whose entries are functions in $L_\infty(0,1)$; $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{n \times m}$ are real matrices with bounded entries; $C(\cdot) = \operatorname{diag}(C_d(\cdot),C_l)$; $C_d(\cdot)$ is a continuous matrix whose entries are functions in $L_\infty(0,1)$; $C_l \in \mathbb{R}^{p \times n}$ is a real matrix with bounded entries; $x_{d,0}(z)$ is a real continuous spacevarying vector and $x_{l,0}$ is a constant vector.

It should be noted that in the above model, the control variable u(t) acts through the ODE part on the boundaries of the PDEs; however, the direct effect of the control variable on the PDEs is also taken into account by term $B_d(z)u(t)$.

The model (1)–(6) can be stated in an infinite-dimensional state-space in the *Hilbert* space $\mathcal{H} = L_2(0, 1)^n$ (Curtain & Zwart, 1995):

$$\dot{x}_d(t) = \mathcal{A}x_d(t) + \mathcal{B}_d u(t) \tag{7}$$

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

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

$$\mathscr{B}_h \mathsf{X}_d(t) = \mathsf{X}_l(t). \tag{10}$$

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

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

with the following domain:

$$D(\mathscr{A}) = \left\{ h(z) \in \mathscr{H} : h(z) \text{ is a.c., and } \frac{dh(z)}{dz} \in \mathscr{H} \right\}$$
 (12)

where a.c. means absolutely continuous.

 $\mathscr{B}_b \in \mathscr{L}(\mathscr{H}, \mathbb{R}^n)$ is a linear boundary operator defined as:

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

$$D(\mathcal{B}_b) = \{ h(z) \in \mathcal{H} : h(z) \text{ is a.c.} \}$$
 (14)

 $\mathscr{B}_d \in \mathscr{L}(\mathbb{R}^m, \mathscr{H})$ is given by $\mathscr{B}_d = B_d(\cdot)I$, and $\mathscr{C} \in \mathscr{L}(\mathscr{H} \oplus \mathbb{R}^n, \mathscr{Y} \oplus \mathbb{R}^p)$ is given by $\mathscr{C} = C(\cdot)I$, where I is the identity operator.

Remark 1. The assumption that the entries of the matrices M(z), $B_d(z)$, and $C_d(z)$ are functions in $L_{\infty}(0, 1)$, guarantees the boundedness of the matrix M(z) and the linear operators \mathcal{B}_d and \mathscr{C} .

The infinite-dimensional state-space system (7)–(10) with an inhomogeneous boundary condition can be transformed to a new system with a homogenous boundary condition using *boundary control transformation* (see Curtain & Zwart, 1995, Section 3.3 and Fattorini, 1968, Section 1). This is one way to prove the *exponential stabilizability* and *exponential detectability* properties of the system and also required to solve the resulting ORE (see Sections 3 and 4). We assume that there is a $\mathfrak{B} \in \mathcal{L}(\mathbb{R}^n, \mathcal{H})$ such that for all $x_l(t), \mathfrak{B}x_l(t) \in D(\mathscr{A})$ and:

$$\mathscr{B}_{h}\mathfrak{B}x_{l}(t) = x_{l}(t). \tag{15}$$

Operator $\mathfrak B$ satisfying the above conditions exists and also $\mathscr A\mathfrak B$ is an element of $\mathcal L(\mathbb R^n,\mathscr H)$ (see the proof of Theorem 3). Indeed, $\mathscr A\mathfrak B=M(z)I$ and since the entries of M(z) are functions in $L_\infty(0,1)$, then $\mathscr A\mathfrak B$ is bounded. Now, by assuming that $x_l(t)$ is sufficiently smooth, the state transformation $\omega(t)=x_d(t)-\mathfrak Bx_l(t)$ can be used to have (Curtain & Zwart, 1995, Definition 3.3.2 and Theorem 3.3.3):

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

Then:

$$\dot{\omega}(t) = \mathscr{F}\omega(t) + \mathscr{A}\mathfrak{B}x_l(t) + \mathscr{B}_d u(t) - \mathfrak{B}\dot{x}_l(t)$$

$$\omega(0) = \omega_0 \tag{16}$$

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 \mathcal{F} is defined as:

$$D(\mathscr{F}) = D(\mathscr{A}) \cap \ker(\mathscr{B}_b) = \left\{ h(z) \in \mathscr{H} : h(z) \right\}$$
is a.c., $\frac{dh(z)}{dz} \in \mathscr{H}$, and $h(0) = 0$. (17)

By combining (8) and (16) we obtain the new infinite-dimensional state-space representation of the DPS-LPS on $\mathcal{H} \oplus \mathbb{R}^n$ as:

$$\begin{bmatrix} \dot{\omega}(t) \\ \dot{x}_{l}(t) \end{bmatrix} = \begin{bmatrix} \mathcal{F} & \mathfrak{A} \\ 0 & A \end{bmatrix} \begin{bmatrix} \omega(t) \\ x_{l}(t) \end{bmatrix} + \begin{bmatrix} \bar{\mathcal{B}}_{d} \\ B \end{bmatrix} u(t)$$

$$y(t) = \mathcal{C}[\omega(t), x_{l}(t)]^{T}$$

$$\omega(0) = \omega_{0}, \qquad x_{l}(0) = x_{l,0}$$

$$\text{where } \mathfrak{A} = \mathcal{A}\mathfrak{B} - \mathfrak{B}A; \ \bar{\mathcal{B}}_{d} = \mathcal{B}_{d} - \mathfrak{B}B \in \mathcal{L}(\mathbb{R}^{m}, \mathcal{H}); \text{ and}$$

$$(18)$$

$$\mathbf{C} = \mathcal{C} \begin{bmatrix} I & \mathfrak{B} \\ \mathbf{0} & I \end{bmatrix} \in \mathcal{L}(\mathcal{H} \oplus \mathbb{R}^n, \mathcal{Y} \oplus \mathbb{R}^p).$$

Remark 2. System (18) has a homogeneous boundary condition as $\mathcal{B}_b\omega(t)=0$. Moreover, operator \mathscr{F} is the infinitesimal generator of a C_0 -semigroup on \mathscr{H} (Aksikas et al., 2009, Theorem 2) and therefore, system (18) is well-posed on $\mathscr{H} \oplus \mathbb{R}^n$ (Curtain & Zwart, 1995, Theorem 3.3.3).

We define the state variables for system (18) as $x(t) = [\omega(t), x_l(t)]^T \in \mathcal{H} \oplus \mathbb{R}^n$. Now, the system is written as:

$$\dot{x}(t) = \mathcal{A}x(t) + \mathcal{B}u(t)
y(t) = \mathcal{C}x(t)
x_0 = [\omega_0, x_{l,0}]^T \in \mathcal{H} \oplus \mathbb{R}^n$$
(19)

where A and B are linear operators, and defined as:

$$\mathcal{A} = \begin{bmatrix} \mathcal{F} & \mathfrak{A} \\ 0 & A \end{bmatrix}, \qquad \mathcal{B} = \begin{bmatrix} \bar{\mathcal{B}}_d \\ B \end{bmatrix}.$$

3. Dynamical properties

In this section, dynamical properties of the system given by (19) including *stability*, *stabilizability*, and *detectability* are studied. The following theorem, which is a special case of Curtain and Zwart (1995, Lemma 3.2.2), deals with the open-loop stability of system (19).

Theorem 3. If \mathscr{F} provides an exponentially stable C_0 -semigroup on \mathscr{H} and $\psi(t) = e^{At}$ is exponentially stable on \mathbb{R}^n , then operator \mathscr{A} provides an exponentially stable C_0 -semigroup on $\mathscr{H} \oplus \mathbb{R}^n$.

Proof. Let T(t) be C_0 -semigroup on \mathcal{H} generated by \mathscr{F} and $\psi(t) = e^{At}$ be state transition matrix generated by matrix A on \mathbb{R}^n . We also assume that there exist $m_1, m_2, \alpha_1, \alpha_2 > 0$ such that:

$$||T(t)|| < m_1 e^{-\alpha_1 t}, \qquad ||\psi(t)|| < m_2 e^{-\alpha_2 t}.$$

According to Curtain and Zwart (1995, Theorem 3.2.1), for operator $\mathcal A$ to be *infinitesimal generator* of a C_0 -semigroup on $\mathcal H \oplus \mathbb R^n$, the perturbation $\mathfrak A$ has to be bounded. First, we prove that this condition holds.

32 can be found from (15) as:

$$\mathcal{B}_b \mathfrak{B} x_l(t) = \mathcal{B}_b \mathfrak{B}_0(z) x_l(t) = x_l(t)$$

where $\mathfrak{B}_0(z) \in L_{\infty}(0, 1)^{n \times n}$. Then:

$$\mathfrak{B}_0(0) = I, \quad \mathfrak{B}_0(z) = I.$$

By using (11) we have:

$$\mathcal{A}\mathfrak{B}x_{l}(t) = \mathcal{A}\mathfrak{B}_{0}(z)x_{l}(t)$$

$$= V\frac{d[\mathfrak{B}_{0}(z)x_{l}(t)]}{dz} + M(z)\mathfrak{B}_{0}(z)x_{l}(t). \tag{20}$$

Let us substitute expression for $\mathfrak{B}_0(z)$, which yields:

$$\mathscr{A}\mathfrak{B}x_l(t) = M(z)x_l(t)$$

or:

$$\mathscr{A}\mathfrak{B} = M(z)I \tag{21}$$

where *I* is the identity operator. By using the triangular inequality of the induced norm by inner product in the *Hilbert* space, we have:

$$\|\mathscr{A}\mathfrak{B} - \mathfrak{B}A\| < \|\mathscr{A}\mathfrak{B}\| + \|\mathfrak{B}A\|$$

or:

$$\|\mathscr{A}\mathfrak{B} - \mathfrak{B}A\| \leq \|M\| + \|A\|.$$

Since the entries of M(z) are functions in $L_{\infty}(0, 1)$ and matrix A has real bounded elements, $\|\mathscr{A}\mathfrak{B} - \mathfrak{B}A\| = \|\mathfrak{A}\| < \infty$ and therefore, $\mathfrak{A} \in \mathscr{L}(\mathbb{R}^n, \mathscr{H})$.

Now, we prove the *exponential stability* of the C_0 -semigroup generated by A. By using (Curtain & Zwart, 1995, Theorem 3.2.1, Definition 3.1.4, and Lemma 3.2.2), the *mild solution* of (19) is given by:

$$x(t) = \bar{T}(t)x_0 + \int_0^t \bar{T}(t-s)\mathcal{B}u(s)ds$$
 (22)

where

$$\bar{T}(t) = \begin{bmatrix} T(t) & S(t) \\ 0 & \psi(t) \end{bmatrix}$$

is the C_0 -semigroup generated by \mathcal{A} , and operator S(t) is defined as:

$$S(t)h = \int_0^t T(t-s)\mathfrak{A}\psi(s)hds.$$

Then, by the same argument used in Curtain and Zwart (1995, Lemma 3.2.2), it can be shown:

$$\left\| \bar{T}(t) \begin{bmatrix} \omega \\ x_l \end{bmatrix} \right\| \le me^{-\alpha t} \left\| \begin{bmatrix} \omega \\ x_l \end{bmatrix} \right\|, \quad \alpha, m > 0. \quad \Box$$

Now, we explore *stabilizability* and *detectability* of system (19) in the following theorem. These properties are crucial in solving the LQ control problem in the next section.

Theorem 4. If the finite-dimensional system (A, B, C_l) is exponentially stabilizable and exponentially detectable on \mathbb{R}^n , so will be system (19) on $\mathcal{H} \oplus \mathbb{R}^n$.

Proof. Since operator \mathscr{F} and its adjoint operator \mathscr{F}^* are generators of exponentially stable C_0 -semigroups on \mathscr{H} (Aksikas et al., 2009, Theorem 2 and Remark 3) and the perturbation \mathfrak{A} is bounded (see the proof of Theorem 3), the proof can be done by using the same argument made in the proof of Curtain and Zwart (1995, Theorems 5.2.6 and 5.2.7). \square

4. LQ control synthesis

In this section, we are interested in LQ control synthesis for the DPS-LPS system (19). The design is based on the minimization of an infinite-time horizon, quadratic objective function that requires the solution of an ORE (see Curtain & Zwart, 1995, Section 6.2 and Bensoussan et al., 2007, Part V). The solution of the ORE can be achieved by converting it to an equivalent set of *matrix Riccati equations*. The optimal feedback operator can then be found by solving the resulting *matrix Riccati equations*.

Let us consider the following infinite-time horizon quadratic objective function:

$$J(x_0, u) = \int_0^\infty (\langle \mathcal{C}x(t), \mathcal{P}\mathcal{C}x(t)\rangle + \langle u(t), Ru(t)\rangle)dt$$
 (23)

where $\mathcal{P} = PI \in \mathcal{L}(\mathcal{Y} \oplus \mathbb{R}^p)$, in which

$$P = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \in \mathbb{R}^{2p \times 2p}$$

and $R \in \mathbb{R}^{m \times m}$ are positive symmetric matrices. The minimization of the above objective function subject to system (19) results in solving the following ORE (see Curtain & Zwart, 1995, Section 6.2):

$$[A^*Q + QA + C^*PC - QBR^{-1}B^*Q]x = 0.$$
 (24)

According to Curtain and Zwart (1995, Theorem 6.2.7), ORE (24) has a unique, non-negative, and self-adjoint solution $\mathcal{Q} \in \mathcal{L}(\mathcal{H} \oplus \mathbb{R}^n)$, if system (19) is *exponentially optimizable* (*stabilizable*) and *exponentially detectable*. Under these conditions, the minimum cost function is given by $J(x_0, u_{\text{opt}}) = \langle x_0, \mathcal{Q} x_0 \rangle$ and for any initial condition $x_0 \in \mathcal{H} \oplus \mathbb{R}^n$ the unique optimal control variable u_{opt} , which minimizes the objective function (23), is obtained on $t \geq 0$ as:

$$u_{\rm opt}(t) = Kx(t) \tag{25}$$

where

$$K = -R^{-1}\mathcal{B}^*\mathcal{Q}. \tag{26}$$

In addition, A + BK generates an exponentially stable C_0 -semigroup.

Remark 5. In cost functional (23), operator $\mathcal{P}^{1/2}\mathcal{C}$ plays the same role as operator \mathcal{C} in Curtain and Zwart (1995, Theorem 6.2.7). Since matrix P is assumed to be positive symmetric, if pair $(\mathcal{C}, \mathcal{A})$ is *exponentially detectable* on $\mathcal{H} \oplus \mathbb{R}^n$, so is pair $(\mathcal{P}^{1/2}\mathcal{C}, \mathcal{A})$ on $\mathcal{H} \oplus \mathbb{R}^n$. Indeed, there exists a feedback operator $\bar{F} \in \mathcal{L}(\mathcal{H} \oplus \mathcal{C})$

 \mathbb{R}^n , $\mathscr{Y} \oplus \mathbb{R}^p$) such that $A^* + C^* \bar{F}$ generates an exponentially stable C_0 -semigroup on $\mathscr{H} \oplus \mathbb{R}^n$. Then, we can find

$$\bar{F}' = \mathcal{P}^{-1/2}\bar{F} \in \mathcal{L}(\mathcal{H} \oplus \mathbb{R}^n, \mathcal{Y} \oplus \mathbb{R}^p)$$

such that $\mathcal{A}^* + \mathcal{C}^* \mathcal{P}^{1/2} \bar{F}'$ generates an exponentially stable C_0 -semigroup on $\mathcal{H} \oplus \mathbb{R}^n$. It should be noted that since P is positive symmetric, its square root is also positive symmetric (see e.g., Bernstein, 2005, P. 278), and therefore, $\mathcal{P}^{-1/2} = P^{-1/2}I$ exists.

It can be concluded from Theorem 4 and Remark 5 that if the finitedimensional system is *exponentially stabilizable* and *exponentially detectable*, ORE (24) has a unique, non-negative, and self-adjoint solution $\mathcal{Q} \in \mathcal{L}(\mathcal{H} \oplus \mathbb{R}^n)$. In order to solve the ORE, let us consider the following form of the solution:

$$\mathcal{Q} := \begin{bmatrix} \Phi_0 I & 0 \\ 0 & \Psi_0 I \end{bmatrix} \tag{27}$$

where Φ_0 , $\Psi_0 \in \mathbb{R}^{n \times n}$ are non-negative diagonal and non-negative symmetric matrices, respectively and I is the identity operator. Solutions of the form given in (27) help to convert ORE (24) into an equivalent set of *matrix Riccati equations*, which permits the use of a numerical scheme to solve the control design equations. Indeed, by substituting for \mathcal{A} , \mathcal{B} , \mathcal{C} , and \mathcal{Q} in (24), one obtains:

$$\mathscr{F}^*\Phi + \Phi\mathscr{F} + \mathscr{C}_d^*\mathscr{P}_{11}\mathscr{C}_d - \Phi\bar{\mathscr{B}}_d R^{-1}\bar{\mathscr{B}}_d^*\Phi = 0$$
 (28)

$$\Phi \mathfrak{A} + \mathcal{C}_d^* \mathcal{P}_{11} \mathcal{C}_d \mathfrak{B} + \mathcal{C}_d^* \mathcal{P}_{12} \mathcal{C}_l - \Phi \bar{\mathcal{B}}_d R^{-1} B^* \Psi = 0$$
 (29)

$$\mathfrak{A}^* \Phi + \mathfrak{B}^* \mathscr{C}_d^* \mathscr{P}_{11} \mathscr{C}_d + \mathscr{C}_l^* \mathscr{P}_{21} \mathscr{C}_d - \Psi B R^{-1} \bar{\mathscr{D}}_d^* \Phi = 0$$
 (30)

$$\mathbf{A}^*\Psi + \Psi\mathbf{A} + \mathfrak{B}^*\mathscr{C}_d^*\mathscr{P}_{11}\mathscr{C}_d\mathfrak{B} + \mathscr{C}_l^*\mathscr{P}_{21}\mathscr{C}_d\mathfrak{B}$$

$$+\mathfrak{B}^*\mathcal{C}_d^*\mathcal{P}_{12}\mathcal{C}_l+\mathcal{C}_l^*\mathcal{P}_{22}\mathcal{C}_l-\Psi BR^{-1}B^*\Psi=0$$
(31)

where
$$\Phi = \Phi_0 I$$
; $\Psi = \Psi_0 I$; $\mathscr{C}_d = C_d(\cdot) I$; $\mathscr{C}_l = C_l I$; $\mathscr{P}_{11} = P_{11} I$; $\mathscr{P}_{12} = P_{12} I$; $\mathscr{P}_{21} = P_{21} I$ and $\mathscr{P}_{22} = P_{22} I$.

Eq. (28) is an ORE, which can be converted to the following *matrix Riccati differential equation* (see Aksikas et al., 2009, Theorem 5):

$$V\frac{d\Phi_0}{dz} = M^*\Phi_0 + \Phi_0 M + C_d^* P_{11} C_d - \Phi_0 \bar{B}_d R^{-1} \bar{B}_d^* \Phi_0$$

$$\Phi_0(1) = 0$$
(32)

where $\bar{B}_d = B_d - \mathfrak{B}_0 B$.

The following *algebraic matrix equation* can be obtained from (21) and (29):

$$\Phi_0 M \mathfrak{B}_0 - \Phi_0 \mathfrak{B}_0 A + C_d^* P_{11} C_d \mathfrak{B}_0
+ C_d^* P_{12} C_l - \Phi_0 \bar{B}_d R^{-1} B^* \Psi_0 = 0.$$
(33)

Eq. (30) is the adjoint of (29) as $P_{21} = P_{12}^*$; therefore, these two equations are the same. The equivalent *algebraic matrix Riccati* equation for (31) is:

$$A^*\Psi_0 + \Psi_0 A + \mathfrak{B}_0^* C_d^* P_{11} C_d \mathfrak{B}_0 + C_l^* P_{12}^* C_d \mathfrak{B}_0 + \mathfrak{B}_0^* C_d^* P_{12} C_l + C_l^* P_{22} C_l - \Psi_0 B R^{-1} B^* \Psi_0 = 0.$$
 (34)

Eqs. (32)–(34) form a set of differential and algebraic equations (DAEs), in which Φ_0 is the differential variable, and Ψ_0 and P_{12} are the algebraic variables. Now, we are in a position to show the existence of solution (27) of ORE (24) in the following lemma and theorem.

Lemma 6. Let us consider positive symmetric matrices P_{11} and R. Then matrix Riccati differential equation (32) has a unique and nonnegative solution Φ_0 .

Proof. Since *V* is a negative diagonal matrix, *matrix Riccati differential equation* (32) can be written as:

$$\tilde{V}\frac{d\Phi_0}{dz} = -M^*\Phi_0 - \Phi_0 M - C_d^* P_{11} C_d + \Phi_0 \bar{B}_d R^{-1} \bar{B}_d^* \Phi_0$$

$$\Phi_0(1) = 0$$

where $\tilde{V}=-V$ is positive diagonal and P_{11} and R are positive symmetric. When $\tilde{V}=I$, it was proven in Abou-Kandil, Freiling, Ionescu, and Jank (2003, Theorem 4.1.6) that the above *matrix Riccati differential equation* has a unique and non-negative solution. This result can be extended to our case where Φ_0 is diagonal and \tilde{V} is constant positive diagonal. The key issue is to extend the assertion (a) of Abou-Kandil et al. (2003, Theorem 4.1.4). Let us use the notation of the above reference. We consider $\tilde{V}\dot{X}_i=\mathcal{R}(X_i;H_i),\ i=1,2,$ and define $X=\tilde{V}(X_2-X_1)$. Since, in our case, X, X_1 and X_2 are diagonal, they and \tilde{V} commute. Therefore, by the same argument used in the proof of Abou-Kandil et al. (2003, Theorem 4.1.4), it can be shown:

$$\dot{X} \leq \tilde{A}X + X\tilde{A}^*, \qquad X(t_0) = \tilde{V}(X_2 - X_1) \geq 0$$

where $\tilde{A} = \frac{1}{2}X\tilde{V}^{-1}S_2\tilde{V}^{-1} + X_1S_2\tilde{V}^{-1} - A_2^*\tilde{V}^{-1}$. Then, following from Abou-Kandil et al. (2003, Theorem 4.1.2):

$$X = \tilde{V}(X_2 - X_1) > 0$$

or $X_2 \ge X_1$. Consequently, Abou-Kandil et al. (2003, Theorem 4.1.6) can be easily extended to this case. Therefore, *matrix Riccati differential equation* (32) has a unique and non-negative solution Φ_0 .

Theorem 7. Let us consider positive symmetric matrices P_{11} and R and let Φ_0 be the unique and non-negative solution of matrix Riccati differential equation (32). Suppose (i) there exists a positive symmetric matrix P_{22} such that algebraic matrix equations (33)–(34) yield solutions Ψ_0 and P_{12} , and (ii) the resulting P_{12} is such that matrix P_{12} is positive. Then $Q_1 = \operatorname{diag}(\Phi_0 I, \Psi_0 I)$ is a non-negative solution of ORE (24).

Proof. Given positive symmetric P_{11} and R, it is proven in Lemma 6 that matrix Riccati differential equation (32) has a unique and non-negative solution Φ_0 . Given a positive symmetric matrix P_{22} , according to assumption (i), algebraic matrix equations (33)–(34) yield solutions Ψ_0 and P_{12} . On the other hand, algebraic matrix Riccati equation (34) can be written as:

$$A^*\Psi_0 + \Psi_0 A + \begin{bmatrix} \mathfrak{B}_0 C_d \\ C_l \end{bmatrix}^* \begin{bmatrix} P_{11} & P_{12} \\ P_{12}^* & P_{22} \end{bmatrix} \begin{bmatrix} \mathfrak{B}_0 C_d \\ C_l \end{bmatrix} - \Psi_0 B R^{-1} B^* \Psi_0 = 0.$$

Since (A,B) is stabilizable, and according to assumption (ii)

$$P = \begin{bmatrix} P_{11} & P_{12} \\ P_{12}^* & P_{22} \end{bmatrix} > 0,$$

following from Abou-Kandil et al. (2003, Corollary 2.3.8), (34) has a unique and non-negative solution Ψ_0 . Therefore, under assumptions (i) and (ii), DAEs (32)–(34) lead to unique and non-negative solutions Φ_0 and Ψ_0 and, subsequently, $\mathcal{Q} = \operatorname{diag}(\Phi_0 I, \Psi_0 I)$ is a solution of ORE (24). Moreover, the fact that Φ_0 and Ψ_0 are non-negative implies that \mathcal{Q} is non-negative. Indeed, for any $x \in \mathcal{H} \oplus \mathbb{R}^n$

$$\langle \mathcal{Q}x, x \rangle = \int_0^1 x^T \begin{bmatrix} \Phi_0 & 0 \\ 0 & \Psi_0 \end{bmatrix} x dz. \quad \Box$$

DAE system (32)–(34) can be solved by choosing weighting matrices P_{11} , P_{22} , and R to yield Φ_0 , Ψ_0 , and P_{12} ; however, the calculated P_{12} , should result in a positive matrix P. In order to satisfy this condition, we explore the characterization

of partitioned positive matrices. The conditions for symmetric partitioned matrix

$$P = \begin{bmatrix} P_{11} & P_{12} \\ P_{12}^* & P_{22} \end{bmatrix}$$

to be positive, are (see e.g., Zhang, 2005, Theorem 1.12):

$$P_{11} > 0$$
, and $P_{22} - P_{12}^* P_{11}^{-1} P_{12} > 0$

 $P_{22} - P_{12}^* P_{11}^{-1} P_{12}$ is the *Schur complement* of *P*. By using the above conditions, the following algorithm is proposed for solving DAEs (32)–(34):

- (1) Choose a positive symmetric P_{11} and R. Solve *matrix Riccati differential equation* (32), numerically, to find Φ_0 . This can be done using direct Runge–Kutta methods or other algorithms available in the literature (see e.g., Kenney & Leipnik, 1985).
- available in the literature (see e.g., Kenney & Leipnik, 1985). (2) Given Φ_0 , substitute $P_{22} = P_{12}^* P_{11}^{-1} P_{12} + \epsilon I$, $\epsilon > 0$ in (34) and solve the set of algebraic matrix equations (33)–(34) to find Ψ_0 and P_{12} .
- (3) Given P_{12} , choose a new $P_{22} > P_{12}^* P_{11}^{-1} P_{12} + \epsilon I$ and resolve (33)–(34) to find a new Ψ_0 .

The last step is optional and it may be done if it helps to achieve a more satisfactory control performance. Notice that by using the above algorithm, *P* can be ensured to be positive.

Remark 8. Although no convergence guarantee has been developed for the algorithm presented above, our experience has been that a solution is found within a small number of iterations through the steps of the algorithm. Our experience is based on a set of case studies, which have ranged from the illustrative example presented here to a detailed model of a catalytic distillation process.

Finally, the state feedback operator can be calculated from (26) as:

$$K = -R^{-1} \begin{bmatrix} \bar{\mathscr{B}}_d^* \Phi & B^* \Psi \end{bmatrix}. \tag{35}$$

It should be noted that this solution exists when the finitedimensional part is *exponentially stabilizable* and *exponentially detectable*.

Remark 9. The LQ control developed in this work is based on a late lumping approach, and the merits of late lumping versus early lumping approaches are well discussed in Harmon Ray (1980, Section 4) and Christofides (2001, Section 1.3). The only limitation of the proposed method is that in order to ensure the desired control performance, some restrictions on the choice of state weight P are required. Indeed, this restriction is being imposed by assuming the block-diagonal solution (27) to the ORE (24), which helps to convert the ORE (24) to the *matrix Riccati equations* (32)–(34). Nevertheless, the method gives the exact solution to the LQ control problem for the full infinite-dimensional model without using any approximation.

5. Case study

In this section, we consider a CSTR-PFR configuration shown in Fig. 1 as an interacting lumped and hyperbolic distributed parameter system. This reactor configuration is recommended for some types of chemical reactions (see e.g., Fogler, 2005, Section 2.5.3), and may be used to carry out Van de Vusse reaction to achieve the maximum conversion to the desired product (see e.g., Schweiger & Floudas, 1999, Section 5). Here, we assume reactions and kinetics:

$$A \longrightarrow B, \qquad -r_1 = k_1 e^{-E_1/RT} C_A$$

$$B \longrightarrow C, \qquad -r_2 = k_2 e^{-E_2/RT} C_B$$

$$2A \longrightarrow D, \qquad -r_3 = k_3 e^{-E_3/RT} C_A^2$$

$$(36)$$

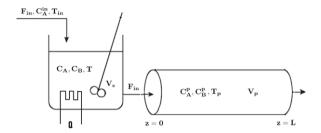


Fig. 1. CSTR-PFR system.

where k_1 , k_2 , and k_3 are pre-exponential constants; E_1 , E_2 , and E_3 are the activation energy and R is the universal gas constant. The exothermic reactions take place in both CSTR and PFR, and component B is the desired product.

The objective is to control both the components' concentration and the temperature within the reactors by using inlet flow rate $(F_{\rm in})$ and cooling rate from the CSTR (Q) as manipulated variables. It should be noticed that $F_{\rm in}$ and Q act on the boundary of PFR through the CSTR; however, when the liquid level is perfectly controlled in the CSTR, $F_{\rm in}$ has a direct effect on the boundary of the PFR as well.

With the assumptions of negligible diffusion in the PFR, perfect level control in the CSTR, no transportation lags in the connecting lines, constant fluid velocity in the PFR with respect to spatial coordinate, constant physical properties, and incompressible fluid, the mathematical model of the system is given as:

$$\frac{dC_A}{dt} = \frac{F_{\rm in}}{V_c} (C_A^{\rm in} - C_A) - k_1 e^{\frac{-E_1}{RT}} C_A - k_3 e^{\frac{-E_3}{RT}} C_A^2$$
 (37)

$$\frac{dC_B}{dt} = -\frac{F_{\rm in}}{V_{\rm s}} C_B + k_1 e^{\frac{-E_1}{RT}} C_A - k_2 e^{\frac{-E_2}{RT}} C_B \tag{38}$$

$$\frac{dT}{dt} = \frac{1}{\rho c_p} \left[k_1 e^{\frac{-E_1}{RT}} C_A(-\Delta H_1) + k_2 e^{\frac{-E_2}{RT}} C_B(-\Delta H_2) + k_3 e^{\frac{-E_3}{RT}} C_A^2(-\Delta H_3) \right] + \frac{F_{\text{in}}}{V_s} (T_{\text{in}} - T) + \frac{Q}{\rho c_n V_s}$$
(39)

$$\frac{\partial C_A^p}{\partial t} = -\upsilon \frac{\partial C_A^p}{\partial z} - k_1 e^{\frac{-E_1}{RT}} C_A^p - k_3 e^{\frac{-E_3}{RT}} C_A^{p2}$$

$$\tag{40}$$

$$\frac{\partial C_B^p}{\partial t} = -\upsilon \frac{\partial C_B^p}{\partial z} + k_1 e^{\frac{-E_1}{R^{\dagger}}} C_A^p - k_2 e^{\frac{-E_2}{R^{\dagger}}} C_B^p \tag{41}$$

$$\frac{\partial T_p}{\partial t} = -\upsilon \frac{\partial T_p}{\partial z} + \frac{k_1}{\rho c_p} e^{\frac{-E_1}{RT}} C_A^p (-\Delta H_1)
+ \frac{k_2}{\rho c_p} e^{\frac{-E_2}{RT}} C_B^p (-\Delta H_2) + \frac{k_3}{\rho c_p} e^{-E_3/RT} C_A^{p^2} (-\Delta H_3)$$
(42)

$$C_A^p(t,0) = C_A \tag{43}$$

$$C_p^p(t,0) = C_R \tag{44}$$

$$T_n(t,0) = T (45)$$

where C_A and C_B are the concentration of the components A and B in the CSTR, respectively; T is the temperature in the CSTR; C_A^p and C_B^p are the concentration of the components A and B in the PFR, respectively; T_p is the temperature in the PFR; $z \in [0, L]$ is the spatial coordinate; $t \in [0, \infty]$ is the time; $F_{\rm in}$, $C_A^{\rm in}$, and $T_{\rm in}$ are the volumetric flow-rate, concentration, and temperature of the feed to the CSTR; V_s and V_p are the volumes of the CSTR and the PFR, respectively; v is the fluid velocity in the PFR, which is given by $v = \frac{F_{\rm in}L}{V_p}$; ΔH_1 , ΔH_2 , and ΔH_3 are the heat of reaction for reactions 1, 2, and 3, respectively; ρ and c_p are the average fluid density and specific heat.

The model parameters used in this case study are given in Table 1. In the table, subscript "ss" denotes the steady-state

Table 1 Model parameters.

Parameter	Value
k_1	$225.2250 \times 10^6 \mathrm{s}^{-1}$
k_2	$225.2250 \times 10^6 \mathrm{s}^{-1}$
k_3	$1.583 \times 10^6 \text{ s}^{-1}$
$F_{\rm in,ss}$	$174.845 \times 10^{-6} \text{ m}^3/\text{s}$
Q_{ss}	−1.36 kJ/s
$Q_{ m ss} \ C_A^{ m in}$	5.1 kmol/m ³
$T_{\rm in}$	403.15 K
ΔH_1	-4200 kJ/kmol
ΔH_2	−11 000 kJ/kmol
ΔH_3	−41 850 kJ/kmol
E_1/R	9758.3 K
E_2/R	9758.3 K
E_3/R	8560.0 K
V_s	0.01 m^3
V_p	0.005 m ³
ho	934.2 kg/m^3
c_p	3.01 kJ/kg K

condition. In order to find the equilibrium condition for the system, the model equations (37)–(45) are solved at steady-state in gPROMS® Process systems enterprise (1997–2012). Simulation yields $C_{A,ss}$, $C_{B,ss}$, and T_{ss} ; 2.71 kmol/m³, 1.07 kmol/m³, and 409.79 K, respectively. The $C_{A,ss}^p$, $C_{B,ss}^p$, and $T_{p,ss}$ profiles are shown in Fig. 2. The model equations are linearized around the steady-state condition to yield the linear system (1)–(6) on $L_2(0,1)^3 \oplus \mathbb{R}^3$. Here $x_d = \begin{bmatrix} \bar{C}_p^p & \bar{C}_p^p & \bar{T}_p \end{bmatrix}^T \in L_2(0,1)^3$ where \bar{C}_A^p , \bar{C}_B^p and \bar{T}_p are the deviation distributed states; $x_l = \begin{bmatrix} \bar{C}_A & \bar{C}_B & \bar{T} \end{bmatrix}^T \in \mathbb{R}^3$ where \bar{C}_A , \bar{C}_B and \bar{T} are the deviation lumped states; $u = \begin{bmatrix} \bar{F}_{in} & \bar{Q} \end{bmatrix}^T \in \mathbb{R}^2$ where \bar{F}_{in} and \bar{Q} are the deviation input variables; $M(z) \in L_\infty(0,1)^{3\times3}$ is the Jacobian matrix of the functions at the right parts of (40)–(42) with respect to C_A^p , C_B^p , and T_p , evaluated at steady-state; $V = -\frac{F_{in,ss}L}{V_D}$ diag(1,1,1); $B_d(z) \in L_\infty(0,1)^{3\times2}$ is given by:

$$B_d(z) = -\frac{L}{V_p} \begin{bmatrix} \frac{\partial C_{A,ss}^p}{\partial z} & 0\\ \frac{\partial C_{B,ss}^p}{\partial z} & 0\\ \frac{\partial T_{p,ss}}{\partial z} & 0 \end{bmatrix}.$$

 $A \in \mathbb{R}^{3 \times 3}$ is the Jacobian matrix of the functions at the right parts of (37)–(39) with respect to C_A , C_B , and T, evaluated at steady-state and $B \in \mathbb{R}^{3 \times 2}$ is given by:

$$B = \begin{bmatrix} \frac{C_A^{\text{in}} - C_{A,ss}}{V_s} & 0\\ -\frac{C_{B,ss}}{V_s} & 0\\ \frac{T_{\text{in}} - T_{ss}}{V_s} & \frac{1}{\rho c_p V_s} \end{bmatrix}.$$

5.1. Controller design

We use the proposed optimal policy to control the components' concentration and the temperature in the CSTR and their profiles in the PFR. Since it is assumed that all the states in the reactors are measured, $C_d(z)$ and C_l are equal to diag(1, 1, 1). In order to find the LQ controller for this system, we apply the results obtained in Section 4 to the linearized process model, which satisfies all the conditions mentioned in Sections 2 and 4. The controller can be calculated by finding Φ_0 and Ψ_0 through solving the set of differential and algebraic equations (32)–(34) by using the proposed computational method, as follows:

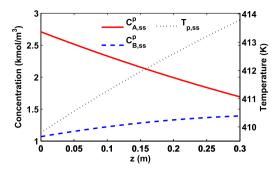


Fig. 2. Steady-state profiles in the PFR.

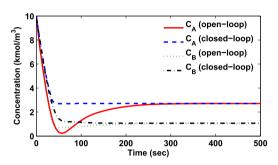


Fig. 3. Concentration responses in the CSTR.

- We choose $P_{11} = \text{diag}(110, 110, 110)$ and R = diag(0.01, 0.0001) and find Φ_0 through solving the differential equation (32)
- We consider $P_{22} = P_{12}^* P_{11}^{-1} P_{12} + \epsilon I$ and solve (33) and (34) to obtain Ψ_0 and P_{12} .
- In order to have a better control performance, we choose a new $P_{22} = \text{diag}(320, 320, 320)$, which satisfies $P_{22} > P_{12}^* P_{11}^{-1} P_{12} + \epsilon I$ and resolve (33) and (34) to get new Ψ_0 and P_{12} .

Finally, the feedback operator is obtained using (35).

5.2. Simulation results

In order to assess the performance of the control policy, the designed feedback operator is used with the original non-linear system (37)-(45). The set of coupled non-linear PDEs and ODEs are solved using orthogonal collocation on finite element method in gPROMS. We use $C_A(0) = 10 \text{ kmol/m}^3$, $C_B(0) = 10 \text{ kmol/m}^3$, T(0) = 406 K, $C_A^p(0, z) = 1 \text{ kmol/m}^3$, $C_B^p(0, z) = 1 \text{ kmol/m}^3$, and $T_p(0, z) = 403$ K as the initial conditions. To have a measure of how good the designed controller is, the responses of open-loop and closed-loop systems for the concentrations and the temperature in the CSTR and at the outlet of the PFR are compared in Figs. 3–5. As it can be seen, the controlled system is able to reject the effect of the initial condition about 3 times faster (with respect to the residence time) than the open-loop system, and it converges to the desired steady-state condition, accurately, Moreover, the open-loop inverse-responses appearing at the outlet of the PFR have disappeared. The variations of the control inputs are also shown in Fig. 6. The control efforts are not particularly aggressive, and are physically realizable.

6. Summary

In this work, the LQ control problem for a class of composite lumped and distributed parameter systems is formulated and solved by using ORE approach. In such system, the boundary control actuation involves finite-dimensional dynamics, i.e., the manipulated input acts through the lumped system on the

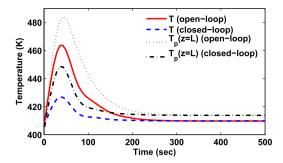


Fig. 4. Temperature responses in the CSTR and at the outlet of the PFR.

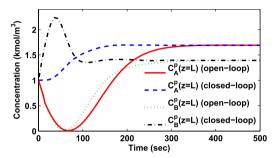


Fig. 5. Concentration responses at the outlet of the PFR.

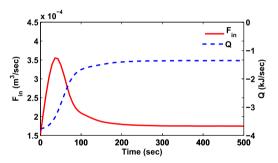


Fig. 6. Control input profiles.

boundaries of the distributed system. The LQ control problem is formulated based on an infinite-dimensional state-space representation of the system, which is obtained via a state transformation from the original system using the *boundary control transformation* method. The solution of the LQ control problem is achieved by solving the *matrix Riccati equations* that result from the ORE of the infinite-dimensional state-space representation. The designed optimal control policy is implemented on an interacting CSTR-PFR system through a numerical study. The simulations show that the controller results in a high performance closed-loop system.

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