University of Alberta

INFINITE-DIMENSIONAL LQ CONTROL FOR COMBINED LUMPED AND DISTRIBUTED PARAMETER SYSTEMS

by

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This thesis is dedicated to *my wife and parents*

Abstract

Transport-reaction processes are extensively present in chemical engineering practice. Typically, these processes involve phase equilibria and/or are combined with well-mixed processes. Examples include counter-current two-phase contactors, interconnected CSTR-PFR systems and distillation columns. These processes belong to the class of distributed parameter systems and their mathematical description involves combinations of partial differential equations (PDEs) , ordinary differential equations (ODEs) and algebraic equations. The commonly used techniques for controlling such distributed parameter systems involve approximation of the PDEs with a set of ODEs and applying standard control methods for lumped parameter systems. It is recognized that such approximate methods may result in significant errors in the analysis and control synthesis for distributed parameter systems. Therefore, the accurate analysis and control synthesis for these systems require the development of methods based on the infinite-dimensional control system theories.

The thesis focuses on the development of infinite-dimensional linear quadratic (LQ) control for distributed parameter systems described by combinations of hyperbolic PDEs, ODEs and algebraic equations. In order to solve the optimal control problem, the dynamical properties of the systems considered, including C_0-semigroup generation, exponential stabilizability and exponential detectability, are explored. These properties provide guarantees of the existence and uniqueness of the solution to the optimal control problem. The technique used to design the LQ controller is based on solving an operator Riccati

equation (ORE). This is achieved through finding the equivalent matrix Riccati equation, which can be solved numerically by using proposed algorithms. Several numerical simulation studies, including an interconnected CSTR-PFR process, a continuous counter-current adsorption process of two interacting components in a moving-bed adsorber and a catalytic distillation process, are performed to demonstrate the theoretical results.

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List of Abbreviations and Symbols

Abbreviations

a.c. Absolutely continuous

CD Catalytic distillation

CSTR Continuous stirred tank reactor

DAEs Differential and algebraic equations

DME Dimethyl ether

DPS Distributed parameter system

err Error

IAE Integral of absolute errors

LPS Lumped parameter system

LQ Linear quadratic

LTI Linear time-invariant

MOL Method of lines

MPC Model predictive control

ODEs Ordinary differential equations

ORE Operator Riccati equation

PDAEs Partial differential and algebraic equations

PDEs Partial differential equations

PFR Plug flow reactor

PI Proportional integral

RD Reactive distillation

Mathematical Symbols

$[h, g]^T$ Transpose of $[h, g]$

$\langle h, g \rangle$ Inner product of h and g

$\mathbb{C}$ Set of complex numbers

$\mathbb{R}$ Set of real numbers

$\mathbb{R}^n$ Space of real vectors

$\mathbb{R}^{n \times n}$ Space of real matrices

$\mathcal{L}(X)$ Space of bounded linear operators from X into X

$\mathcal{L}(X, Y)$ Space of bounded linear operators from X into Y

$\mathscr{A}^*$ Adjoint of $\mathscr{A}$

$\mathscr{H} \oplus \mathbb{R}^n$ Direct sum of $\mathscr{H}$ and $\mathbb{R}^n$

$\mathscr{H}$ State space

$\mathscr{U}$ Input space

$\mathscr{Y}$ Output space

$\overline{D(\mathscr{A})}$ Closure of $D(\mathscr{A})$

$\Re(\zeta, \mathscr{A})$ Resolvent operator of $\mathscr{A}$

$\rho(\mathscr{A})$ Resolvent set of $\mathscr{A}$

$D(\mathscr{A})$ Domain of $\mathscr{A}$

$diag(h_1, h_2, \ldots, h_n)$ Diagonal matrix with elements $h_1, h_2, \ldots, h_n$

$h(\cdot)$ $h(z)$

I Identity operator

$ker(\mathscr{A})$ Kernel of $\mathscr{A}$

$L_2(a, b)^n$ Hilbert space of measurable integrable real-valued functions $[a, b] \rightarrow \mathbb{R}^n$

$L_\infty(a, b)$ Space of bounded measurable real-valued functions $[a, b] \rightarrow \mathbb{R}^n$

$L_\infty(a, b)^{n \times n}$ Space of bounded measurable real-valued functions $[a, b] \rightarrow \mathbb{R}^{n \times n}$

$max(h, g)$ Maximum of h and g

$Re(h)$ Real part of h

Chapter 1

Introduction

Transport-reaction processes are commonly used in chemical and biochemical engineering for synthesis and separation of chemical products. Plug flow reactors (PFRs) are an example, in which the reactants are continuously converted to the products (reaction phenomenon) as they flow down the length of the reactor (transport phenomenon). These processes belong to the class of distributed parameter systems (DPS), meaning that the process variables are functions of both time and spatial position. Since the value of the process variables at each spatial position is a function solely of time, and there are an infinite number of spatial points, distributed parameter systems are also called infinite-dimensional systems. The dynamics of such processes can be described by partial differential equations (PDEs)[1]. The commonly used approach for controlling distributed parameter systems is the so-called early lumping methods (Ray, 1980). In these approaches, the system dynamics are approximated by a finite-dimensional model by discretizing the spatial derivatives of the PDE model at a finite number of points. This allows the use of standard ODE-based control methods; however, there remains the question regarding to what extent these approximate models represent the dynamics of the original distributed parameter system. Depending on the discretization scheme and the number and location of

[1]It should be noted that the mathematical description of the distributed parameter systems may also involve ordinary differential, algebraic and integral equations (Oh and Pantelides, 1996). The scope of the thesis does not include the integral equations. The presence of ordinary differential and algebraic equations are considered, which is discussed in Section 1.2.

discretization points, one might obtain different approximate models with different levels of accuracy. Therefore, applying the early lumping approaches may lead to significant errors in the analysis and controller synthesis for distributed parameter systems. For instance, using discretized models may result in erroneous conclusions regarding the dynamical properties of the open-loop system, such as controllability and observability, and also, the stability of the closed-loop system. Motivated by these considerations, a considerable effort has been made to develop control methods in the context of infinite-dimensional system representation. A review of these methods is given in the following section. This review is not intended to be exhaustive, but to provide the necessary background for the methods developed for the PDE systems that arise from mathematical modelling of transport-reaction processes.

1.1 PDE Systems - Control Background

In contrast to finite-dimensional systems, there is no general approach that can deal with the analysis and control synthesis for infinite-dimensional systems. The methods for the solution of the infinite-dimensional control problems strongly depend on the characteristics of the PDE models. To describe this, let us consider the general form of the linear PDE models, which represents the transport-reaction processes, in the following:

$$\frac{\partial x(t,z)}{\partial t} = \underbrace{D(z)\frac{\partial^2 x(t,z)}{\partial z^2}}_{\text{Axial dispersion}} + \underbrace{V(z)\frac{\partial x(t,z)}{\partial z}}_{\text{Convection}} + \underbrace{M(z)x(t,z)}_{\text{Reaction}} + \underbrace{B(z)u_d(t,z)}_{\text{Distributed control}} \tag{1.1}$$

$$D(z)\frac{\partial x(t,z)}{\partial z}\bigg|_{z=0} = \underbrace{V(z)|_{z=0}(x(t,z)|_{z=0} - u_b(t))}_{\text{Boundary control}}; \quad D(z)\frac{\partial x(t,z)}{\partial z}\bigg|_{z=L} = 0$$

where $x(t,z)$ is the distributed state variable; t is the time; $z \in [0, L]$ is the spatial coordinate; $D(z)$ is the dispersion coefficient matrix; $V(z)$ is the velocity matrix; $M(z)$ and $B(z)$ are matrix functions; $u_d(t,z)$ is the distributed control input variable; and $u_b(t)$ is the boundary control input variable.

The properties of the above PDE model are determined by the physical applications of the transport-reaction processes. There are many physical considerations that can contribute toward these properties; however, the contribution of the convection and/or axial dispersion mechanisms in the transport-reaction phenomena, the type of control actuation used and the number of fluid and/or solid phases involved are among the most important factors that have been considered in the literature. In the following, these physical considerations are demonstrated and used to classify the control methods developed for transport-reaction systems.

1.1.1 Transport Mechanism

The transport mechanism in a transport-reaction process includes convection and axial dispersion. Such a process can be described by parabolic PDE, which involves convection, diffusion and reaction terms. When the diffusion mechanism is dominant (highly dissipative parabolic PDE), the fact that the dynamics of the system are usually determined by a finite number of modes, motivates the use of modal analysis approaches to derive ODE models that capture the dominant dynamics of the system. These ODE models are subsequently used for controller design (Ray, 1980; Christofides and Baker, 1999; Baker and Christofides, 2000; Christofides, 2001; Dubljevic and Christofides, 2006*a*). In these methods, the number of the dominant modes (the order of the derived ODE model) depends on the contribution of the convection mechanism. As the effect of the convection increases, a higher order ODE model should be used to capture the dominant dynamics. When the convection mechanism is dominant (convection-dominated parabolic PDE), then the dynamics of the system are determined by a huge number of ODEs and therefore, the modal decomposition methods are not practical for these systems. For convection-dominated parabolic systems, a combination of the method of characteristics and finite difference approximation was used in (Shang *et al.*, 2007). This work, however, approximated the diffusion term by a discretization scheme, which introduced some error in the model used

for control design.

When the axial dispersion is negligible in comparison to the convection mechanism, the PDE model that describes the transport-reaction process does not involve the diffusion term and is of first-order hyperbolic type. The standard approach to deal with first-order hyperbolic PDE systems is the method of characteristics (Rhee *et al.*, 1986), which converts the underlying hyperbolic PDEs into equivalent ODE systems along the characteristic curves. This method was used in combination with ODE-based control methods such as model predictive control (Shang *et al.*, 2004) and sliding mode techniques (Sira-Ramirez, 1989; Hanczyc and Palazoglu, 1995). Applicability of these characteristic-based methods is restricted to systems having one or two characteristics with linear characteristic curves, which is not the case for the general applications of multi-component transport-reaction systems. For this reason, alternative methods were developed in the literature to address the control problem for first-order hyperbolic systems. The geometric control approach was used for a class of first-order quasi-linear hyperbolic systems (Christofides and Daoutidis, 1996; Christofides and Daoutidis, 1998). Moreover, a linear quadratic (LQ) regulator for first-order linear hyperbolic PDEs was studied in (Aksikas *et al.*, 2009) (using an operator Riccati equation (ORE) approach for a given infinite-dimensional state-space model) and in (Aksikas *et al.*, 2007) (using spectral factorization method for transfer function models). This work assumed that the velocity matrix in the transport operator is constant symmetric with negative eigenvalues. This assumption is not valid for some of the applications such as a counter-current two-phase contactors, where chemical equilibrium is established (see Section 1.2.2).

It can be concluded from the above discussion that the control design for convection-dominated transport-reaction systems (described by convection-dominated parabolic or first-order hyperbolic PDEs) is considered a harder problem to address. This is because of the fact that all the eigenmodes of the spatial differential operator for these systems

contain the same amount of energy. Some effort has been made in the literature to address the control problem for these systems. The existing methods involve some limitations and more research in this area seems to be required.

1.1.2 Control Actuation

The control actuation for transport-reaction systems is typically spatially distributed (in-domain control). Examples include heating/cooling jacket-equipped fixed-bed reactors. In the model equations representing such processes, both input and output variables belong to the distributed domain. This means that the input and output operators are bounded. As a result of this advantage, developing control methods for these systems is less challenging and has received more attention in the literature (Ray, 1980; Curtain and Zwart, 1995; Christofides, 2001; Bensoussan *et al.*, 2007).

In most physical applications of transport-reaction processes the control actuation is applied through the boundaries (boundary control). For example, consider a tubular reactor that is being controlled by manipulating the inlet concentration of the reactants. Although boundary control actuation is physically more realistic, boundary control problems are considered to be harder to solve. One of the main issues in solving boundary control problems is that the input and output operators for these systems are unbounded (Krstic and Smyshlyaev, 2008). As a result of this mathematical difficulty, fewer methods have been developed in this area. Stability and boundary feedback stabilization for boundary control systems containing a single PDE were addressed in (Fattorini, 1968; Curtain, 1985; Lasiecka and Triggiani, 1983; Emirsjlow and S.Townley, 2000; Slemrod, 1976; Krstic and Smyshlyaev, 2008). Optimal control of theses systems was also addressed in (Casas, 1997; Mordukhovich and Raymond, 2004; Hasanov, 2009). These contributions were mainly devoted to deriving necessary optimality conditions using optimal control theory for PDE systems and did not address the solution of the optimal control problem for application purposes. In (Dubljevic and Christofides, 2006*b*), predictive boundary control

for parabolic PDEs was addressed by using a modal decomposition technique to obtain a finite-dimensional approximation. This work only considered a single PDE; and moreover, the method cannot be applied to hyperbolic systems.

Regarding the preceding review of methods for boundary control systems, it can be concluded that the most of these only deal with transport-reaction systems described by a single PDE. Furthermore, there is no solid research work that can address the optimal control for these systems. Therefore, more research work on developing optimal boundary control methods for transport-reaction systems described by systems of PDEs is necessary.

1.2 Thesis Motivation

Transport-reaction processes are not limited to simple systems such as tubular reactors and, depending on the process design considerations, these processes may have more complicated configurations. The model equations representing such processes involve particular characterizations that require new treatment for system analysis and control synthesis. In the following, several examples are provided to show the variety of transport-reaction processes and the complexities they may have in the context of infinite-dimensional system representation.

1.2.1 Coupled Lumped/Distributed Parameter Systems

In some industrial applications, the transport-reaction processes may be used in combination with well-mixed processes. For example, consider the hybrid bioreactor shown in Figure (1.1) (Yeom, 2007). This process is used for the treatment of volatile organic compounds such as benzene. Wastewater containing volatile pollutants is fed to a bubble column bioreactor in which biodegradation and vaporization of the pollutants occur, simultaneously. The vaporized pollutant is then degraded in a biofilter section. In this process, the bubble column bioreactor, which may be considered a lumped parameter

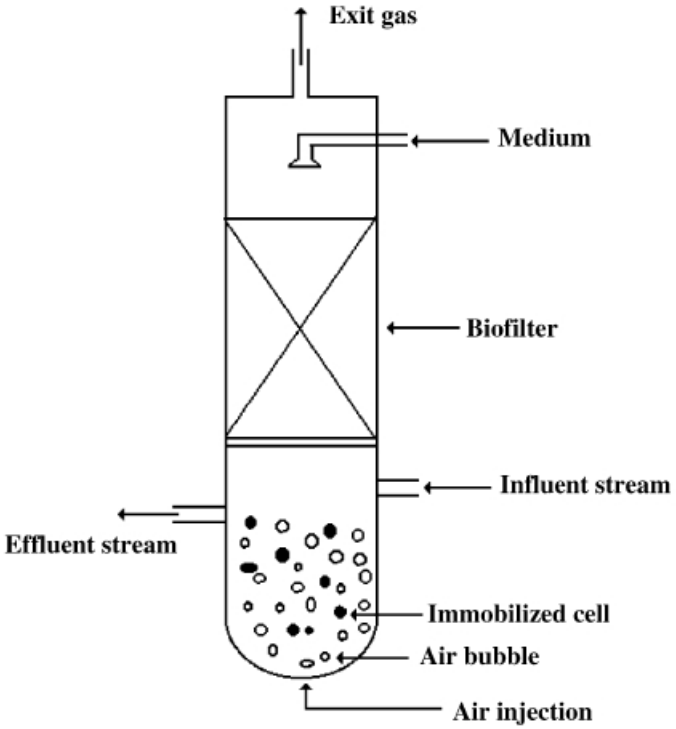

Figure 1.1: Hybrid bioreactor

system, is interconnected with the biofilter, which is a distributed parameter system, through the interface. The air injection flowrate as the manipulated input is indirectly applied on the biofilter through the bubble column bioreactor, i.e., the boundary control actuation of the biofilter involves finite-dimensional dynamics. The model equations for this system involve a combination of partial and ordinary differential equations (PDEs-ODEs). More examples for processes modelled by coupled PDEs-ODEs can be found in (Wang, 1966; Tzafestas, 1970*a*; Oh and Pantelides, 1996; Borsche *et al.*, 2010). Composite PDE-ODE models can also be used to describe the transportation delay accompanied by other chemical processes such as chemical reactions or mixing, where differential-difference equations fail to model the system (Hiratsuka and Ichikawa, 1969). In such systems, the transportation delay can be modelled by hyperbolic PDEs and the other portion of the system can be described by ODEs.

These processes belong to the class of boundary control problems; however, the boundary control actuation in these systems involves finite-dimensional dynamics. This introduces new challenges in the analysis and control synthesis for the underlying boundary control system. 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 (Weiss and Zhao, 2009; Borsche *et al.*, 2012). Boundary feedback stabilization of such systems involving a single PDE was also addressed using backstepping technique (Krstic and Smyshlyaev, 2008*a*; Krstic, 2009; Susto and Krstic, 2010; Bekiaris and Krstic, 2011; Tang and Xie, 2011). Most studies on optimal control of PDE-ODE systems have dealt with deriving necessary optimality conditions using optimal control theory for PDE systems, without providing a realistic method to solve the optimal control problem (Wang, 1966; Tzafestas, 1970*b*; Tzafestas, 1970*a*; Thowsen and Perkins, 1973; Thowsen and Perkins, 1975).

1.2.2 Two-Phase Systems

Typically, transport-reaction processes are fluid-solid or fluid-fluid contactors. These processes can be either in co-current or counter-current configuration and the contact between the phases can be either direct or indirect. Due to the interaction between the fluid and/or solid phases, the PDE models representing such transport-reaction systems involve special properties, which introduce issues in the development of control methods. For instance, the model equations for a fixed-bed catalytic reactor (in which a fluid phase is in a direct contact with a solid phase) may typically involve a system of coupled hyperbolic and parabolic PDEs (Tavazzi *et al.*, 2006). The approaches used for solving the control problems for hyperbolic and parabolic systems are totally different (Section 1.1.1) and new methods that combine these approaches must be developed in order to address the control problem for coupled hyperbolic and parabolic systems. Another

example includes a counter-current heat exchanger, in which two transport systems are interacting through an indirect contact. The model equations representing such a system comprise two heterodirectional hyperbolic PDEs (Maidi *et al.*, 2009). These systems are susceptible to open-loop instability (Christofides and Daoutidis, 1996). This, in particular, affects the verification of stabilizability and detectability properties, which are difficult to address for infinite-dimensional systems (Christofides and Daoutidis, 1996). Finally, consider a continuous counter-current adsorption process of two interacting components in a moving-bed adsorber (Rhee *et al.*, 1986, vol II). In such a process, two transport-reaction processes are exchanging mass and energy through a direct contact. When chemical equilibrium is established, this system is modelled by a combination of coupled partial differential and algebraic equations (PDAEs), in which the PDEs describe the transport-reaction phenomena, while the algebraic equations represent the equilibrium condition. The presence of the algebraic equations makes the velocity matrix in the transport operator spatially varying, non-diagonal, and not necessarily negative through of the domain. In contrast to transport operators with a constant, negative and diagonal velocity matrix (which is the case for most single-phase systems), dealing with the well-posedness (existence and uniqueness of the solution for the open-loop system) of such systems is not a standard argument (Russell, 1978). Moreover, solving the optimal control problem for systems involving such a transport operator is a challenging issue (Aksikas *et al.*, 2009).

Research in the area of feedback control for two-phase systems is really scarce. Most research work in this area concerned two heterodirectional hyperbolic PDEs representing a counter-current heat exchanger. Exponential stability property of these systems was studied in (Xu and Sallet, 2002). Also, boundary feedback stabilization of a 2×2 counter-current hyperbolic system was addressed in (Vazquez *et al.*, 2011; Coron *et al.*, 2007; Bastin and Coron, 2011). There is no solid research study on developing practical control methods for PDE models that arise from modelling of two-phase transport-reaction processes.

1.3 Thesis Scope and Contributions

The objective of this research work is to develop control methods for a class of transport-reaction systems coupled with lumped parameter processes, and also a class of two-phase transport-reaction systems. The transport-reaction processes considered in this thesis are described by system of first-order hyperbolic PDEs. This is motivated by the veriety of applications and specific theoritical characterizations of hyperbolic systems. Furthermore, the focus of the thesis is on optimal control methods to address the multivariate nature of transport-reaction processes.

Model predictive control (MPC) and LQ control are the most common optimal control strategies used in process control practice. The only available developed MPC method for first-order hyperbolic systems, that respects the infinite-dimensional characteristics of the system and can be realized in practice, is characteristic-based MPC presented in (Shang *et al.*, 2004). This method is based on equivalent ODE realizations obtained by the method of characteristics; however, the applicability of the method of characteristics is restricted to systems having one or two characteristics with linear characteristic curves, which is not the case for most multi-component transport-reaction systems. This limitation is mainly imposed by the state prediction problem. Therefore, LQ controller, which is based on an explicit design, seems to be more promising method for a wide range of transport-reaction processes represented by first-order hyperbolic PDEs. LQ control for these systems was addressed in (Aksikas *et al.*, 2009) using an ORE approach for a given infinite-dimensional state-space model, and in (Aksikas *et al.*, 2007) using spectral factorization method for transfer function models. This work made two main assumptions: 1) the control actuation is distributed (in-domain control) and the boundary control problem, which is the case for a large number of transport-reaction processes, was not addressed; and 2) the velocity matrix in the transport operator is constant symmetric with negative eigenvalues, which is not valid for the two-phase applications that are widely present in chemical engineering

processes. Furthermore, this work only considered the regulation problem and did not address the problem of rejecting disturbances, which is one of the main issues in process control practice.

This thesis is intended to make a contribution in the area of optimal control for transport-reaction processes. In particular, the thesis focuses on the development of infinite-dimensional LQ control for transport-reaction processes described by combinations of multivariate hyperbolic PDEs, ODEs and algebraic equations, which are extensively present in chemical engineering practice. To this end, infinite-dimensional systems theory is used to develop high-performance, computationally efficient and industrially realizable control methods. The main contributions of the thesis can be summarized as follows:

- Convection-dominated transport-reaction processes under boundary control actuation are considered. To address a wider range of systems, it is considered that the boundary control actuation involves finite-dimensional dynamics. A boundary control method is used to represent the resulting coupled PDE/ODE model in an infinite-dimensional state-space setting. Stability, stabilizability, and detectability properties of the system are analyzed. The infinite-time horizon LQ control problem for the system is formulated, and the related ORE is solved by converting it to a set of matrix Riccati equations for which the existence and uniqueness of the solution are proved. The results are applied to a CSTR-PFR process.

- Two-phase convection-dominated transport-reaction processes are treated. The C_0-semigroup generation and exponential stability of the hyperbolic operator resulting from coupled PDE/Algebraic equation model are proved. The ORE associated with the infinite-time horizon LQ control problem is solved through finding an equivalent matrix Riccati differential equation. The results are applied to a counter-current adsorption process.

- The results obtained for coupled PDE/Algebraic equation system are applied to the

detailed model of a catalytic distillation process. These results are then extended to develop an optimal infinite-dimensional proportional plus integral LQ controller, which can reject the effect of load losses.

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Chapter 2

Boundary Optimal (LQ) Control of Coupled Hyperbolic PDEs and ODEs

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2.1 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 (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 (Orlov and Utkin, 1987; Christofides, 2001), optimal control (Curtain and Zwart, 1995; Bensoussan *et al.*, 2007; Shang *et al.*, 2004; Dubljevic *et al.*, 2005), using backstepping approach (Krstic and Smyshlyaev, 2008), and Lyapunov methods (Orlov, 2000; Coron *et al.*, 2007) 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 (Wang, 1966; Tzafestas, 1970*a*; Oh and Pantelides, 1996; Borsche *et al.*, 2010) 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 and 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. (Weiss and Zhao, 2009; Borsche *et al.*, 2012; Littman and Markus, 1988)). Stability and boundary feedback stabilization of such systems were also addressed (Krstic and Smyshlyaev, 2008*a*; Krstic, 2009; Susto and Krstic, 2010; Bekiaris and Krstic, 2011; Tang and Xie, 2011; d'Andréa Novel *et al.*, 1994; Rasmussen and Michel, 1976). 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, 1970*b*) 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, 1970*a*), and necessary optimality conditions were found by applying Green's identity together with functional analysis techniques. In (Tzafestas, 1970*a*), 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 infinite-dimensional (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 and Winkin, 1990). This technique was applied in (Aksikas *et al.*, 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 and Zwart, 1995). This method

was used in (Aksikas *et al.*, 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 state-space setting with distributed input and output (Aksikas *et al.*, 2009; Aksikas and Forbes, 2010). When a state-space 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 ORE-based 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 finite-dimensional 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 analyzed. 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.

2.2 Problem Statement

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

$$\frac{\partial x_d}{\partial t}(t,z) = V\frac{\partial x_d}{\partial z}(t,z) + M(z)x_d(t,z) + B_d(z)u(t) \tag{2.1}$$

$$\frac{dx_l}{dt}(t) = Ax_l(t) + Bu(t) \tag{2.2}$$

$$y(t) = C(\cdot)[x_d(t,\cdot), x_l(t)]^T \tag{2.3}$$

with the following boundary and initial conditions:

$$x_d(t,0) = x_l(t) \tag{2.4}$$

$$x_d(0,z) = x_{d,0}(z) \tag{2.5}$$

$$x_l(0) = x_{l,0} \tag{2.6}$$

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; $V = diag(\upsilon_1, \upsilon_2, \ldots, \upsilon_n) < 0$ is a real 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; $C(\cdot) = diag(C_d(\cdot), C_l)$; $C_d(\cdot)$ 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 space-varying 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 (2.1) to (2.6) can be stated in an infinite-dimensional state-space in the Hilbert space $\mathscr{H} = L_2(0,1)^n$ (Curtain and Zwart, 1995):

$$\dot{x}_d(t) = \mathscr{A}x_d(t) + \mathscr{B}_d u(t) \tag{2.7}$$

$$\dot{x}_l(t) = Ax_l(t) + Bu(t) \tag{2.8}$$

$$y(t) = \mathscr{C}[x_d(t), x_l(t)]^T \tag{2.9}$$

$$\mathscr{B}_b x_d(t) = x_l(t) \tag{2.10}$$

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

$$\mathscr{A}h(z) = V\frac{dh(z)}{dz} + M(z)h(z) \tag{2.11}$$

with the following domain:

$$D(\mathscr{A}) = \{h(z) \in \mathscr{H} : h(z) \text{ is a.c., and } \frac{dh(z)}{dz} \in \mathscr{H}\} \tag{2.12}$$

where a.c. means absolutely continuous.

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

$$\mathscr{B}_b h(z) = h(0) \tag{2.13}$$

$$D(\mathscr{B}_b) = \{h(z) \in \mathscr{H} : h(z) \text{ is a.c.}\} \tag{2.14}$$

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

Remark 2.2.1 *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 $\mathscr{B}_d$ and $\mathscr{C}$.*

The infinite-dimensional state-space system (2.7) to (2.10) with an inhomogeneous boundary condition can be transformed to a new system with a homogenous boundary condition using boundary control transformation (see (Curtain and 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 2.3 and 2.4). We assume that there is a $\mathfrak{B} \in \mathcal{L}(\mathbb{R}^n, \mathscr{H})$ such that for all $x_l(t)$, $\mathfrak{B}x_l(t) \in D(\mathscr{A})$ and:

$$\mathscr{B}_b \mathfrak{B} x_l(t) = x_l(t) \tag{2.15}$$

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 2.3.1). 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 $\omega(t) = x_d(t) - \mathfrak{B}x_l(t)$ can be used to have (Curtain and 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:

$$\begin{aligned} \dot{\omega}(t) &= \mathscr{F}\omega(t) + \mathscr{A}\mathfrak{B}x_l(t) + \mathscr{B}_d u(t) - \mathfrak{B}\dot{x}_l(t) \\ \omega(0) &= \omega_0 \end{aligned} \tag{2.16}$$

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:

$$\begin{aligned} D(\mathscr{F}) = D(\mathscr{A}) \cap ker(\mathscr{B}_b) = \{h(z) \in \mathscr{H} : h(z) \\ \text{is a.c.}, \frac{dh(z)}{dz} \in \mathscr{H}, \text{and } h(0) = 0\} \end{aligned} \tag{2.17}$$

By combining (2.8) and (2.16) we obtain the new infinite-dimensional state-space representation of the DPS-LPS on $\mathscr{H} \oplus \mathbb{R}^n$ as:

$$\begin{aligned} &\begin{bmatrix} \dot{\omega}(t) \\ \dot{x}_l(t) \end{bmatrix} = \begin{bmatrix} \mathscr{F} & \mathfrak{A} \\ 0 & A \end{bmatrix} \begin{bmatrix} \omega(t) \\ x_l(t) \end{bmatrix} + \begin{bmatrix} \bar{\mathscr{B}}_d \\ B \end{bmatrix} u(t) \\ &y(t) = \mathcal{C}[\omega(t), x_l(t)]^T \\ &\omega(0) = \omega_0, x_l(0) = x_{l,0} \end{aligned} \tag{2.18}$$

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

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

Remark 2.2.2 *System (2.18) has a homogeneous boundary condition as $\mathscr{B}_b\omega(t) = 0$. 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 (2.18) is well-posed on $\mathscr{H} \oplus \mathbb{R}^n$ (Curtain and Zwart, 1995, Theorem 3.3.3).*

We define the state variables for system (2.18) as $x(t) = [\omega(t), x_l(t)]^T \in \mathscr{H} \oplus \mathbb{R}^n$. Now, the system is written as:

$$\begin{aligned} \dot{x}(t) &= \mathcal{A}x(t) + \mathcal{B}u(t) \\ y(t) &= \mathcal{C}x(t) \\ x_0 &= [\omega_0, x_{l,0}]^T \in \mathscr{H} \oplus \mathbb{R}^n \end{aligned} \tag{2.19}$$

where $\mathcal{A}$ and $\mathcal{B}$ are linear operators, and defined as:

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

2.3 Dynamical Properties

In this section, dynamical properties of the system given by (2.19) 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 (2.19).

Theorem 2.3.1 *If $\mathscr{F}$ generates an exponentially stable C_0-semigroup on $\mathscr{H}$ and $\psi(t) = e^{At}$ is exponentially stable on $\mathbb{R}^n$, then operator $\mathcal{A}$ generates an exponentially stable C_0-semigroup on $\mathscr{H} \oplus \mathbb{R}^n$.*

Proof: Let $T(t)$ be C_0-semigroup on $\mathscr{H}$ 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:

$$\|T(t)\| \leq m_1 e^{-\alpha_1 t}, \quad \|\psi(t)\| \leq m_2 e^{-\alpha_2 t}$$

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

$\mathfrak{B}$ can be found from (2.15) as:

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

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

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

By using (2.11) we have:

$$\mathscr{A}\mathfrak{B}x_l(t) = \mathscr{A}\mathfrak{B}_0(z)x_l(t) = V\frac{d[\mathfrak{B}_0(z)x_l(t)]}{dz} + M(z)\mathfrak{B}_0(z)x_l(t) \tag{2.20}$$

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

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

or:

$$\mathscr{A}\mathfrak{B} = M(z)I \tag{2.21}$$

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

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

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, $\mathfrak{A} \in \mathcal{L}(\mathbb{R}^n, \mathscr{H})$.

Now, we prove the exponential stability of the C_0-semigroup generated by $\mathcal{A}$. By using (Curtain and Zwart, 1995, Theorem 3.2.1, Definition 3.1.4, and Lemma 3.2.2), the mild solution of (2.19) is given by:

$$x(t) = \bar{T}(t)x_0 + \int_0^t \bar{T}(t-s)\mathcal{B}u(s)ds \tag{2.22}$$

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:

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

□

Now, we explore stabilizability and detectability of system (2.19) in the following Theorem. These properties are crucial in solving the LQ control problem in the next section.

Theorem 2.3.2 *If the finite-dimensional system (A, B, C_l) is exponentially stabilizable and exponentially detectable on $\mathbb{R}^n$, so will be system (2.19) on $\mathscr{H} \oplus \mathbb{R}^n$.*

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 2.3.1), 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).

□

2.4 LQ Control Synthesis

In this section, we are interested in LQ control synthesis for the DPS-LPS system (2.19). The design is based on the minimization of an infinite-time horizon, quadratic objective function that requires the solution of an ORE (see (Curtain and 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:

$$J(x_0, u) = \int_0^\infty (\langle \mathcal{C}x(t), \mathcal{P}\mathcal{C}x(t)\rangle + \langle u(t), Ru(t)\rangle)dt \tag{2.23}$$

where $\mathcal{P} = PI \in \mathcal{L}(\mathscr{Y} \oplus \mathbb{R}^p)$, 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 (2.19) results in solving the following ORE (see (Curtain and Zwart, 1995, Section 6.2)):

$$[\mathcal{A}^*\mathcal{Q} + \mathcal{Q}\mathcal{A} + \mathcal{C}^*\mathcal{P}\mathcal{C} - \mathcal{Q}\mathcal{B}R^{-1}\mathcal{B}^*\mathcal{Q}]x = 0 \tag{2.24}$$

According to (Curtain and Zwart, 1995, Theorem 6.2.7), ORE (2.24) has a unique, non-negative, and self-adjoint solution $\mathcal{Q} \in \mathcal{L}(\mathscr{H} \oplus \mathbb{R}^n)$, if system (2.19) is exponentially stabilizable and exponentially detectable. Under these conditions, the minimum cost function is given by $J(x_0, u_{opt}) = \langle x_0, \mathcal{Q}x_0\rangle$ and for any initial condition $x_0 \in \mathscr{H} \oplus \mathbb{R}^n$ the unique optimal control variable u_{opt}, which minimizes the objective function (2.23), is obtained on $t \geq 0$ as:

$$u_{opt}(t) = Kx(t) \tag{2.25}$$

where

$$K = -R^{-1}\mathcal{B}^*\mathcal{Q} \tag{2.26}$$

In addition, $\mathcal{A} + \mathcal{B}K$ generates an exponentially stable C_0-semigroup.

Remark 2.4.1 *In cost functional (2.23), 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 $\mathscr{H} \oplus \mathbb{R}^n$, so is pair $(\mathcal{P}^{1/2}\mathcal{C}, \mathcal{A})$ on*

$\mathscr{H} \oplus \mathbb{R}^n$. Indeed, there exists a feedback operator $\bar{F} \in \mathcal{L}(\mathscr{H} \oplus \mathbb{R}^n, \mathscr{Y} \oplus \mathbb{R}^p)$ such that $\mathcal{A}^* + \mathcal{C}^*\bar{F}$ generates an exponentially stable C_0-semigroup on $\mathscr{H} \oplus \mathbb{R}^n$. Then, we can find

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

such that $\mathcal{A}^* + \mathcal{C}^*\mathcal{P}^{1/2}\bar{F}'$ generates an exponentially stable C_0-semigroup on $\mathscr{H} \oplus \mathbb{R}^n$. 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 2.3.2 and Remark 2.4.1 that if the finite-dimensional system is exponentially stabilizable and exponentially detectable, ORE (2.24) has a unique, non-negative, and self-adjoint solution $\mathcal{Q} \in \mathcal{L}(\mathscr{H} \oplus \mathbb{R}^n)$. In order to solve the ORE, let us consider the following form of the solution:

$$\mathcal{Q} := \begin{bmatrix} \Phi_0 I & 0 \\ 0 & \Psi_0 I \end{bmatrix} \tag{2.27}$$

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 (2.27) help to convert ORE (2.24) 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 (2.24), one obtains:

$$\mathscr{F}^*\Phi + \Phi\mathscr{F} + \mathscr{C}_d^*\mathscr{P}_{11}\mathscr{C}_d - \Phi\bar{\mathscr{B}}_d R^{-1}\bar{\mathscr{B}}_d{}^*\Phi = 0 \tag{2.28}$$

$$\Phi\mathfrak{A} + \mathscr{C}_d^*\mathscr{P}_{11}\mathscr{C}_d\mathfrak{B} + \mathscr{C}_d^*\mathscr{P}_{12}\mathscr{C}_l - \Phi\bar{\mathscr{B}}_d R^{-1}B^*\Psi = 0 \tag{2.29}$$

$$\mathfrak{A}^*\Phi + \mathfrak{B}^*\mathscr{C}_d^*\mathscr{P}_{11}\mathscr{C}_d + \mathscr{C}_l^*\mathscr{P}_{21}\mathscr{C}_d - \Psi B R^{-1}\bar{\mathscr{B}}_d{}^*\Phi = 0 \tag{2.30}$$

$$A^*\Psi + \Psi A + \mathfrak{B}^*\mathscr{C}_d^*\mathscr{P}_{11}\mathscr{C}_d\mathfrak{B} + \mathscr{C}_l^*\mathscr{P}_{21}\mathscr{C}_d\mathfrak{B} + \mathfrak{B}^*\mathscr{C}_d^*\mathscr{P}_{12}\mathscr{C}_l + \mathscr{C}_l^*\mathscr{P}_{22}\mathscr{C}_l - \Psi B R^{-1}B^*\Psi = 0 \tag{2.31}$$

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 $\mathscr{P}_{22} = P_{22}I$.

Equation (2.28) is an ORE, which can be converted to the following matrix Riccati differential equation (see (Aksikas *et al.*, 2009, Theorem 5)):

$$\begin{aligned} V\frac{d\Phi_0}{dz} &= M^*\Phi_0 + \Phi_0 M + C_d^* P_{11} C_d - \Phi_0 \bar{B}_d R^{-1} \bar{B}_d^* \Phi_0 \\ \Phi_0(1) &= 0 \end{aligned} \tag{2.32}$$

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

The following algebraic matrix equation can be obtained from (2.21) and (2.29):

$$\Phi_0 M\mathfrak{B}_0 - \Phi_0\mathfrak{B}_0 A + C_d^* P_{11} C_d \mathfrak{B}_0 + C_d^* P_{12} C_l - \Phi_0 \bar{B}_d R^{-1} B^* \Psi_0 = 0 \tag{2.33}$$

Equation (2.30) is the adjoint of (2.29) as $P_{21} = P_{12}^*$; therefore, these two equations are the same. The equivalent algebraic matrix Riccati equation for (2.31) is:

$$\begin{aligned} A^*\Psi_0 + \Psi_0 A + \mathfrak{B}_0^* C_d^* P_{11} C_d \mathfrak{B}_0 + C_l^* P_{12}^* C_d \mathfrak{B}_0 + \\ \mathfrak{B}_0^* C_d^* P_{12} C_l + C_l^* P_{22} C_l - \Psi_0 B R^{-1} B^* \Psi_0 = 0 \end{aligned} \tag{2.34}$$

Equations (2.32), (2.33), and (2.34) 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 (2.27) of ORE (2.24) in the following Lemma and Theorem.

Lemma 2.4.1 *Let us consider positive symmetric matrices P_{11} and R. Then matrix Riccati differential equation (2.32) has a unique and non-negative solution Φ_0.*

Proof: Since V is a negative diagonal matrix, matrix Riccati differential equation (2.32) can be written as:

$$\begin{aligned} \tilde{V}\frac{d\Phi_0}{dz} &= -M^*\Phi_0 - \Phi_0 M - C_d^* P_{11} C_d + \Phi_0 \bar{B}_d R^{-1} \bar{B}_d^* \Phi_0 \\ \Phi_0(1) &= 0 \end{aligned}$$

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 *et al.*, 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:

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

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):

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

or $X_2 \geq X_1$. Consequently, (Abou-Kandil *et al.*, 2003, Theorem 4.1.6) can be easily extended to this case. Therefore, matrix Riccati differential equation (2.32) has a unique and non-negative solution Φ_0.

□

Theorem 2.4.1 *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 (2.32). Suppose i) there exists a positive symmetric matrix P_{22} such that algebraic matrix equations (2.33)-(2.34) yield solutions Ψ_0 and P_{12}, and ii) the resulting P_{12} is such that matrix P is positive. Then $\mathcal{Q} = diag(\Phi_0 I, \Psi_0 I)$ is a non-negative solution of ORE (2.24).*

Proof: Given positive symmetric P_{11} and R, it is proven in Lemma 2.4.1 that matrix Riccati differential equation (2.32) has a unique and non-negative solution Φ_0. Given a positive symmetric matrix P_{22}, according to assumption (i), algebraic matrix equations (2.33)-(2.34) yield solutions Ψ_0 and P_{12}. On the other hand, algebraic matrix Riccati equation (2.34) 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), (2.34) has a unique and non-negative solution Ψ_0. Therefore, under assumptions (i) and (ii), DAEs (2.32)-(2.34) lead to unique and non-negative solutions Φ_0 and Ψ_0 and, subsequently, $\mathcal{Q} = diag(\Phi_0 I, \Psi_0 I)$ is a solution of ORE (2.24). Moreover, the fact that Φ_0 and Ψ_0 are non-negative implies that $\mathcal{Q}$ is non-negative. Indeed, for any $x \in \mathscr{H} \oplus \mathbb{R}^n$

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

□

DAE system (2.32)-(2.34) 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 and Fuzhen, 2005, Theorem 1.12)):

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

$P_{22} - P_{12}^* P_{11}^{-1} P_{12}$ is the Schur complement of P. By using the above conditions, the following algorithm is proposed for solving DAEs (2.32)-(2.34):

1. Choose a positive symmetric P_{11} and R. Solve matrix Riccati differential equation (2.32), 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 and Leipnik, 1985));

2. Given Φ_0, substitute $P_{22} = P_{12}^* P_{11}^{-1} P_{12} + \epsilon I$, $\epsilon > 0$ in (2.34) and solve the set of algebraic matrix equations (2.33)-(2.34) 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 (2.33)-(2.34) 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 2.4.2 *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 (2.26) as:

$$K = -R^{-1} \left[\bar{\mathscr{B}}_d^* \Phi \quad B^* \Psi \right] \tag{2.35}$$

It should be noted that this solution exists when the finite-dimensional part is exponentially stabilizable and exponentially detectable.

Remark 2.4.3 *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 (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 (2.27) to the ORE (2.24), which helps to convert the ORE (2.24) to the matrix Riccati equations (2.32) to (2.34). Nevertheless, the method gives the exact solution to the LQ control problem for the full infinite-dimensional model without using any approximation.*

2.5 Case Study

In this section we consider a CSTR-PFR configuration shown in Figure 2.1 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 and Floudas, 1999, Section 5)). Here, we assume reactions and kinetics:

$$\begin{aligned} A &\longrightarrow B, \qquad -r_1 = k_1 e^{-E_1/RT} C_A \\ B &\longrightarrow C, \qquad -r_2 = k_2 e^{-E_2/RT} C_B \\ 2A &\longrightarrow D, \quad -r_3 = k_3 e^{-E_3/RT} C_A^2 \end{aligned} \tag{2.36}$$

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

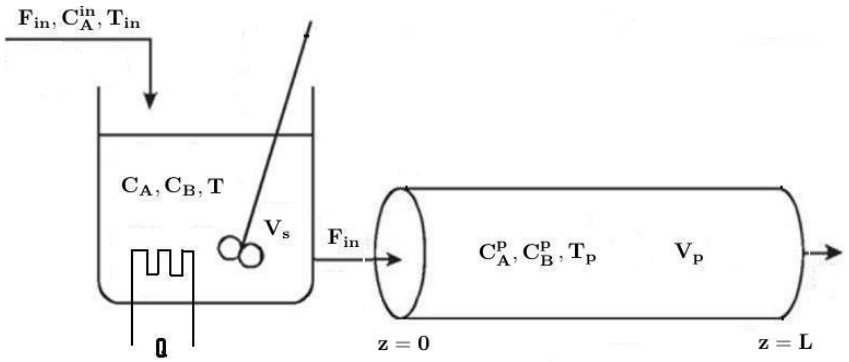

Figure 2.1: CSTR-PFR system

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:

$$\frac{dC_A}{dt} = \frac{F_{in}}{V_s}(C_A^{in} - C_A) - k_1 e^{\frac{-E_1}{RT}} C_A - k_3 e^{\frac{-E_3}{RT}} C_A^2 \tag{2.37}$$

$$\frac{dC_B}{dt} = -\frac{F_{in}}{V_s} C_B + k_1 e^{\frac{-E_1}{RT}} C_A - k_2 e^{\frac{-E_2}{RT}} C_B \tag{2.38}$$

$$\frac{dT}{dt} = \frac{1}{\rho c_p}[k_1 e^{\frac{-E_1}{RT}} C_A(-\Delta H_1) + k_2 e^{\frac{-E_2}{RT}} C_B(-\Delta H_2) + k_3 e^{\frac{-E_3}{RT}} C_A^2(-\Delta H_3)] + \frac{F_{in}}{V_s}(T_{in} - T) + \frac{Q}{\rho c_p V_s} \tag{2.39}$$

$$\frac{\partial C_A^p}{\partial t} = -\upsilon \frac{\partial C_A^p}{\partial z} - k_1 e^{\frac{-E_1}{RT}} C_A^p - k_3 e^{\frac{-E_3}{RT}} {C_A^p}^2 \tag{2.40}$$

$$\frac{\partial C_B^p}{\partial t} = -\upsilon \frac{\partial C_B^p}{\partial z} + k_1 e^{\frac{-E_1}{RT}} C_A^p - k_2 e^{\frac{-E_2}{RT}} C_B^p \tag{2.41}$$

$$\frac{\partial T_p}{\partial t} = -\upsilon \frac{\partial T_p}{\partial z} + \frac{k_1}{\rho c_p} e^{\frac{-E_1}{RT}} C_A^p(-\Delta H_1) + \frac{k_2}{\rho c_p} e^{\frac{-E_2}{RT}} C_B^p(-\Delta H_2) + \frac{k_3}{\rho c_p} e^{-E_3/RT} {C_A^p}^2(-\Delta H_3) \tag{2.42}$$

$$C_A^p(t, 0) = C_A \tag{2.43}$$

$$C_B^p(t, 0) = C_B \tag{2.44}$$

$$T_p(t, 0) = T \tag{2.45}$$

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_{in}, C_A^{in}, and T_{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; υ is the fluid velocity in the PFR, which is given by $\upsilon = \frac{F_{in} L}{V_p}$; ΔH_1, ΔH_2, and ΔH_3 are the heat of reaction for reactions 1, 2, and 3, respectively; and ρ and c_p are the average fluid density and specific heat.

The model parameters used in this case study are given in Table 2.1. In the table,

Table 2.1: Model parameters

Parameter	**Value**	**Parameter**	**Value**
k_1	$225.2250 \times 10^6\, sec^{-1}$	E_1/R	$9758.3\, K$
k_2	$225.2250 \times 10^6\, sec^{-1}$	E_2/R	$9758.3\, K$
k_3	$1.583 \times 10^6\, sec^{-1}$	E_3/R	$8560.0\, K$
$F_{in,ss}$	$174.845 \times 10^{-6}\, m^3/sec$	V_s	$0.01\, m^3$
Q_{ss}	$-1.36\, kJ/sec$	V_p	$0.005\, m^3$
C_A^{in}	$5.1\, kmol/m^3$	ρ	$934.2\, kg/m^3$
T_{in}	$403.15\, K$	c_p	$3.01\, kJ/kgK$
ΔH_1	$-4200\, kJ/kmol$		
ΔH_2	$-11000\, kJ/kmol$		
ΔH_3	$-41850\, kJ/kmol$		

subscript "ss" denotes the steady-state condition. In order to find the equilibrium condition for the system, the model equations (2.37) to (2.45) are solved at steady-state in gPROMS® (*Process Systems Enterprise, gPROMS. www.psenterprise.com*, 1997-2012). Simulation yields $C_{A,ss}$, $C_{B,ss}$, and T_{ss}; $2.71\ kmol/m^3$, $1.07\ kmol/m^3$, and $409.79\ K$, respectively. The $C^p_{A,ss}$, $C^p_{B,ss}$, and $T_{p,ss}$ profiles are shown in Figure 2.2. The model equations are linearized around the steady-state condition to yield the linear system (2.1) to (2.6) on $L_2(0,1)^3 \oplus \mathbb{R}^3$. Here $x_d = \begin{bmatrix}\bar{C}^p_A & \bar{C}^p_B & \bar{T}_p\end{bmatrix}^T \in L_2(0,1)^3$ where $\bar{C}^p_A$, $\bar{C}^p_B$ 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; $M(z) \in L_\infty(0,1)^{3\times 3}$ is the Jacobian matrix of the functions at the right parts of (2.40) to (2.42) with respect to C^p_A, C^p_B, and T_p, evaluated at steady-state; $V = -\frac{F_{in,ss}L}{V_p} diag(1,1,1)$; $B_d(z) \in L_\infty(0,1)^{3\times 2}$ is given by:

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

$A \in \mathbb{R}^{3\times 3}$ is the Jacobian matrix of the functions at the right parts of (2.37) to (2.39) with

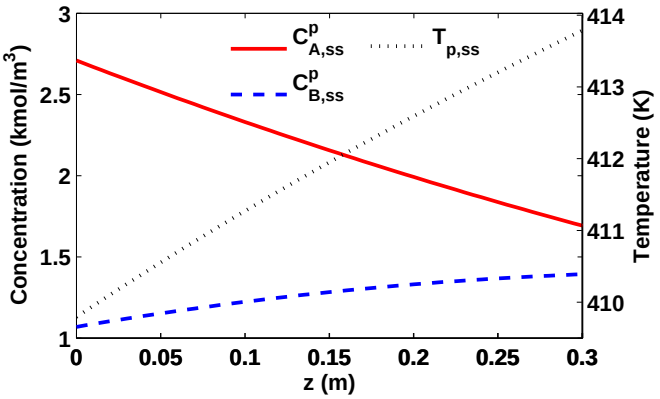

Figure 2.2: Steady-state profiles in the PFR

respect to C_A, C_B, and T, evaluated at steady-state; and $B \in \mathbb{R}^{3\times 2}$ is given by:

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

2.5.1 Controller Design

We use the proposed optimal policy to control the concentration of components A and B 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 2.4 to the linearized process model, which satisfies all the conditions mentioned in Sections 2.2 and 2.4. The controller can be calculated by finding Φ_0 and Ψ_0 through solving the set of differential and algebraic equations (2.32) to (2.34) by using the proposed computational method, as follows:

- We choose $P_{11} = diag(110, 110, 110)$ and $R = diag(0.01, 0.0001)$ and find Φ_0 through solving the differential equation (2.32);
- We consider $P_{22} = P_{12}^* P_{11}^{-1} P_{12} + \epsilon I$ and solve (2.33) and (2.34) to obtain Ψ_0 and P_{12};

- In order to have a better control performance, we choose a new $P_{22} = diag(320, 320, 320)$, which satisfies $P_{22} > P_{12}^{*} P_{11}^{-1} P_{12} + \epsilon I$ and resolve (2.33) and (2.34) to get new Ψ_0 and P_{12};

Finally, the feedback operator is obtained using (2.35).

2.5.2 Simulation Results

In order to assess the performance of the control policy, the designed feedback operator is used with the original non-linear system (2.37) to (2.45). The set of coupled non-linear PDEs and ODEs are solved using orthogonal collocation on finite element method in gPROMS. We use $C_A(0) = 10\ kmol/m^3$, $C_B(0) = 10\ kmol/m^3$, $T(0) = 406\ K$, $C_A^p(0, z) = 1\ kmol/m^3$, $C_B^p(0, z) = 1\ kmol/m^3$, 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 Figure 2.3 to Figure 2.5. 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 Figure 2.6. The control efforts are not particularly aggressive, and are physically realizable.

2.6 Conclusions

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 boundaries of the distributed system. The LQ

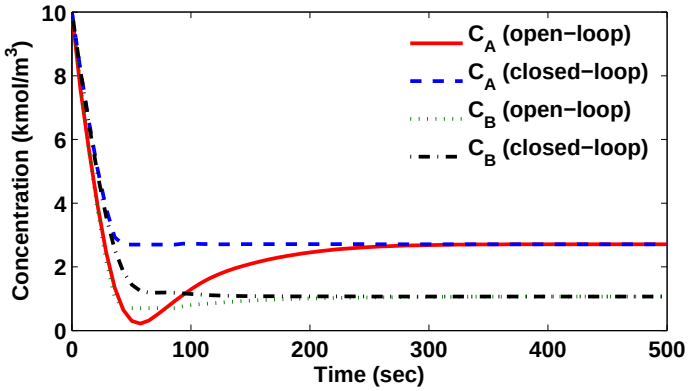

Figure 2.3: Concentration responses in the CSTR

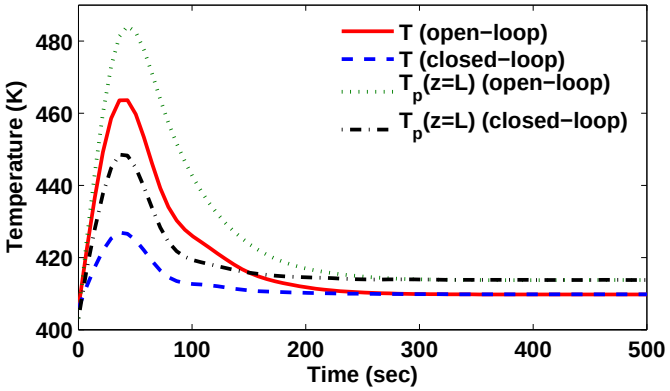

Figure 2.4: Temperature responses in the CSTR and at the outlet of the PFR

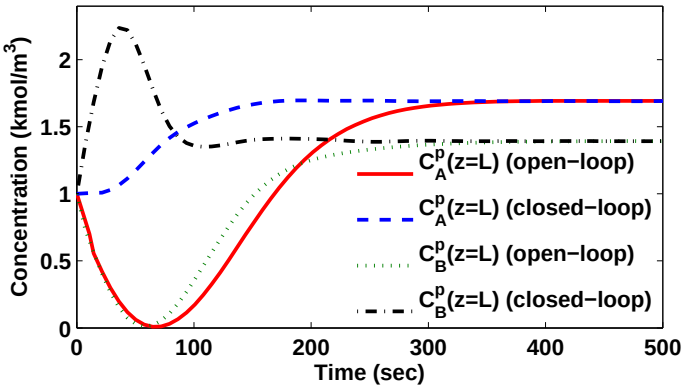

Figure 2.5: Concentration responses at the outlet of the PFR

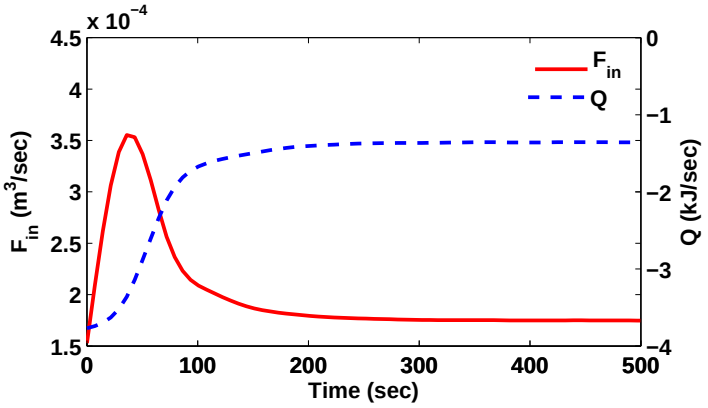

Figure 2.6: Control input profiles

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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Chapter 3

LQ (Optimal) Control of Hyperbolic PDAEs

The material of this chapter has been submitted in Systems & Control Letters.

3.1 Introduction

A range of distributed parameter processes in chemical and biochemical engineering are modelled by first-order hyperbolic PDAEs. Examples include, counter-current two-phase contactors such as multi-component (reactive) distillation (Noeres *et al.*, 2003) and adsorption in a moving bed adsorber (Rhee *et al.*, 1986) (see (Rhee *et al.*, 1986) for more examples). In such processes, the two phases are in direct contact with each other while moving in opposite directions. Model equations of these systems involve hyperbolic PDEs describing transport-reaction phenomena and algebraic equations representing the mass and energy transfer between the phases. Typically, where chemical equilibrium is assumed, the algebraic equations can be solved for the algebraic variables to yield a set of pure PDEs in which the velocity matrix is spatially varying, non-symmetric, and its eigenvalues are not necessarily negative through of the domain.

Developing control methods for PDE systems using infinite-dimensional approaches has been widely addressed in the literature. Modal analysis (Ray, 1980), non-linear control methods (Orlov and Utkin, 1987; Christofides, 2001), backstepping approach (Krstic and Smyshlyaev, 2008), optimal control techniques (Curtain and Zwart, 1995; Bensoussan *et al.*, 2007), and Lyapunov methods (Orlov, 2000) have been applied to design high-performance controllers. First-order hyperbolic PDE systems have been of particular interest due to their specific characterizations and verity of physical applications. An important characterization of hyperbolic PDEs is that the modal decomposition method is not applicable to them. The method of characteristics was used in (Ray, 1980; Shang *et al.*, 2004) to convert hyperbolic PDEs to equivalent ODE system; however, applicability of the method of characteristics is restricted to systems having one or two characteristics with linear characteristic curves. In (Christofides and Daoutidis, 1996) the geometric control approach was used for a class of quasi-linear hyperbolic systems. This work assumed a symmetric velocity matrix with partially negative eigenvalues to preserve the C_0-semigroup generation property. In (Winkin *et al.*, 2000) dynamical properties such as observability and reachability of a class of first-order hyperbolic systems containing two PDEs with constant negative diagonal velocity matrix were explored.

Linear quadratic (LQ) regulator is a classical method in the optimal control techniques. This control policy for infinite-dimensional systems has been addressed in the literature using spectral factorization method for transfer function models (Aksikas *et al.*, 2007), and operator Riccati equation (ORE) method for state-space models (Curtain and Zwart, 1995; Aksikas *et al.*, 2008; Aksikas *et al.*, 2009).

In previous research effort (Moghadam *et al.*, 2013), LQ control problem for a set of hyperbolic PDEs coupled with a set of ODEs through the interface was treated. In such systems, the boundary control actuation of a transport-reaction system involves finite-dimensional dynamics. Using the boundary control transformation method, the system was

represented in an infinite-dimensional state-space setting $L_2(0,1)^n \oplus \mathbb{R}^n$, which involves a coupling between both PDE and ODE parts. The C_0-semigroup generation and exponential stability properties of the coupled system were proved by using the well-posedness of the transformed system and by taking advantage of the constant negative diagonal velocity matrix for the PDE part. Moreover, it was shown that the ORE for the mixed system can be converted to a system of coupled differential and algebraic matrix Riccati equations, which has a unique and non-negative solution provided that the velocity matrix associated with the PDE part is constant negative diagonal (Moghadam *et al.*, 2013). Then, a computational algorithm was proposed for solving the coupled differential and algebraic matrix Riccati equations.

In the present work, we address the LQ control problem for a system of hyperbolic PDEs coupled with a system of algebraic equations (PDAEs). In such systems, a transport-reaction process is constrained by equilibrium condition. The coupling between the PDEs and algebraic equations results in a set of pure hyperbolic PDEs in which the velocity matrix is non-constant, non-symmetric and not necessarily negative. The C_0-semigroup generation property of the underlying hyperbolic operator is proved using the Hille-Yosida theorem and its exponential stability property is shown by proving the conditions of (Luo *et al.*, 1999, Theorem 3.35). These properties provide guarantees of the existence and uniqueness of the solution to the ORE. This solution is then found through converting the ORE to an equivalent matrix Riccati differential equation, which can be solved numerically to find the optimal feedback operator. To demonstrate the theory, an illustrative example is given at the end.

3.2 Problem Statement

The general mathematical formulation of the PDAE system considered is given as follows:

$$\frac{\partial \mathbf{x}}{\partial t} = u_1 \mathbf{V}_x \frac{\partial \mathbf{x}}{\partial z} + u_2 \mathbf{V}_w \frac{\partial \mathbf{w}}{\partial z} + \mathbf{V}_t \frac{\partial \mathbf{w}}{\partial t} + \mathbf{Q}(\mathbf{x}, \mathbf{w}) \tag{3.1}$$

$$\mathbf{w} = \mathbf{f}(\mathbf{x}) \tag{3.2}$$

with the following boundary and initial conditions:

$$\mathbf{x}(0,t) = 0, \quad \mathbf{w}(1,t) = \mathbf{w}_{in} \tag{3.3}$$

$$\mathbf{x}(z,0) = \mathbf{x}_e(z), \quad \mathbf{w}(z,0) = \mathbf{f}(\mathbf{x}_e(z)) \tag{3.4}$$

where $\mathbf{x}(.,t) = [x_1(.,t), \ldots, x_n(.,t)]^T \in \mathscr{H} = L_2(0,1)^n$ is the vector of distributed variables; $L_2(0,1)^n$ denotes the Hilbert space of measurable integrable real-valued functions $[0,1] \rightarrow \mathbb{R}^n$; $\mathbf{w}(.,t) = [w_1(.,t), \ldots, w_n(.,t)]^T \in L_2(0,1)^n$ is the vector of algebraic variables; $u_1(t), u_2(t) \in \mathbb{R}$ are the input variables; $\mathbf{V}_x = diag(\nu_{x,1}, \ldots, \nu_{x,n})$, $\mathbf{V}_w = diag(\nu_{w,1}, \ldots, \nu_{w,n})$, $\mathbf{V}_t = diag(\nu_{t,1}, \ldots, \nu_{t,n})$ with $\nu_{x,i}, \nu_{t,i} < 0, \nu_{w,i} > 0, i = 1, \ldots, n$, are constant diagonal matrices; $\mathbf{Q}(\mathbf{x}, \mathbf{w})$, and $\mathbf{f}(\mathbf{x})$ are real continuously differentiable vector functions; $\mathbf{w}_{in}$ is a constant vector; $\mathbf{x}_e(z)$ is the equilibrium profile of $\mathbf{x}$; $t \in [0, \infty)$ is the time; and $z \in [0,1]$ is the spatial coordinate.

Remark 3.2.1 *System (3.1)-(3.4) describes the mathematical model for counter-current two-phase contactors in chemical engineering processes in which chemical equilibrium is established. Here,* $\mathbf{x}(z,t)$ *and* $\mathbf{w}(z,t)$ *denote the concentration of the components in the phases;* $u_1(t)$ *and* $u_2(t)$ *denote the velocity of the phases;* $\mathbf{Q}(\mathbf{x}, \mathbf{w})$ *represents the reaction rate; and* $\mathbf{f}(\mathbf{x})$ *describes the equilibrium between the phases.*

By taking the derivative of (3.2) with respect to the spatial coordinate and substituting it into (3.1), we obtain:

$$\frac{\partial \mathbf{x}}{\partial t} = \tilde{\mathbf{V}}(\mathbf{x}, \mathbf{u}) \frac{\partial \mathbf{x}}{\partial z} + \tilde{\mathbf{Q}}(\mathbf{x}) \tag{3.5}$$

where $\mathbf{u} = [u_1, u_2]^T$; $\tilde{\mathbf{V}}(\mathbf{x}, \mathbf{u}) = (I - \mathbf{V}_t \frac{\partial \mathbf{f}}{\partial \mathbf{x}})^{-1}(u_1 \mathbf{V}_x + u_2 \mathbf{V}_w \frac{\partial \mathbf{f}}{\partial \mathbf{x}})$; and $\tilde{\mathbf{Q}}(\mathbf{x}) = (I - \mathbf{V}_t \frac{\partial \mathbf{f}}{\partial \mathbf{x}})^{-1} \mathbf{Q}(\mathbf{x}, \mathbf{f}(\mathbf{x}))$.

Remark 3.2.2 *It is assumed that* $I - \mathbf{V}_t \frac{\partial \mathbf{f}}{\partial \mathbf{x}}$ *is invertible. This assumption is satisfied in most physical systems as* $\mathbf{V}_t$ *is diagonal and* $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}$ *is a full-rank matrix function.*

Linearizing (3.5) around the equilibrium profiles $(\mathbf{x}_e, \mathbf{u}_e)$ yields:

$$\begin{aligned} \frac{\partial \bar{\mathbf{x}}}{\partial t} &= \mathbf{V}(z)\frac{\partial \bar{\mathbf{x}}}{\partial z} + \mathbf{M}(z)\bar{\mathbf{x}} + \mathbf{B}(z)\bar{\mathbf{u}}, \quad \bar{\mathbf{x}}(0,t) = 0 \\ \bar{\mathbf{y}} &= \mathbf{C}(z)\bar{\mathbf{x}} \end{aligned} \tag{3.6}$$

where $\bar{\mathbf{x}}(z,t) = \mathbf{x}(z,t) - \mathbf{x}_e(z) \in \mathscr{H}$ is the state variable in deviation form; $\bar{\mathbf{u}}(z,t) = \mathbf{u}(z,t) - \mathbf{u}_e(z) \in \mathscr{U} = L_2(0,1)^2$ is the input variable in deviation form; $\bar{\mathbf{y}}(z,t) = \mathbf{y}(z,t) - \mathbf{y}_e(z) \in \mathscr{Y} = L_2(0,1)^p$ with $\mathbf{y}(z,t) = \mathbf{C}(z)\mathbf{x}(z,t)$ and $\mathbf{y}_e(z) = \mathbf{C}(z)\mathbf{x}_e(z)$ denotes the output variable in deviation form; $\mathbf{C}(z) \in L_\infty(0,1)^{p\times n}$ is a real continuous matrix function; and $\mathbf{V}(z)$, $\mathbf{M}(z) \in L_\infty(0,1)^{n\times n}$ and $\mathbf{B}(z) \in L_\infty(0,1)^{n\times 2}$ are given by:

$$\mathbf{V}(z) = \tilde{\mathbf{V}}(\mathbf{x}_e, \mathbf{u}_e) \tag{3.7}$$

$$\mathbf{M}(z) = [\frac{\partial \tilde{\mathbf{V}}}{\partial \mathbf{x}}]_{\mathbf{x}=\mathbf{x}_e, \mathbf{u}=\mathbf{u}_e} \frac{d\mathbf{x}_e}{dz} + [\frac{\partial \tilde{\mathbf{Q}}}{\partial \mathbf{x}}]_{\mathbf{x}=\mathbf{x}_e} \tag{3.8}$$

$$\mathbf{B}(z) = [\frac{\partial \tilde{\mathbf{V}}}{\partial \mathbf{u}}]_{\mathbf{x}=\mathbf{x}_e, \mathbf{u}=\mathbf{u}_e} \frac{d\mathbf{x}_e}{dz} \tag{3.9}$$

Comment 3.2.1 *Matrix* $\mathbf{V}(z)$ *is spatially varying, non-symmetric, and its eigenvalues are not necessarily negative through of the domain; however, we assume that it has* n *real and distinct eigenvalues. Morover, since vector functions* $\mathbf{Q}$ *and* $\mathbf{f}$ *are continuously differentiable, so are the eigenvalues of* $\mathbf{V}(z)$.

Comment 3.2.2 *Although the input variable* $\mathbf{u}(t)$ *in (3.6) may be finite-dimensional in practice, here we consider a spatially distributed input variable* $\mathbf{u}(z,t)$ *to represent system (3.6) as an infinite-dimensional state-space with distributed input and distributed output.*

Remark 3.2.3 *Besides PDAE model (3.1)-(3.4), system (3.6) can also represent the linearized version of quasi-linear hyperbolic PDEs describing the majority of convection-reaction processes (Rhee* et al.*, 1986).*

Now, let us represent system (3.6) in an infinite-dimensional state-space in the Hilbert space $\mathscr{H}$ (Curtain and Zwart, 1995):

$$\begin{aligned} \dot{\bar{\mathbf{x}}}(t) &= \mathscr{A}\bar{\mathbf{x}}(t) + \mathscr{B}\bar{\mathbf{u}}(t) \\ \bar{\mathbf{y}}(t) &= \mathscr{C}\bar{\mathbf{x}}(t) \end{aligned} \tag{3.10}$$

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

$$\mathscr{A}\mathbf{h}(z) = \mathbf{V}(z)\frac{d\mathbf{h}(z)}{dz} + \mathbf{M}(z)\mathbf{h}(z) \tag{3.11}$$

with the following domain:

$$D(\mathscr{A}) = \{\mathbf{h}(z) \in \mathscr{H} : \mathbf{h}(z) \text{ is a.c., and } \frac{d\mathbf{h}(z)}{dz} \in \mathscr{H}, \mathbf{h}(0) = 0\} \tag{3.12}$$

where a.c. means absolutely continuous; $\mathscr{B} \in (\mathscr{U}, \mathscr{H})$ is given by $\mathscr{B} = \mathbf{B}(\cdot)I$; and $\mathscr{C} \in (\mathscr{H}, \mathscr{Y})$ is given by $\mathscr{C} = \mathbf{C}(\cdot)I$, where I is the identity operator.

3.3 LQ Control Synthesis

In this section, we are interested in developing an LQ controller for system (3.10), which results from the linearization of system (3.1)-(3.4). Let us consider the following infinite-time horizon quadratic objective function (Curtain and Zwart, 1995; Bensoussan *et al.*, 2007):

$$J(\bar{\mathbf{x}}_0, \bar{\mathbf{u}}) = \int_0^\infty (\langle \mathscr{C}\bar{\mathbf{x}}(t), \mathscr{P}\mathscr{C}\bar{\mathbf{x}}(t)\rangle + \langle \bar{\mathbf{u}}(t), \mathscr{R}\bar{\mathbf{u}}(t)\rangle)dt \tag{3.13}$$

where $\mathscr{P} = \mathbf{P}I \in \mathcal{L}(\mathscr{Y})$ with $\mathbf{P} \in \mathbb{R}^{p\times p}$ is a non-negative and symmetric matrix; $\bar{\mathbf{x}}_0 \in \mathscr{H}$ is an initial condition; and $\mathscr{R} = \mathbf{R}I \in \mathcal{L}(\mathscr{U})$ with $\mathbf{R} \in \mathbb{R}^{2\times 2}$ is a positive symmetric matrix. The minimization of the above objective function subject to system (3.10) requires solving the following ORE (see (Curtain and Zwart, 1995) and the references therein):

$$[\mathscr{A}^*\mathscr{Q} + \mathscr{Q}\mathscr{A} + \mathscr{C}^*\mathscr{P}\mathscr{C} - \mathscr{Q}\mathscr{B}\mathscr{R}^{-1}\mathscr{B}^*\mathscr{Q}]\bar{\mathbf{x}} = 0 \tag{3.14}$$

According to (Curtain and Zwart, 1995, Theorem 6.2.7), ORE (3.14) has a unique, non-negative, and self-adjoint solution $\mathscr{Q} \in \mathcal{L}(\mathscr{H})$, if system (3.10) is exponentially

stabilizable and exponentially detectable. Under these conditions, the minimum cost function is given by $J(\bar{\mathbf{x}}_0, \bar{\mathbf{u}}_{opt}) = \langle \bar{\mathbf{x}}_0, \mathscr{Q}\bar{\mathbf{x}}_0 \rangle$ and for any initial condition $\bar{\mathbf{x}}_0 \in \mathscr{H}$, the unique optimal control variable $\bar{\mathbf{u}}_{opt}$, which minimizes the objective function (3.13), is obtained on $t \geq 0$ as:

$$\bar{\mathbf{u}}_{opt}(t) = \mathbf{K}\bar{\mathbf{x}}(t) \tag{3.15}$$

where

$$\mathbf{K} = -\mathscr{R}^{-1}\mathscr{B}^*\mathscr{Q} \tag{3.16}$$

In addition, $\mathscr{A} + \mathscr{B}\mathbf{K}$ generates an exponentially stable C_0-semigroup (Curtain and Zwart, 1995).

In order to satisfy the conditions of (Curtain and Zwart, 1995, Theorem 6.2.7), we explore the stabilizability and detectability characteristics of system (3.10). In (Aksikas *et al.*, 2009, Theorem 2), it is proven that if matrix $\mathbf{V}$ is negative symmetric with constant elements, then operator $\mathscr{A}$ given by (3.11) and (3.12) generates an exponentially stable C_0-semigroup and whence, $(\mathscr{A}, \mathscr{B})$ is exponentially stabilizable and $(\mathscr{P}^{1/2}\mathscr{C}, \mathscr{A})$ is exponentially detectable; however, matrix $\mathbf{V}(z)$ in (3.10) is spatially varying, non-symmetric, and not necessarily negative. Therefore, (Aksikas *et al.*, 2009, Theorem 2) cannot be applied to prove the stabilizability and detectability properties of system (3.10). In order to prove these properties, first, we make $\mathbf{V}(z)$ a diagonal matrix, using the following state transformation:

$$\bar{\mathbf{x}} = \mathbf{T}(z)\hat{\mathbf{x}} \tag{3.17}$$

where $\mathbf{T}(z)$ is the transformation matrix whose columns are the eigenvectors of $\mathbf{V}(z)$. By applying this state transformation to (3.6), we have:

$$\begin{aligned} &\frac{\partial \hat{\mathbf{x}}}{\partial t} = \bar{\mathbf{V}}(z)\frac{\partial \hat{\mathbf{x}}}{\partial z} + \bar{\mathbf{M}}(z)\hat{\mathbf{x}} + \bar{\mathbf{B}}(z)\bar{\mathbf{u}}, \quad \hat{\mathbf{x}}(0,t) = 0 \\ &\bar{\mathbf{y}} = \bar{\mathbf{C}}(z)\hat{\mathbf{x}} \end{aligned} \tag{3.18}$$

where $\bar{\mathbf{V}}(z) = \mathbf{T}(z)^{-1}\mathbf{V}(z)\mathbf{T}(z)$ is a diagonal matrix whose elements are the eigenvalues

of $\mathbf{V}(z)$; and $\bar{\mathbf{M}}(z)$, $\bar{\mathbf{B}}(z)$ and $\bar{\mathbf{C}}(z)$ are given by:

$$\bar{\mathbf{M}}(z) = \mathbf{T}(z)^{-1}\mathbf{V}(z)\frac{\partial \mathbf{T}(z)}{\partial z} + \mathbf{T}(z)^{-1}\mathbf{M}(z)\mathbf{T}(z);$$
$$\bar{\mathbf{B}}(z) = \mathbf{T}(z)^{-1}\mathbf{B}(z); \quad \bar{\mathbf{C}}(z) = \mathbf{C}(z)\mathbf{T}(z)$$

The infinite-dimensional state-space representation of (3.18) is:

$$\begin{aligned} \dot{\hat{\mathbf{x}}}(t) &= \bar{\mathscr{A}}\hat{\mathbf{x}}(t) + \bar{\mathscr{B}}\bar{\mathbf{u}}(t) \\ \bar{\mathbf{y}}(t) &= \bar{\mathscr{C}}\hat{\mathbf{x}}(t) \end{aligned} \tag{3.19}$$

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

$$\bar{\mathscr{A}}\mathbf{h}(z) = \bar{\mathbf{V}}(z)\frac{d\mathbf{h}(z)}{dz} + \bar{\mathbf{M}}(z)\mathbf{h}(z),\ D(\bar{\mathscr{A}}) = D(\mathscr{A}) \tag{3.20}$$

$\bar{\mathscr{B}} \in (\mathscr{U}, \mathscr{H})$ is given by $\bar{\mathscr{B}} = \bar{\mathbf{B}}(\cdot)I$; and $\bar{\mathscr{C}} \in (\mathscr{H}, \mathscr{Y})$ is given by $\bar{\mathscr{C}} = \bar{\mathbf{C}}(\cdot)I$.

The ORE for system (3.19) is given by:

$$[\bar{\mathscr{A}}^*\mathscr{Q} + \mathscr{Q}\bar{\mathscr{A}} + \bar{\mathscr{C}}^*\mathscr{P}\bar{\mathscr{C}} - \mathscr{Q}\bar{\mathscr{B}}\mathscr{R}^{-1}\bar{\mathscr{B}}^*\mathscr{Q}]\hat{\mathbf{x}} = 0 \tag{3.21}$$

where $\mathscr{P}$, $\mathscr{R}$ and $\mathscr{Q}$ are defined in (3.13) and (3.14). Now, we explore the stabilizability and detectability properties of system (3.19) in the following two theorems.

Theorem 3.3.1 *Let us consider operator $\bar{\mathscr{A}}$ defined by (3.20) on its domain. Operator $\bar{\mathscr{A}}$ is the infinitesimal generator of a C_0-semigroup on $\mathscr{H}$.*

Proof: Operator $\bar{\mathscr{A}}$ is given by:

$$\begin{aligned} &\bar{\mathscr{A}} = \bar{\mathbf{V}}(z)\frac{d.}{dz} + \bar{\mathbf{M}}(z)I = diag(\lambda_1(z)\frac{d.}{dz}, \lambda_2(z)\frac{d.}{dz}, \ldots, \lambda_n(z)\frac{d.}{dz}) + \bar{\mathbf{M}}(z)I, \\ &D(\bar{\mathscr{A}}) = D(\mathscr{A}) \end{aligned} \tag{3.22}$$

where $\lambda_i(z), i = 1, \ldots, n \in L_\infty(0,1)$ are the eigenvalues of $\mathbf{V}(z)$ (diagonal elements of $\bar{\mathbf{V}}(z)$) and I is the identity operator. First, we prove that $\mathfrak{A}_1 h(z) = \lambda_1(z)\frac{dh(z)}{dz}$, with the following domain,

$$D(\mathfrak{A}_1) = \{h(z) \in L_2(0,1) : h(z) \text{ is a.c., and } \frac{dh(z)}{dz} \in L_2(0,1), h(0) = 0\} \tag{3.23}$$

is the infinitesimal generator of a C_0-semigroup on $L_2(0,1)$. According to (Curtain and Zwart, 1995, Corollary 2.2.3), the sufficient conditions for a closed, densely defined operator on a Hilbert space to be the infinitesimal generator of a C_0-semigroup satisfying $\|S(t)\| \leq e^{\omega t}$ are:

$$Re(\langle \mathfrak{A}_1 h, h\rangle) \leq \omega \|h\|^2 \qquad \text{for } h \in D(\mathfrak{A}_1) \tag{3.24}$$

$$Re(\langle \mathfrak{A}_1^* h, h\rangle) \leq \omega \|h\|^2 \qquad \text{for } h \in D(\mathfrak{A}_1^*) \tag{3.25}$$

First, we prove that operator $\mathfrak{A}_1$, with domain (3.23), is closed. Assume $\{q_n\} \subset D(\mathfrak{A}_1)$ is a sequence such that $\{q_n\} \to q$ and $\lambda_1(z)\frac{dq_n}{dz} \to g$. We should show $q \in D(\mathfrak{A}_1)$ and $\lambda_1(z)\frac{dq}{dz} = g$ (see (Curtain and Zwart, 1995, Definitions A.2.15 and A.3.43)) . Let us define $f \in D(\mathfrak{A}_1)$ by

$$f(\xi) = \int_0^\xi \frac{g(z)}{\lambda_1(z)} dz \tag{3.26}$$

in which $\lambda_1(z)\frac{df}{dz} = g(z)$. By the same argument used in (Curtain and Zwart, 1995, Example A.3.45), it can be shown that $f = q$ and therefore, $\mathfrak{A}_1$ is a closed operator. It also should be noted that the domain of $\mathfrak{A}_1$ is dense on $L_2(0,1)$, i.e. $\overline{D(\mathfrak{A}_1)}$, the closure of $D(\mathfrak{A}_1)$, is equal to $L_2(0,1)$ (see e.g. (Luo *et al.*, 1999, Example 2.21)). Now, we prove that condition (3.24) holds. Since $\lambda_1(z) \in L_\infty(0,1)$ and $h(z) \in L_2(0,1)$ are real, $Re(\langle \mathfrak{A}_1 h, h\rangle) = \langle \mathfrak{A}_1 h, h\rangle$. We have:

$$\begin{aligned}
\langle \mathfrak{A}_1 h, h\rangle &= \int_0^1 \lambda_1(z)\frac{dh(z)}{dz}h(z)dz = [\lambda_1(z)h(z)^2]_0^1 - \int_0^1 h(z)\frac{d(\lambda_1(z)h(z))}{dz}dz \\
&= [\lambda_1(z)h(z)^2]_0^1 - \int_0^1 h(z)(\lambda_1(z)\frac{dh(z)}{dz} + h(z)\frac{d\lambda_1(z)}{dz})dz \\
&= \lambda_1(1)h(1)^2 - \int_0^1 h(z)\lambda_1(z)\frac{dh(z)}{dz}dz - \int_0^1 h(z)^2\frac{d\lambda_1(z)}{dz}dz
\end{aligned}$$

By rearranging the above equation we obtain:

$$2\int_0^1 \lambda_1(z)\frac{dh(z)}{dz}h(z)dz = \lambda_1(1)h(1)^2 - \int_0^1 h(z)^2\frac{d\lambda_1(z)}{dz}dz$$

or,

$$\langle \mathfrak{A}_1 h, h\rangle = \frac{1}{2}\lambda_1(1)h(1)^2 - \frac{1}{2}\int_0^1 h(z)^2\frac{d\lambda_1(z)}{dz}dz$$

Then, we can write:

$$\langle \mathfrak{A}_1 h, h\rangle \leq \frac{1}{2}|\lambda_1(1)|h(1)^2 + \frac{1}{2}|\int_0^1 h(z)^2 \frac{d\lambda_1(z)}{dz} dz|$$

Using the Cauchy-Schwartz inequality on $L_2(0,1)$, we have:

$$\begin{aligned}\langle \mathfrak{A}_1 h, h\rangle \leq \frac{1}{2}|\lambda_1(1)|h(1)^2 + \frac{1}{2}(\int_0^1 h(z)^4 dz \int_0^1 (\frac{d\lambda_1(z)}{dz})^2 dz)^{\frac{1}{2}} \\ \leq \frac{1}{2}|\lambda_1(1)|h(1)^2 + \frac{1}{2}\|h\|^2 \|\frac{d\lambda_1}{dz}\|\end{aligned}$$

Since both $h(1)^2$ and $\|h\|^2$ are bounded values, we can find some $\alpha_1 \geq 1$ such that $h(1)^2 \leq \alpha_1 \|h\|^2$. Subsequently,

$$\langle \mathfrak{A}_1 h, h\rangle \leq \frac{1}{2}\alpha_1|\lambda_1(1)|\|h\|^2 + \frac{1}{2}\|h\|^2\|\frac{d\lambda_1}{dz}\| = \frac{1}{2}(\alpha_1|\lambda_1(1)| + \|\frac{d\lambda_1}{dz}\|)\|h\|^2$$

Hence, condition (3.24) holds for $\omega_1 = \frac{1}{2}(\alpha_1|\lambda_1(1)| + \|\frac{d\lambda_1}{dz}\|)$. Next, we prove condition (3.25). For this purpose, first, we find the adjoint operator $\mathfrak{A}_1^*$. According to (Curtain and Zwart, 1995, Definition A.3.63), for a densely defined operator $\mathfrak{A}_1$ on $L_2(0,1)$, the adjoint operator $\mathfrak{A}_1^*$ can be found through:

$$\langle \mathfrak{A}_1 h, g\rangle = \langle h, \mathfrak{A}_1^* g\rangle \tag{3.27}$$

where $g \in D(\mathfrak{A}_1^*)$. Let us calculate $\mathfrak{A}_1^*$ as follows:

$$\begin{aligned}\langle \mathfrak{A}_1 h, g\rangle &= \int_0^1 \lambda_1(z)\frac{dh}{dz} g dz = [\lambda_1(z)hg]_0^1 - \int_0^1 h\frac{d(\lambda_1(z)g)}{dz}dz \\ &= \lambda_1(1)h(1)g(1) - \int_0^1 h\frac{d(\lambda_1(z)g)}{dz}dz\end{aligned}$$

If $g(1) = 0$, $\frac{dg}{dz} \in L_2(0,1)$, and $\mathfrak{A}_1^* g = -\frac{d(\lambda_1(z)g)}{dz}$, then (3.27) is satisfied. The domain of $\mathfrak{A}_1^*$ will be:

$$D(\mathfrak{A}_1^*) = \{g(z) \in L_2(0,1) : g(z) \text{ is a.c., and } \frac{dg(z)}{dz} \in L_2(0,1), g(1) = 0\} \tag{3.28}$$

Now, let us prove condition (3.25) as follows:

$$\begin{aligned}\langle \mathfrak{A}_1^* h, h\rangle &= \int_0^1 -\frac{d(\lambda_1(z)h(z))}{dz}h(z)dz = -\int_0^1 (\lambda_1(z)\frac{dh(z)}{dz} + h(z)\frac{d\lambda_1(z)}{dz})h(z)dz \\ &= -\int_0^1 \lambda_1(z)\frac{dh(z)}{dz}h(z)dz - \int_0^1 h(z)^2\frac{d\lambda_1(z)}{dz}dz \\ &= [\lambda_1(z)h(z)^2]_1^0 + \int_0^1 \frac{d(\lambda_1(z)h(z))}{dz}h(z)dz - \int_0^1 h(z)^2\frac{d\lambda_1(z)}{dz}dz\end{aligned}$$

By rearranging the above equation we obtain:

$$-2\int_0^1 \frac{d(\lambda_1(z)h(z))}{dz}h(z)dz = \lambda_1(0)h(0)^2 - \int_0^1 h(z)^2\frac{d\lambda_1(z)}{dz}dz$$

or,

$$\langle \mathfrak{A}_1^* h, h\rangle = \frac{1}{2}\lambda_1(0)h(0)^2 - \frac{1}{2}\int_0^1 h(z)^2\frac{d\lambda_1(z)}{dz}dz$$

Then,

$$\langle \mathfrak{A}_1^* h, h\rangle \leq \frac{1}{2}|\lambda_1(0)|h(0)^2 + \frac{1}{2}|\int_0^1 h(z)^2\frac{d\lambda_1(z)}{dz}dz|$$

By the same argument used in proving condition (3.24), it can be shown:

$$\langle \mathfrak{A}_1^* h, h\rangle \leq \frac{1}{2}|\lambda_1(0)|h(0)^2 + \frac{1}{2}\|h\|^2\|\frac{d\lambda_1}{dz}\|$$

Since both $h(0)^2$ and $\|h\|^2$ are bounded values, we can find some $\alpha_2 \geq 1$ such that $h(0)^2 \leq \alpha_2\|h\|^2$. Subsequently,

$$\langle \mathfrak{A}_1^* h, h\rangle \leq \frac{1}{2}(\alpha_2|\lambda_1(0)| + \|\frac{d\lambda_1}{dz}\|)\|h\|^2$$

Hence, condition (3.25) holds for $\omega_2 = \frac{1}{2}(\alpha_2|\lambda_1(0)| + \|\frac{d\lambda_1}{dz}\|)$. Conditions (3.24) and (3.25) hold for $\omega = max(\omega_1, \omega_2)$ and therefore, $\mathfrak{A}_1$ is the infinitesimal generator of a C_0-semigroup on $L_2(0,1)$.

Similarly, it can be concluded that $\mathfrak{A}_i = \lambda_i(z).\frac{d.}{dz},\ D(\mathfrak{A}_i) = D(\mathfrak{A}_1), i = 2,\ldots,n$, are the infinitesimal generators of a C_0-semigroup on $L_2(0,1)$. Therefore, operator $\mathfrak{A}\mathbf{h}(z) = \bar{\mathbf{V}}(z)\frac{d\mathbf{h}(z)}{dz},\ D(\mathfrak{A}) = D(\bar{\mathscr{A}})$, is the infinitesimal generator of a C_0-semigroup on $\mathscr{H}$. Now, observing that $\bar{\mathbf{M}}(z) \in L_\infty(0,1)^{n\times n}$, by using the perturbation theory (Curtain and

Zwart, 1995, Theorem 3.2.1), it can be shown that $\bar{\mathscr{A}} = \bar{\mathbf{V}}(z)\frac{d.}{dz} + \bar{\mathbf{M}}(z)I$, $D(\bar{\mathscr{A}}) = D(\mathscr{A})$, is also the infinitesimal generator of a C_0-semigroup on $\mathscr{H}$.

□

Theorem 3.3.2 *Let us consider operator $\bar{\mathscr{A}}$ defined by (3.20) on its domain. The C_0-semigroup generated by $\bar{\mathscr{A}}$ is exponentially stable.*

Proof: In order to prove exponential stability, we prove the conditions of (Luo *et al.*, 1999, Theorem 3.35). The first condition requires $\{\zeta \mid Re\,\zeta \geq 0\} \subset \rho(\bar{\mathscr{A}})$, where $\rho(\bar{\mathscr{A}})$ is the resolvent set of $\bar{\mathscr{A}}$. In order to prove the first condition, let us solve $(\zeta I - \bar{\mathscr{A}})\mathbf{h}(z) = 0$, $\mathbf{h}(z) \in D(\bar{\mathscr{A}})$, which results in:

$$\bar{\mathbf{V}}(z)\frac{d\mathbf{h}(z)}{dz} = (\zeta I - \bar{\mathbf{M}}(z))\mathbf{h}(z), \quad \mathbf{h}(0) = 0$$

This equation yields $\mathbf{h}(z) = 0$, meaning that $(\zeta I - \bar{\mathscr{A}})$ is injective for all $\zeta \in \mathbb{C}$. On the other hand, let us solve equation $(\zeta I - \bar{\mathscr{A}})\mathbf{h}(z) = \mathbf{g}(z)$, $\mathbf{g}(z) \in D(\Re(\zeta, \bar{\mathscr{A}}))$, where $\Re(\zeta, \bar{\mathscr{A}})$ is the resolvent operator of $\bar{\mathscr{A}}$. This equation has a solution $\mathbf{h}(z) \in D(\bar{\mathscr{A}})$ given by:

$$\mathbf{h}(z) = -\int_0^z \mathcal{K}(z, s, \zeta)\bar{\mathbf{V}}^{-1}(s)\mathbf{g}(s)ds = (\Re(\zeta, \bar{\mathscr{A}})\mathbf{g}(z))(z) \tag{3.29}$$

where $\mathcal{K}(z, s, \zeta)$ is the fundamental matrix for the homogenous system. It follows from (3.29) that the resolvent operator is compact (Curtain and Zwart, 1995, Theorem A.3.24). Therefore, according to (Kato, 1966, Theorem 6.29), the spectrum of $\bar{\mathscr{A}}$ consists entirely of isolated eigenvalues. Consequently, the injectivity of $(\zeta I - \bar{\mathscr{A}})$ for all $\zeta \in \mathbb{C}$ implies that the point spectrum (entire spectrum) is empty and all $\zeta \in \mathbb{C}$ belong to $\rho(\bar{\mathscr{A}})$. Therefore, the first condition of (Luo *et al.*, 1999, Theorem 3.35) holds.

The second condition requires the boundedness of the resolvent operator for all ζ with $Re\,\zeta \geq 0$. In order to show the boundedness of the resolvent operator for small ζ (a strip around the imaginary axis), let us use (3.29) to write:

$$\|\mathbf{g}\|^2 \leq \|\zeta I - \bar{\mathscr{A}}\|^2\|\mathbf{h}\|^2 \tag{3.30}$$

Now, let us find $\|\mathbf{h}\|^2$ as:

$$\|\mathbf{h}\|^2 = \int_0^1 |\mathbf{h}(z)|^2 dz = \int_0^1 | \int_0^z \mathcal{K}(z,s,\zeta)\bar{\mathbf{V}}^{-1}(s)\mathbf{g}(s)ds|^2 dz$$

Using the Cauchy-Schwartz inequality on $\mathscr{H}$, we can write:

$$\|\mathbf{h}\|^2 \leq \int_0^1 [\int_0^z |\mathcal{K}(z,s,\zeta)|^2 ds \int_0^z |\bar{\mathbf{V}}^{-1}(s)\mathbf{g}(s)|^2 ds] dz \leq \|\mathcal{K}\|^2 \|\bar{\mathbf{V}}^{-1}\|^2 \|\mathbf{g}\|^2 \qquad (3.31)$$

By combining (3.30) and (3.31), we obtain:

$$\|\Re(\zeta, \bar{\mathscr{A}})\| \leq \|\mathcal{K}\|^2 \|\bar{\mathbf{V}}^{-1}\|^2$$

Since the elements of $\bar{\mathbf{V}}^{-1}(z)$ and $\bar{\mathbf{M}}(z) \in L_\infty(0,1)$, and the fundamental matrix $\mathcal{K}$ is continuous with respect to ζ (see e.g. (Hale and Lunel, 1993, Section 2.2)), for $|\zeta| \leq \epsilon_1,\ \epsilon_1 > 0$, we have $\|\mathcal{K}\| \leq \epsilon_2,\ \epsilon_2 \geq 0$, and therefore, $\Re(\zeta, \bar{\mathscr{A}})$ is bounded.

On the other hand, for sufficiently large ζ, since operator $\bar{\mathscr{A}}$ is the generator of a C_0-semigroup, by using the Hille-Yosida theorem (Luo *et al.*, 1999, Theorem 2.17), we have:

$$\|\Re(\zeta, \bar{\mathscr{A}})\| \leq \frac{\beta}{\zeta - \eta}, \quad \beta, \eta > 0 \qquad (3.32)$$

This implies the resolvent operator $\Re(\zeta, \bar{\mathscr{A}})$ is bounded by some $\epsilon_3 < 1$.

Consequently, the resolvent operator is bounded for all ζ with $Re\,\zeta \geq 0$. Therefore, the second condition of (Luo *et al.*, 1999, Theorem 3.35) is also satisfied and $\bar{\mathscr{A}}$ is the infinitesimal generator of an exponentially stable C_0-semigroup on $\mathscr{H}$.

□

Since $\bar{\mathscr{A}}$ is the infinitesimal generator of an exponentially stable C_0-semigroup on $\mathscr{H}$, system (3.19) is exponentially stabilizable and exponentially detectable on $\mathscr{H}$, and according to (Curtain and Zwart, 1995, Theorem 6.2.7), ORE (3.21) has a unique, non-negative, and self-adjoint solution $\mathscr{Q} \in \mathcal{L}(\mathscr{H})$. In order to solve the ORE, we convert it to an equivalent matrix Riccati differential equation.

Theorem 3.3.3 *Consider system (3.1)-(3.4) and its linearized and transformed version (3.18), which is stated in an infinite-dimensional state-space representation (3.19) in the Hilbert space $\mathscr{H}$. The unique, non-negative, and self-adjoint solution to the associated ORE (3.21) is:*

$$\mathscr{Q} = \Phi(z)I = diag(\Phi_1(z), \Phi_2(z), \ldots, \Phi_n(z)) \tag{3.33}$$

where $\Phi(z)$ is a non-negative solution to the following matrix Riccati differential equation:

$$\frac{d(\bar{\mathbf{V}}\Phi)}{dz} = \bar{\mathbf{M}}^*\Phi + \Phi\bar{\mathbf{M}} + \bar{\mathbf{C}}^*\mathbf{P}\bar{\mathbf{C}} - \Phi\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Phi, \quad \Phi(1) = 0 \tag{3.34}$$

Proof: First, let us find the adjoint operator $\bar{\mathscr{A}}^*$. By the same argument used in the proof of Theorem 3.3.1, it can be shown the adjoint of $\mathfrak{A}\mathbf{h}(z) = \bar{\mathbf{V}}(z)\frac{d\mathbf{h}(z)}{dz}$, $\mathbf{h}(z) \in D(\mathfrak{A}) = D(\bar{\mathscr{A}})$, is $\mathfrak{A}^*\mathbf{g} = -\frac{d(\bar{\mathbf{V}}\mathbf{g})}{dz}$, $\mathbf{g}(z) \in D(\mathfrak{A}^*)$, where $D(\mathfrak{A}^*)$ is:

$$D(\mathfrak{A}^*) = \{\mathbf{g}(z) \in \mathscr{H} : \mathbf{g}(z) \text{ is a.c., and } \frac{d\mathbf{g}(z)}{dz} \in \mathscr{H}, \mathbf{g}(1) = 0\} \tag{3.35}$$

Now, by using (Curtain and Zwart, 1995, Lemma A.3.65), we can write:

$$\bar{\mathscr{A}}^* = (\mathfrak{A} + \bar{\mathbf{M}})^* = \mathfrak{A}^* + \bar{\mathbf{M}}^*, \quad D(\bar{\mathscr{A}}^*) = D(\mathfrak{A}^*)$$

Next, by substituting (3.33) into (3.21), we get:

$$-\frac{d(\bar{\mathbf{V}}\Phi\hat{\mathbf{x}})}{dz} + \bar{\mathbf{M}}^*\Phi\hat{\mathbf{x}} + \Phi\bar{\mathbf{V}}\frac{d\hat{\mathbf{x}}}{dz} + \Phi\bar{\mathbf{M}}\hat{\mathbf{x}} + \bar{\mathbf{C}}^*\mathbf{P}\bar{\mathbf{C}}\hat{\mathbf{x}} - \Phi\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Phi\hat{\mathbf{x}} = 0 \tag{3.36}$$

On the other hand, we can write:

$$-\frac{d(\bar{\mathbf{V}}\Phi\hat{\mathbf{x}})}{dz} = -\bar{\mathbf{V}}\Phi\frac{d\hat{\mathbf{x}}}{dz} - \frac{d(\bar{\mathbf{V}}\Phi)}{dz}\hat{\mathbf{x}}$$

Since $\bar{\mathbf{V}}$ and Φ are diagonal, then $\Phi\bar{\mathbf{V}} = \bar{\mathbf{V}}\Phi$. Therefore, (3.36) turns into:

$$\frac{d(\bar{\mathbf{V}}\Phi)}{dz} = \bar{\mathbf{M}}^*\Phi + \Phi\bar{\mathbf{M}} + \bar{\mathbf{C}}^*\mathbf{P}\bar{\mathbf{C}} - \Phi\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Phi$$

Moreover, we have $\mathscr{Q}\hat{\mathbf{x}} = \Phi\hat{\mathbf{x}} \in D(\bar{\mathscr{A}}^*)$. If $\Phi(1) = 0$, then $\Phi(1)\hat{\mathbf{x}}(1) = 0$, which implies that $\Phi\hat{\mathbf{x}} \in D(\bar{\mathscr{A}}^*)$. On the other hand, since Φ is a non-negative solution of (3.34) on $[0, 1]$, so will be $\mathscr{Q}$ of (3.21).

□

Once $\Phi(z)$ is calculated, then the optimal control variable can be found from:

$$\bar{\mathbf{u}}_{opt}(z,t) = \mathbf{u}_{opt}(z,t) - \mathbf{u}_e = -\mathbf{R}^{-1}\bar{\mathbf{B}}^*(z)\Phi(z)\hat{\mathbf{x}}(z,t) \tag{3.37}$$

3.4 Case Study

Let us consider a continuous counter-current adsorption process of two interacting components in a moving-bed adsorber, as an example to demonstrate how to apply the theoretical development given above. In this process, which has a wide application in the pharmaceutical and biochemical industries, separation of two chemical components is achieved by selective adsorption on a solid medium. When the axial dispersion is negligible and the system is subject to the equilibrium relations of Langmuir type, the mathematical model of the system describing the concentrations of the two components in the fluid phase is given by (Rhee *et al.*, 1986, vol II, Section 5):

$$\frac{\partial c_{f,1}}{\partial t} = -\upsilon_f \frac{\partial c_{f,1}}{\partial \tilde{z}} + F\upsilon_s \frac{\partial c_{s,1}}{\partial \tilde{z}} - F\frac{\partial c_{s,1}}{\partial t} \tag{3.38}$$

$$\frac{\partial c_{f,2}}{\partial t} = -\upsilon_f \frac{\partial c_{f,2}}{\partial \tilde{z}} + F\upsilon_s \frac{\partial c_{s,2}}{\partial \tilde{z}} - F\frac{\partial c_{s,2}}{\partial t} \tag{3.39}$$

$$c_{s,1} = \frac{a_1 c_{f,1}}{1 + b_1 c_{f,1} + b_2 c_{f,2}} \tag{3.40}$$

$$c_{s,2} = \frac{a_2 c_{f,2}}{1 + b_1 c_{f,1} + b_2 c_{f,2}} \tag{3.41}$$

$$c_{f,1}(0,t) = c_{f,1}^{in},\ c_{f,2}(0,t) = c_{f,2}^{in},\ c_{s,1}(L,t) = c_{s,1}^{in},\ c_{s,2}(L,t) = c_{s,2}^{in} \tag{3.42}$$

$$c_{f,1}(\tilde{z},0) = c_{f,1}^{e}(\tilde{z}), \quad c_{f,2}(\tilde{z},0) = c_{f,2}^{e}(\tilde{z}) \tag{3.43}$$

where $c_{f,i}$ and $c_{s,i}$, $i = 1, 2$, are the concentrations of the components in the fluid and the solid phase, respectively; υ_f is the interstitial velocity of the fluid phase; υ_s is the speed of the adsorbent (solid) phase; F is the phase ratio; a_i and b_i, $i = 1, 2$, are the Langmuir isotherm coefficients; $c_{f,i}^{in}$ and $c_{s,i}^{in}$, $i = 1, 2$, are the inlet concentrations of the components in the fluid and the solid phase, respectively; $c_{f,i}^{e}(\tilde{z})$, $i = 1, 2$, are the equilibrium profiles

Table 3.1: Model parameters

Component		**1**	**2**
Langmuir isotherm coefficient a_i	—	5	6
Langmuir isotherm coefficient b_i	lit/mol	2.5	3
Concentration $c_{f,i}^{in}$	mol/lit	0.06	0.06
Concentration $c_{s,i}^{in}$	mol/lit	0.12	0
Phase ratio F	—	1.5	
Fluid phase velocity v_f	m/sec	0.45	
Solid phase velocity v_s	m/sec	0.1	
Length of the adsorbent L	m	1	

of the components in the fluid phase; $t \in [0, \infty)$ is the time; $\tilde{z} \in [0, L]$ is the spatial coordinate; and L is the length of the adsorber. The numerical values for the parameters used in this case study are given in Table 3.1. By using the following transformations:

$$\bar{c}_{f,1} = \frac{c_{f,1} - c_{f,1}^{in}}{c_{f,1}^{in}}, \quad \bar{c}_{f,2} = \frac{c_{f,2} - c_{f,2}^{in}}{c_{f,2}^{in}}, \quad z = \frac{\tilde{z}}{L} \tag{3.44}$$

model (3.38)-(3.43) can be represented in the form of system (3.1)-(3.4) in which $\mathbf{x} = [\bar{c}_{f,1}, \bar{c}_{f,2}]^T$; $\mathbf{w} = [c_{s,1}, c_{s,2}]^T$; $u_1 = v_f$; $u_2 = v_s$; $\mathbf{V}_x = diag(-1/L, -1/L)$; $\mathbf{V}_w = diag(F/Lc_{f,1}^{in}, F/Lc_{f,2}^{in})$; $\mathbf{V}_t = diag(-F/c_{f,1}^{in}, -F/c_{f,2}^{in})$; $\mathbf{Q}(\mathbf{x}, \mathbf{w}) = 0$; $\mathbf{f}(\mathbf{x})$ is given by the transformed version of (3.40) and (3.41); $\mathbf{w}_{in} = [c_{s,1}^{in}, c_{s,2}^{in}]^T$; $x_{e,1} = (c_{f,1}^{e} - c_{f,1}^{in})/c_{f,1}^{in}$; and $x_{e,2} = (c_{f,2}^{e} - c_{f,2}^{in})/c_{f,2}^{in}$.

Following the model derivation discussed in Section 3.2, we get linear model (3.6). The resulting matrix $\mathbf{V}(z)$ is spatially varying, non-symmetric, and its eigenvalues are not necessarily negative through of the domain. The eigenvalues of $\mathbf{V}(z)$ are shown in Figure 3.1. Since the eigenvalues are distinct, matrix $\mathbf{V}(z)$ is diagonalizable and therefore, transformation (3.17) can be applied to yield system (3.18). The control objective is to regulate the concentrations along the adsorber using v_f and v_s as the control variables. As it was discussed in Section 3.3, the LQ controller can be calculated through solving matrix Riccati differential equation (3.34). Since we are interested in controlling both state variables, the observation matrix $\mathbf{C}(z)$ is set to be the identity matrix. The weighting matrices are chosen such that $\mathbf{P} = diag(0.01, 0.1)$ and $\mathbf{R} =$

$diag(100, 100)$. An arbitrary initial condition $c_{f,1}(z, 0) = 0.15\, mol/lit$ and $c_{f,2}(z, 0) = 0.15\, mol/lit$ is chosen and the controller is implemented on the nonlinear model equations (3.38)-(3.43) through a numerical simulation in gPROMS® (*Process Systems Enterprise, gPROMS. www.psenterprise.com, 1997-2012)*. Backward finite-difference method is used to approximate the spatial derivatives. The profiles for the fluid phase concentrations $c_{f,1}$ and $c_{f,2}$, are shown in Figure 3.2. These figures show how the LQ controller is able to bring the concentration profiles to their desired equilibrium profiles. This is the ideal control and gives us the best achievable performance; however, this control variable is distributed through of the domain and may not be realizable in practice. The following averaged value may be used instead, which results in the best suboptimal controller:

$$\mathbf{u}_{sub}(t) - \mathbf{u}_e = -\int_0^1 \mathbf{R}^{-1}\bar{\mathbf{B}}^*(z)\Phi(z)\hat{\mathbf{x}}(z, t)dz \tag{3.45}$$

To have a measure of how much the control performance is deteriorated by using the suboptimal controller, the spatially averaged control error given as

$$err_{ave,i} = \frac{1}{L}\int_0^L [c_{f,i}(\tilde{z}, t) - c^e_{f,i}(\tilde{z})]d\tilde{z} \tag{3.46}$$

is considered here for comparison. The spatially averaged error for optimal and suboptimal systems are shown in Figure 3.3(a). As it can be seen, the performance of the suboptimal controller is slightly poorer than the optimal controller. Finally, the suboptimal control input profiles are shown in Figure 3.3(b), which indicates that the control efforts are not particularly aggressive, and are physically realizable.

3.5 Conclusion

In this work, LQ control of a set of first-order hyperbolic PDAEs is achieved by using the infinite-dimensional Hilbert state-space representation of the system and the well-known operator Riccati equation (ORE) method. The set of PDAEs is converted to a system

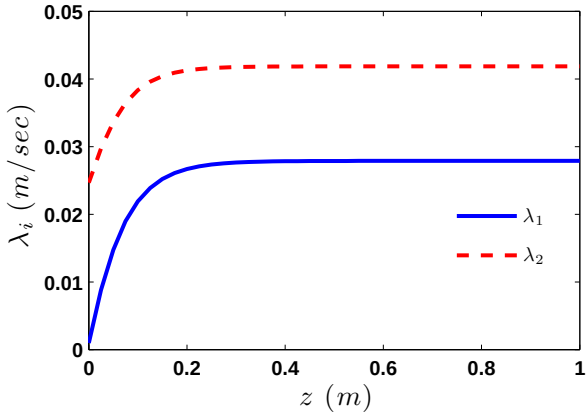
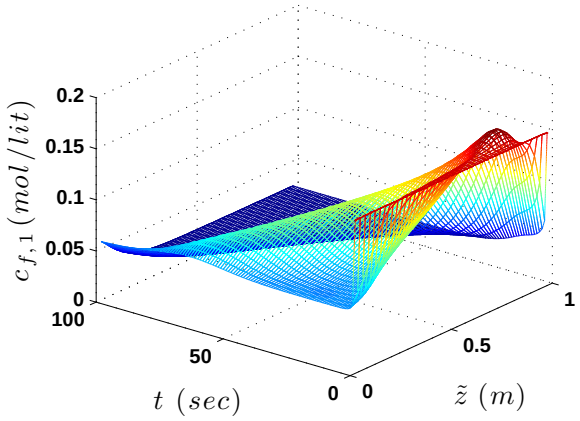
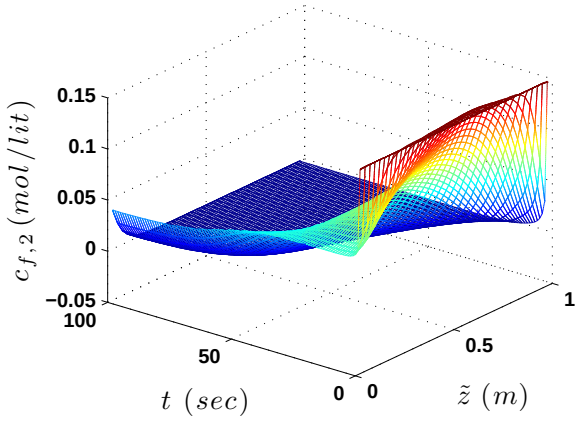


Figure 3.1: Eigenvalues of $\mathbf{V}(z)$

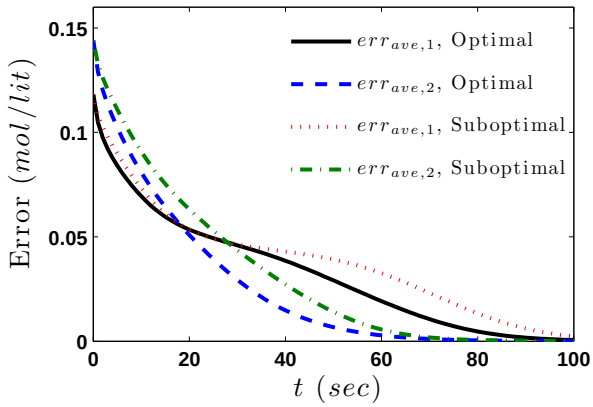


(a) Component 1

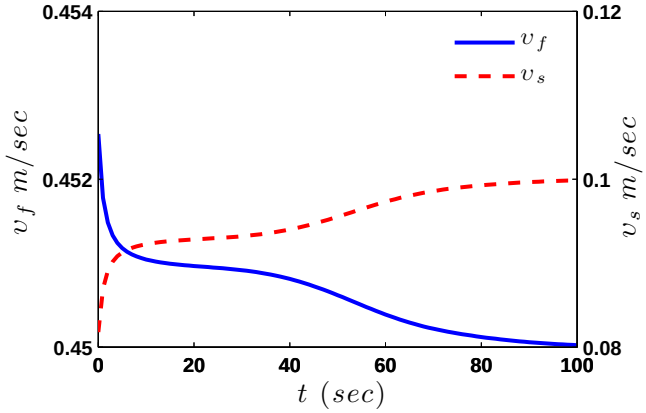


(b) Component 2

Figure 3.2: Concentration of the components



(a) Spatially averaged error



(b) Suboptimal control input profiles

Figure 3.3: Spatially averaged error and suboptimal control input profiles

consisting of a set of pure PDEs in which the velocity matrix is spatially varying, non-symmetric, and its eigenvalues are not necessarily negative through of the domain. The existence and uniqueness of the non-negative solution to the ORE is explored by proving exponential stability of the system. The non-negative solution to the ORE is found through converting it to an equivalent matrix Riccati differential equation. An illustrative example is give at the end to demonstrate the theory.

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Chapter 4

Infinite-Dimensional LQ Optimal Control of a Dimethyl Ether (DME) Catalytic Distillation Column

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4.1 Introduction

Reactive distillation (RD) has received much attention in the literature over recent years due to its advantages and inherent complexities. This process is a combination of chemical reaction and multi-component distillation in a counter-current column. When solid catalyst is used to accelerate the reaction, the process is called catalytic distillation (CD). The most important advantages in use of RD include reduced downstream processing, using the heat of reaction for distillation, overcoming chemical equilibria by removing products from

the reaction zone and etc.; however, the interaction between the simultaneous reaction and distillation introduces challenging problems in controlling the column operating conditions, which include the existence of steady-state multiplicity, strong interactions between process variables and process gain sign change (Khaledi and Young, 2005).

The reactive distillation process can take place either in a trayed or a packed column (Taylor and Krishna, 2000). In the case of packed column, the process belongs to the class of distributed parameter systems, meaning that the process variables are functions of both time and spatial coordinate. Such a system is modelled by a set of coupled PDAEs in which partial differential equations (PDEs) describe the transport-reaction phenomena, while algebraic equations represent the equilibrium condition. In the absence of the axial dispersion, the main transport mechanism is convection and the resulting PDEs are of first-order hyperbolic type (Noeres *et al.*, 2003). The conventional approach to deal with PDE systems is early lumping. In this method the controller is designed using an approximate ODE model, which results from discretizing the PDE system at a finite number of points. This allows the use of standard control methods applicable to ODE systems, which has been widely addressed in the literature (e.g., (Vecchio and Petit, 2005; Georgakis *et al.*, 1977)); however, this approximation results in some mismatch in the dynamical properties of the original distributed parameter and the lumped parameter models (Ray, 1980), which affects the performance of the designed model-based controller. A more rigorous way to cope with such a distributed parameter process is to exploit the infinite-dimensional characteristic of the system (Ray, 1980; Christofides, 2001).

Despite the complexities in control of RD process, a relatively small amount of research work has been reported in this area and most of the publications deal with modelling, simulation, process design and the analysis of steady-state multiplicity (e.g., (Taylor and Krishna, 2000; Noeres *et al.*, 2003; Sharma and Singh, 2010)). A significant portion of the literature in the area of control of RD concerns the effectiveness of different

control structures including conventional proportional integral (PI) controllers (e.g., (Al-Afraj and Luyben, 2000; Al-Arfaj and Luyben, 2002; Kaymak and Luyben, 2005)). Linear model predictive control (MPC) technique has also been applied to control this process based on simplified dynamic models (e.g., (Baldon *et al.*, 1997; Khaledi and Young, 2005)). In addition, a limited number of papers in the literature have dealt with the advanced nonlinear control of the RD process (e.g., (Kumar and Daoutidis, 1999; Grüner *et al.*, 2003; Kawathekar and Riggs, 2007)). All of the existing research work deal with a system of ODEs either by considering a trayed column model or, equivalently, by discretizing a packed (distributed) column model using a finite number of discretization points. Considering the infinite-dimensional characteristic of the packed reactive distillation process, helps to capture all the dynamic modes of the system without using a large number of discretization points. In this approach the controller is designed based on the original PDE model rather than its discretized version; however, it introduces more challenging problem regarding the theoretical developments.

The theory of feedback control for distributed parameter systems in the context of infinite-dimensional system representation has received a lot of attention in the control community. A body of this research work deals with parabolic PDE systems by using modal analysis approach (Ray, 1980; Christofides, 2001). The basic idea in this approach is to derive finite-dimensional systems that capture the dominant dynamics of the parabolic PDE, which are subsequently used for controller design. This method is not applicable to first-order hyperbolic PDE systems where all the eigenmodes of the spatial differential operator contain the same amount of energy. In (Christofides and Daoutidis, 1996) geometric control approach is used for a class of first-order quasi-linear hyperbolic systems. This work assumes a symmetric velocity matrix with partially negative eigenvalues to preserve the C_0-semigroup generation property; however, this assumption is not valid for counter-current two-phase contactors such as multi-component (reactive) distillation

in which the chemical equilibrium is established. These systems are modelled by coupled first-order hyperbolic PDEs and algebraic equations where the algebraic equations can be solved for the algebraic variables to yield a set of pure PDEs in which the velocity matrix is spatially varying, non-symmetric, and its eigenvalues are not necessarily negative through of the domain. A combination of method of characteristics and model predictive control is used in (Shang *et al.*, 2004) to convert hyperbolic PDEs to equivalent ODE system; however, applicability of the method of characteristics is restricted to systems having one or two characteristic curves. In (Dubljevic *et al.*, 2005) a predictive control algorithm is proposed for nonlinear parabolic and first-order hyperbolic PDEs with state and control constraints; however, in case of hyperbolic PDEs, this work assumes that the system under consideration has a very fast dynamics and therefore, the control objectives are satisfied only at the steady-state.

Recently, linear quadratic (LQ) regulator for first-order hyperbolic PDEs has been studied by solving an operator Riccati equation (ORE) for a given infinite-dimensional state-space model. The solution of the ORE is strongly based on the form of the hyperbolic operator, in particular, the velocity matrix. This method is used in (Aksikas *et al.*, 2008) for a class of hyperbolic PDEs in which the velocity matrix is a negative identity matrix. The method is then extended to a more general class of hyperbolic systems where the velocity matrix is diagonal with not necessarily identical entries (Aksikas *et al.*, 2009).

The purpose of the present work is to develop an ORE-based infinite-dimensional LQ control for controlling the concentration profiles in a DME packed catalytic distillation column modelled by a set of first-order hyperbolic PDAEs. The PDAE system is converted to a system of pure first-order hyperbolic PDEs by solving the algebraic equations, and a linear system is then calculated through linearizing the nonlinear PDEs around the desired steady-state profiles. In contrast to the previous work in the area of LQ control of hyperbolic systems (Aksikas *et al.*, 2008; Aksikas *et al.*, 2009), the resulting linear

infinite-dimensional model involves a hyperbolic operator in which the velocity matrix is spatially varying, non-diagonal, and not necessarily negative through of the domain. Therefore, the approaches developed in previous contributions, are not applicable to this kind of operator. In order to solve the LQ control problem, a state transformation is used to make the velocity matrix diagonal. The ORE for the resulting system is then formulated and the existence of its unique and non-negative solution is explored. The solution of the ORE is found through converting it to an equivalent matrix Riccati differential equation which can be solved numerically to calculate the optimal feedback operator. Subsequently, the result is extended to obtain an optimal proportional plus integral controller which can reject the effect of load losses such as changes in the feed flowrate. Finally, a set of numerical simulations is performed to assess the performance of the designed controller.

4.2 Process Model

The process under consideration is shown in Figure 4.1. This catalytic distillation column is used for producing DME through the liquid phase dehydration of methanol. The column has an effective packing height of 4 m, which consists of four sections of 1 m each in height. The rectifying zone at the column top and the stripping zone at the column bottom are filled with packing in which separation is taking place. The two middle sections are catalytically packed reaction zones in which the following reaction is taking place:

$$2\,Methanol \Longleftrightarrow DME + Water \tag{4.1}$$

The reaction rate is given by (Hosseininejad, 2010):

$$r_D = \frac{k_s x_2^2}{(x_2 + \frac{K_W}{K_M}(1 - x_1 - x_2))^2} \tag{4.2}$$

where r_D is the rate of the reaction in $\frac{mol}{kgcat.sec}$; x_1 and x_2 are the mole fractions of DME and methanol in the liquid phase, respectively; and

$$k_s = k_1 exp(\frac{-k_2}{RT})$$
$$\frac{K_W}{K_M} = exp(-k_3 + \frac{k_4}{T})$$

where T is the temperature in Kelvin; k_1, k_2, k_3 and k_4 are the kinetic constants; and R is the universal gas constant.

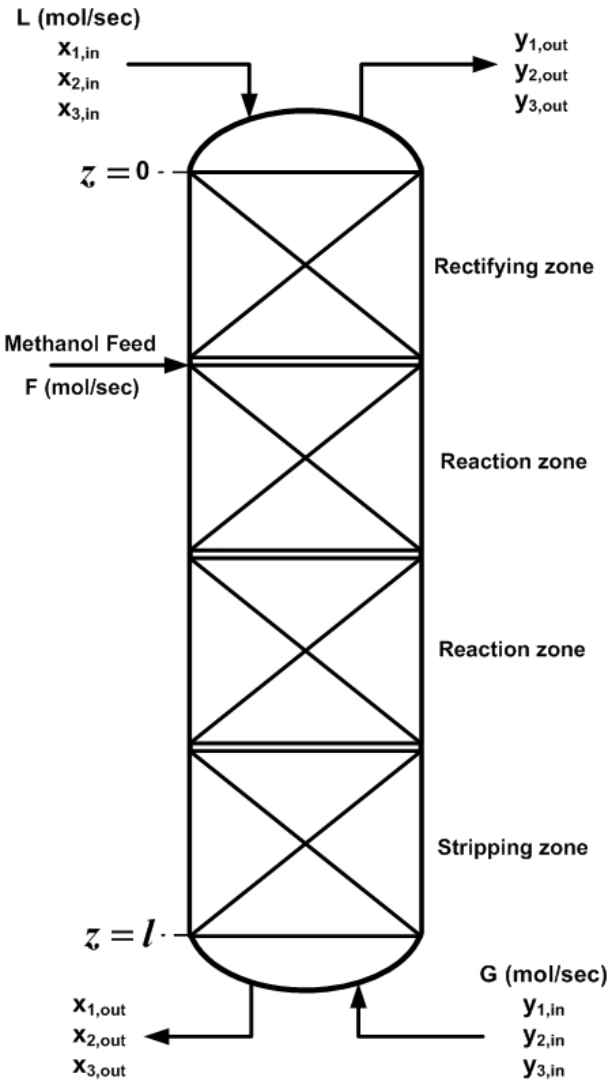


Figure 4.1: Catalytic distillation column

Methanol feed, with flowrate F (50% liquid and 50% gas), enters the column at the top of the reaction zone and the liquid and gas with flowrates L and G enter the column at the top and bottom, respectively. Due to the difference between the vapor pressures of DME, methanol and water, the concentration of methanol in the reaction zone is higher than the other two components, which favours the reaction to occur in the forward direction. The light and heavy products, DME and water, are withdrawn at the column top and bottom, receptively. For the sake of simplicity, we consider a total condenser and a thermosiphon reboiler with negligible liquid and gas hold-ups.

Various types of models, involving different levels of complexity, can be used to simulate the dynamics of this reactive distillation column. In this work, we consider the simple and generic reactive distillation model studied in (Al-Afraj and Luyben, 2000). It should be noted that in (Al-Afraj and Luyben, 2000), gas and liquid rates through the stripping and rectifying zones are constant and these rates change in the reaction zone because the heat of reaction vaporizes some liquid. Since the heat of reaction (4.1) is negligible (Hosseininejad, 2010), we assume constant liquid and gas rates all through the column. Therefore, the model structure of the catalytic distillation column is developed based on the following assumptions:

- Negligible gas hold-up
- Constant liquid hold-up
- Spatially constant gas and liquid rates
- Gas-liquid equilibrium
- No chemical reaction in the gas phase
- Perfect mixing in radial direction
- Fast heat transfer in comparison to mass transfer

- Constant operating pressure
- Ideal vapor-liquid equilibrium according to Raoult's law
- Constant relative volatilities

Using the above assumptions, the nonlinear process model describing the system under study is:

$$U_L \frac{\partial x_1}{\partial t} = -L\frac{\partial x_1}{\partial z} + G\frac{\partial y_1}{\partial z} + r_D\phi \tag{4.3}$$

$$U_L \frac{\partial x_2}{\partial t} = -L\frac{\partial x_2}{\partial z} + G\frac{\partial y_2}{\partial z} - 2r_D\phi \tag{4.4}$$

$$x_1 + x_2 + x_3 = 1 \tag{4.5}$$

$$y_1 = \frac{\alpha_1 x_1}{\alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3} \tag{4.6}$$

$$y_2 = \frac{\alpha_2 x_2}{\alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3} \tag{4.7}$$

$$y_1 + y_2 + y_3 = 1 \tag{4.8}$$

$$T = \frac{B_{vp,D}}{A_{vp,D} - \log_{10}(\frac{\alpha_1 P}{\alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3})} - C_{vp,D} \tag{4.9}$$

subject to the boundary and initial conditions:

$$x_1(0,t) = x_{1,in}, \quad x_2(0,t) = x_{2,in}, \quad y_1(l,t) = y_{1,in}, \quad y_2(l,t) = y_{2,in} \tag{4.10}$$

$$x_1(z,0) = x_{1,e}(z), \quad x_2(z,0) = x_{2,e}(z) \tag{4.11}$$

where $t \in [0, \infty)$ is the time; $z \in [0, l]$ is the spatial coordinate; x_1, x_2 and x_3 are the mole fractions of DME, methanol and water in the liquid phase, respectively; y_1, y_2 and y_3 are the mole fractions of DME, methanol and water in the gas phase, respectively; U_L is the liquid hold-up; ϕ is the catalyst loading; P is the pressure; α_1, α_2 and α_3 are the relative volatilities of DME, methanol and water with respect to water (least volatile component), respectively; $A_{vp,D}$, $B_{vp,D}$ and $C_{vp,D}$ are the Antoine equation parameters for DME; $x_{1,in}$, $x_{2,in}$, $y_{1,in}$ and $y_{2,in}$ are the inlet mole fractions of DME and methanol in the liquid and

Table 4.1: Model parameters

Parameter	**Value**	**Parameter**	**Value**
l	$4\,m$	$y_{3,in}$	0.95
U_L	$10\,\frac{mol}{m}$	α_1	21.3
P	$9 \times 10^5\,Pa$	α_2	3.13
ϕ	$3.5\,\frac{kg}{m}$	α_3	1
F	$0.025\,\frac{mol}{sec}$	$A_{vp,D}$	4.441
L_e	$0.11\,\frac{mol}{sec}$	$B_{vp,D}$	1025.560
G_e	$0.11\,\frac{mol}{sec}$	$C_{vp,D}$	-17.1
$x_{1,in}$	0.95	k_1	$6.12 \times 10^{10}\,\frac{mol}{kgcat.sec}$
$x_{2,in}$	0.05	k_2	$98\,\frac{kJ}{mol}$
$x_{3,in}$	0.0	k_3	6.46
$y_{1,in}$	0.0	k_4	2964
$y_{2,in}$	0.05		

gas phases, respectively; and $x_{1,e}(z)$ and $x_{2,e}(z)$ are the equilibrium profiles of x_1 and x_2, respectively.

It should be noted that the reaction terms in (4.3) and (4.4) for the rectifying and stripping zones are zero, as no reaction is taking place in these sections. The model parameters that are used in this work are given in Table 4.1. In the table, subscript "e" denotes the equilibrium or the steady-state condition. For finding the steady-state mole fraction profiles, we solve the open-loop dynamic system (4.3) to (4.11) in gPROMS® (*Process Systems Enterprise, gPROMS. www.psenterprise.com, 1997-2012)* using an initial condition (see Section 4.5 for the details of the numerical method used), and since the open-loop system is stable, it converges to the equilibrium profiles. The steady-state mole fraction and temperature profiles are shown in Figures 4.2 to 4.4. It can be observed from the figures that the concentration of methanol (the reactant) in the middle section of the column (the reaction zone) is maximum due to the difference between the volatilities of methanol and DME. This helps the reaction to occur in the forward direction. In the top of the column (the rectifying zone) DME separates from methanol and therefore, the top

product mainly contains DME. In the bottom of the column (the stripping zone) water separates from methanol and leaves the column in the bottom product. The equilibrium temperature profile is such that its range in the middle of the column is suitable for the highest achievable reaction rates (Hosseininejad, 2010).

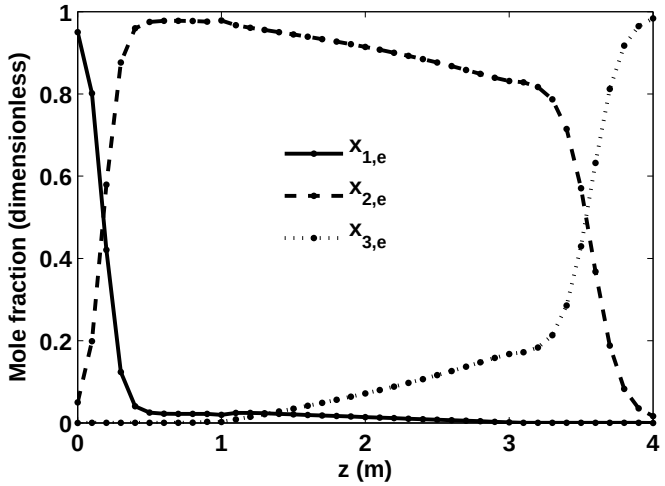


Figure 4.2: Equilibrium liquid phase mole fraction profiles

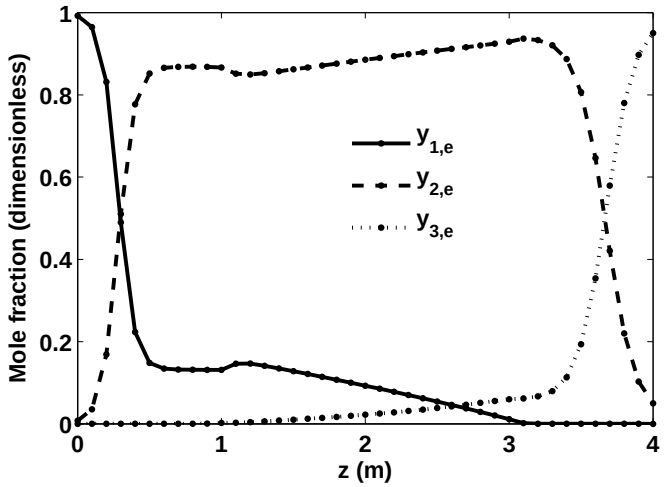


Figure 4.3: Equilibrium gas phase mole fraction profiles

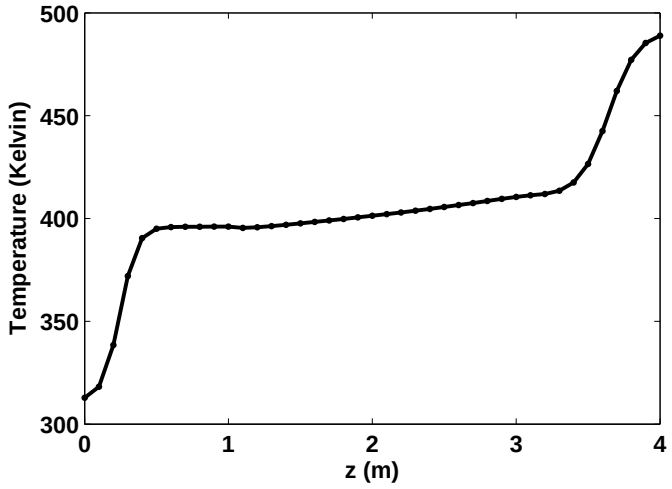


Figure 4.4: Equilibrium temperature profile

4.3 Infinite-Dimensional State-Space Representation

In this section we derive an infinite-dimensional state-space setting for PDAE model (4.3) to (4.11) which is used for formulating the LQ control problem in the next section. Let us use notation $\mathbf{x} = [x_1, x_2]$, $u_1 = L$, $u_2 = G$ and $\mathbf{u} = [u_1, u_2]$. By taking the derivatives of y_1 and y_2 in (4.6) and (4.7) with respect to the spatial coordinate, and by substituting them into (4.3) and (4.4), we get:

$$\begin{aligned} &\frac{\partial \mathbf{x}}{\partial t} = \mathbf{F}(\mathbf{x}, \mathbf{u})\frac{\partial \mathbf{x}}{\partial z} + \mathbf{Q}(\mathbf{x}) \\ &\mathbf{x}(0,t) = \mathbf{x}_{in}, \quad \mathbf{x}(z,0) = \mathbf{x}_e(z) \end{aligned} \tag{4.12}$$

where

$$\frac{\partial \mathbf{x}}{\partial t} = [\frac{\partial x_1}{\partial t}, \frac{\partial x_2}{\partial t}]^T, \quad \frac{\partial \mathbf{x}}{\partial z} = [\frac{\partial x_1}{\partial z}, \frac{\partial x_2}{\partial z}]^T, \quad \mathbf{Q}(\mathbf{x}) = [\frac{r_D\phi}{U_L}, -\frac{2r_D\phi}{U_L}]^T,$$
$$\mathbf{x}_{in} = [x_{1,in}, x_{2,in}]^T, \quad \mathbf{x}_e(z) = [x_{1,e}(z), x_{2,e}(z)]^T$$

and

$$\mathbf{F}(\mathbf{x}, \mathbf{u}) = \begin{bmatrix} f_{11}(\mathbf{x}, \mathbf{u}) & f_{12}(\mathbf{x}, \mathbf{u}) \\ f_{21}(\mathbf{x}, \mathbf{u}) & f_{22}(\mathbf{x}, \mathbf{u}) \end{bmatrix} \tag{4.13}$$

in which $f_{11}(\mathbf{x},\mathbf{u})$, $f_{12}(\mathbf{x},\mathbf{u})$, $f_{21}(\mathbf{x},\mathbf{u})$ and $f_{22}(\mathbf{x},\mathbf{u})$ are nonlinear functions of $\mathbf{x}$ and $\mathbf{u}$ and given as:

$$
\begin{aligned}
f_{11}(\mathbf{x},\mathbf{u}) &= \frac{u_2\alpha_1}{U_L}\frac{\alpha_2 x_2+\alpha_3(1-x_2)}{[\alpha_1 x_1+\alpha_2 x_2+\alpha_3(1-x_1-x_2)]^2}-\frac{u_1}{U_L}\\
f_{12}(\mathbf{x},\mathbf{u}) &= \frac{u_2\alpha_1}{U_L}\frac{x_1(\alpha_3-\alpha_2)}{[\alpha_1 x_1+\alpha_2 x_2+\alpha_3(1-x_1-x_2)]^2}\\
f_{21}(\mathbf{x},\mathbf{u}) &= \frac{u_2\alpha_2}{U_L}\frac{x_2(\alpha_3-\alpha_1)}{[\alpha_1 x_1+\alpha_2 x_2+\alpha_3(1-x_1-x_2)]^2}\\
f_{22}(\mathbf{x},\mathbf{u}) &= \frac{u_2\alpha_2}{U_L}\frac{\alpha_1 x_1+\alpha_3(1-x_1)}{[\alpha_1 x_1+\alpha_2 x_2+\alpha_3(1-x_1-x_2)]^2}-\frac{u_1}{U_L}
\end{aligned}
$$

In order to make the boundary condition in system (4.12) homogenous, let us consider the following state transformation:

$$
\tilde{x}_1=\frac{x_1-x_{1,in}}{x_{1,in}},\quad \tilde{x}_2=\frac{x_2-x_{2,in}}{x_{2,in}} \tag{4.14}
$$

where $x_{1,in}$ and $x_{2,in}$ are assumed constant and given in Table 4.1. By substituting for x_1 and x_2 from (4.14) into (4.12), we obtain the following equivalent representation of model (4.12):

$$
\begin{aligned}
&\frac{\partial\tilde{\mathbf{x}}}{\partial t}=\tilde{\mathbf{F}}(\tilde{\mathbf{x}},\mathbf{u})\frac{\partial\tilde{\mathbf{x}}}{\partial z}+\tilde{\mathbf{Q}}(\tilde{\mathbf{x}})\\
&\tilde{\mathbf{x}}(0,t)=0,\quad \tilde{\mathbf{x}}(z,0)=\tilde{\mathbf{x}}_e(z)
\end{aligned} \tag{4.15}
$$

Linearizing model (4.15) about its equilibrium profile by using the Taylor series expansion leads to the following linear model on the Hilbert space $\mathscr{H}=L_2(0,l)^2$:

$$
\begin{aligned}
&\frac{\partial\bar{\mathbf{x}}}{\partial t}=\mathbf{V}(z)\frac{\partial\bar{\mathbf{x}}}{\partial z}+\mathbf{M}(z)\bar{\mathbf{x}}+\mathbf{B}(z)\bar{\mathbf{u}}\\
&\bar{\mathbf{y}}=\mathbf{C}(z)\bar{\mathbf{x}}\\
&\bar{\mathbf{x}}(0,t)=0
\end{aligned} \tag{4.16}
$$

where $\bar{\mathbf{x}}=\tilde{\mathbf{x}}(z,t)-\tilde{\mathbf{x}}_e(z)\in\mathscr{H}$ is the state variable in deviation form; $\bar{\mathbf{u}}(t)=\mathbf{u}(t)-\mathbf{u}_e\in\mathbb{R}^2$ is the input variable in deviation form; $\bar{\mathbf{y}}=\mathbf{y}-\mathbf{y}_e\in\mathscr{Y}=L_2(0,l)^2$

with $\mathbf{y} = \mathbf{C}(z)\tilde{\mathbf{x}}(z,t)$ and $\mathbf{y}_e = \mathbf{C}(z)\tilde{\mathbf{x}}_e(z)$ denotes the output variable in deviation form; $\mathbf{V}(z)$, $\mathbf{M}(z)$ and $\mathbf{B}(z) \in L_\infty(0,l)^{2\times 2}$ are given in the Appendix; and $\mathbf{C}(z) \in L_\infty(0,l)^{2\times 2}$ is a real continuous space-varying matrix function. It should be noted that although the input variable may be finite-dimensional in practice, here we consider a spatially distributed input variable $\bar{\mathbf{u}}_d(z,t) = \mathbf{u}_d(z,t) - \mathbf{u}_e \in \mathscr{U} = L_2(0,l)^2$ to represent system (4.16) as an infinite-dimensional state-space setting with distributed input and distributed output.

Before stating system (4.16) in an infinite-dimensional state-space setting, we shall make $\mathbf{V}(z)$ a diagonal matrix. This is required to prove the stabilizability and detectability properties of system (4.16) and also to solve the resulting ORE for the LQ control problem in the next section. The eigenvalues of $\mathbf{V}(z)$ are shown in Figure 4.5. As it can be seen, $\mathbf{V}(z)$ has two distinct eigenvalues all through of the domain and therefore, is diagonalizable. It should be noted that $\mathbf{V}(z)$ is not symmetric and its eigenvalues are functions of the spatial coordinate and not necessarily negative all through of the domain. This is not the case considered in (Christofides and Daoutidis, 1996) where a symmetric velocity matrix with partially negative eigenvalues is assumed. Now, let us use the following similarity transformation:

$$\bar{\mathbf{x}} = \mathbf{T}(z)\hat{\mathbf{x}} \tag{4.17}$$

where $\mathbf{T}(z)$ is the transformation matrix whose columns are the eigenvectors of $\mathbf{V}(z)$. By applying this state transformation to (4.16), we obtain:

$$\begin{aligned} \frac{\partial \hat{\mathbf{x}}}{\partial t} &= \bar{\mathbf{V}}(z)\frac{\partial \hat{\mathbf{x}}}{\partial z} + \bar{\mathbf{M}}(z)\hat{\mathbf{x}} + \bar{\mathbf{B}}(z)\bar{\mathbf{u}}_d \\ \bar{\mathbf{y}} &= \bar{\mathbf{C}}(z)\hat{\mathbf{x}} \\ \hat{\mathbf{x}}(0,t) &= 0 \end{aligned} \tag{4.18}$$

where:

$$\bar{\mathbf{V}}(z) = \mathbf{T}(z)^{-1}\mathbf{V}(z)\mathbf{T}(z)$$

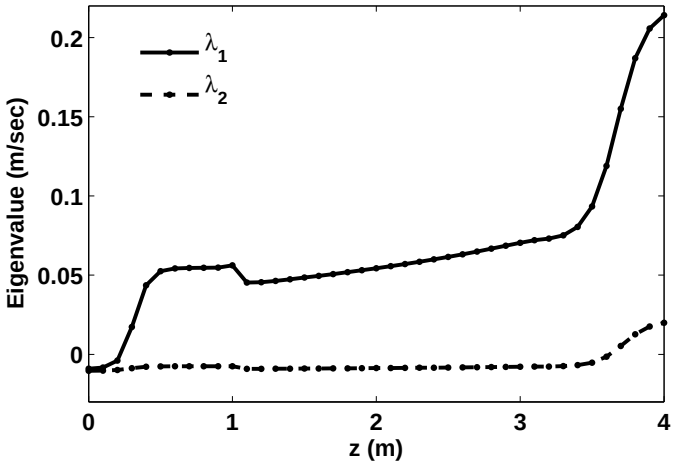


Figure 4.5: Eigenvalues of $\mathbf{V}(z)$

is a diagonal matrix whose elements are the eigenvalues of $\mathbf{V}(z)$; and $\bar{\mathbf{M}}(z)$, $\bar{\mathbf{B}}(z)$ and $\bar{\mathbf{C}}(z)$ are given by:

$$\begin{aligned}
\bar{\mathbf{M}}(z) &= \mathbf{T}(z)^{-1}\mathbf{V}(z)\frac{\partial \mathbf{T}(z)}{\partial z} + \mathbf{T}(z)^{-1}\mathbf{M}(z)\mathbf{T}(z) \\
\bar{\mathbf{B}}(z) &= \mathbf{T}(z)^{-1}\mathbf{B}(z) \\
\bar{\mathbf{C}}(z) &= \mathbf{C}(z)\mathbf{T}(z)
\end{aligned}$$

Model (4.18) can be stated in the following infinite-dimensional state-space setting in the Hilbert space $\mathscr{H}$ (Curtain and Zwart, 1995):

$$\begin{aligned}
\dot{\hat{\mathbf{x}}}(t) &= \mathscr{A}\hat{\mathbf{x}}(t) + \mathscr{B}\bar{\mathbf{u}}_d(t) \\
\bar{\mathbf{y}}(t) &= \mathscr{C}\hat{\mathbf{x}}(t)
\end{aligned} \tag{4.19}$$

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

$$\mathscr{A}h(z) = \bar{\mathbf{V}}(z)\frac{d\mathbf{h}(z)}{dz} + \bar{\mathbf{M}}(z)\mathbf{h}(z) \tag{4.20}$$

with the following domain:

$$D(\mathscr{A}) = \{\mathbf{h}(z) \in \mathscr{H} : \mathbf{h}(z) \text{ is a.c., and } \frac{d\mathbf{h}(z)}{dz} \in \mathscr{H}, \mathbf{h}(0) = 0\} \tag{4.21}$$

where a.c. means absolutely continuous; $\mathscr{B} \in \mathcal{L}(\mathscr{U}, \mathscr{H})$ is given by $\mathscr{B} = \bar{\mathbf{B}}(\cdot)I$; and $\mathscr{C} \in \mathcal{L}(\mathscr{H}, \mathscr{Y})$ is given by $\mathscr{C} = \bar{\mathbf{C}}(\cdot)I$ where I is the identity operator.

4.4 LQ Control Synthesis

In this section, we are interested in developing an LQ control policy in order to regulate the mole fraction profiles along the catalytic distillation column modelled by PDAE system (4.3) to (4.11) and represented in infinite-dimensional state-space setting (4.19). The multivariate nature of the catalytic distillation process and its high energy requirements justify the use of an optimal control policy. Model predictive control (MPC) and LQ control are the most common optimal control strategies in the process control area. The only available MPC design for hyperbolic PDE systems, which considers the infinite-dimensional characteristic of the system, is characteristic-based MPC method proposed in (Shang *et al.*, 2004); however, applicability of this method is restricted to systems having one or two characteristics with linear characteristic curves which is not the case for multi-component distillation column under study. These limitations are mainly imposed by the state prediction problem. Therefore, LQ controller, which is based on an explicit design, is more convenient for this particular process. The LQ control can be achieved through the minimization of an infinite-time horizon, quadratic objective function that requires the solution of an ORE (Curtain and Zwart, 1995; Bensoussan *et al.*, 2007). The solution of the ORE can be obtained by converting it to a matrix Riccati differential equation. The optimal feedback operator can then be found by solving the resulting matrix Riccati equation. In the first part of this section, we shall consider the regulation problem. In such a problem, the objective is to find a state feedback such that the response caused by some non-zero initial conditions (impulse disturbance) dies out at a desired rate. In the second part of this section, we consider the disturbance rejection problem in which the objective is to design a state feedback and an integrator such that the control system maintains the mole fractions at their desired equilibrium profiles in the presence of load losses such as changes in the feed flowrate.

4.4.1 Regulation Problem

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

$$J(\hat{\mathbf{x}}_0, \bar{\mathbf{u}}_d) = \int_0^\infty (\langle \mathscr{C}\hat{\mathbf{x}}(t), \mathscr{P}\mathscr{C}\hat{\mathbf{x}}(t)\rangle + \langle \bar{\mathbf{u}}_d(t), \mathscr{R}\bar{\mathbf{u}}_d(t)\rangle)dt \tag{4.22}$$

where $\mathscr{P} = \mathbf{P}I \in \mathcal{L}(\mathscr{Y})$ with $\mathbf{P} \in \mathbb{R}^{2\times 2}$ is a non-negative and symmetric matrix; and $\mathscr{R} = \mathbf{R}I \in \mathcal{L}(\mathscr{U})$ with $\mathbf{R} \in \mathbb{R}^{2\times 2}$ is a positive definite symmetric matrix. The minimization of objective function (4.22) subject to system (4.19) requires solving the following ORE (see (Curtain and Zwart, 1995) and the references therein):

$$[\mathscr{A}^*\mathscr{Q} + \mathscr{Q}\mathscr{A} + \mathscr{C}^*\mathscr{P}\mathscr{C} - \mathscr{Q}\mathscr{B}\mathscr{R}^{-1}\mathscr{B}^*\mathscr{Q}]\hat{\mathbf{x}} = 0 \tag{4.23}$$

According to (Curtain and Zwart, 1995, Theorem 6.2.7), ORE (4.23) has a unique, non-negative, and self-adjoint solution $\mathscr{Q} \in \mathcal{L}(\mathscr{H})$, if system (4.19) is exponentially stabilizable and exponentially detectable. Under these conditions, the minimum cost function is given by $J(\hat{\mathbf{x}}_0, \bar{\mathbf{u}}_{d,opt}) = \langle \hat{\mathbf{x}}_0, \mathscr{Q}\hat{\mathbf{x}}_0\rangle$ and for any initial condition $\hat{\mathbf{x}}_0 \in \mathscr{H}$, the unique optimal control variable $\bar{\mathbf{u}}_{d,opt}$, which minimizes objective function (4.22), is obtained on $t \geq 0$ as:

$$\bar{\mathbf{u}}_{d,opt}(t) = \mathbf{K}\hat{\mathbf{x}}(t) \tag{4.24}$$

where

$$\mathbf{K} = -\mathscr{R}^{-1}\mathscr{B}^*\mathscr{Q} \tag{4.25}$$

In addition, $\mathscr{A} + \mathscr{B}\mathbf{K}$ generates an exponentially stable C_0-semigroup (Curtain and Zwart, 1995). Operator $\mathscr{A}$ defined by (4.20) and (4.21) is the infinitesimal generator of an exponentially stable C_0-semigroup on $\mathscr{H}$ (Moghadam, 2013). Consequently, system (4.19) is exponentially stabilizable and exponentially detectable on $\mathscr{H}$, and according to (Curtain and Zwart, 1995, Theorem 6.2.7), ORE (4.23) has a unique, non-negative, and self-adjoint solution $\mathscr{Q} \in \mathcal{L}(\mathscr{H})$. In order to solve the ORE, we convert it to an equivalent matrix Riccati differential equation in the following Theorem.

Theorem 4.4.1 *Let us consider PDAE system (4.3) to (4.11) and its infinite-dimensional state-space representation (4.19). The unique, non-negative, and self-adjoint solution to the associated ORE (4.23) is:*

$$\mathscr{Q} = \Phi(z)I = \begin{bmatrix} \Phi_1(z) & 0 \\ 0 & \Phi_2(z) \end{bmatrix} I \tag{4.26}$$

where $\Phi(z)$ is the solution to the following matrix Riccati differential equation:

$$\begin{aligned} &\frac{d(\bar{\mathbf{V}}\Phi)}{dz} = \bar{\mathbf{M}}^*\Phi + \Phi\bar{\mathbf{M}} + \bar{\mathbf{C}}^*\mathbf{P}\bar{\mathbf{C}} - \Phi\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Phi \\ &\Phi(l) = 0 \end{aligned} \tag{4.27}$$

Proof: First, let us find the adjoint operator $\mathscr{A}^*$. By using (Curtain and Zwart, 1995, Definition A.3.63), it can be shown that the adjoint of $\mathfrak{A}\mathbf{h}(z) = \bar{\mathbf{V}}(z)\frac{d\mathbf{h}(z)}{dz}$, $\mathbf{h}(z) \in D(\mathfrak{A}) = D(\mathscr{A})$ is $\mathfrak{A}^*\mathbf{g} = -\frac{d(\bar{\mathbf{V}}\mathbf{g})}{dz}$, $\mathbf{g}(z) \in D(\mathfrak{A}^*)$ where $D(\mathfrak{A}^*)$ is:

$$D(\mathfrak{A}^*) = \{\mathbf{g}(z) \in \mathscr{H} : \mathbf{g}(z) \text{ is a.c., and } \frac{d\mathbf{g}(z)}{dz} \in \mathscr{H}, \mathbf{g}(l) = 0\} \tag{4.28}$$

Now, by using (Curtain and Zwart, 1995, Lemma A.3.65), we can write:

$$\mathscr{A}^* = (\mathfrak{A} + \bar{\mathbf{M}})^* = \mathfrak{A}^* + \bar{\mathbf{M}}^*, \quad D(\mathscr{A}^*) = D(\mathfrak{A}^*)$$

Next, by substituting (4.26) into (4.23), we get:

$$-\frac{d(\bar{\mathbf{V}}\Phi\hat{\mathbf{x}})}{dz} + \bar{\mathbf{M}}^*\Phi\hat{\mathbf{x}} + \Phi\bar{\mathbf{V}}\frac{d\hat{\mathbf{x}}}{dz} + \Phi\bar{\mathbf{M}}\hat{\mathbf{x}} + \bar{\mathbf{C}}^*\mathbf{P}\bar{\mathbf{C}}\hat{\mathbf{x}} - \Phi\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Phi\hat{\mathbf{x}} = 0 \tag{4.29}$$

On the other hand, we can write:

$$-\frac{d(\bar{\mathbf{V}}\Phi\hat{\mathbf{x}})}{dz} = -\bar{\mathbf{V}}\Phi\frac{d\hat{\mathbf{x}}}{dz} - \frac{d(\bar{\mathbf{V}}\Phi)}{dz}\hat{\mathbf{x}}$$

Since $\bar{\mathbf{V}}$ and Φ are diagonal, then $\Phi\bar{\mathbf{V}} = \bar{\mathbf{V}}\Phi$. Therefore, (4.29) turns into:

$$\frac{d(\bar{\mathbf{V}}\Phi)}{dz} = \bar{\mathbf{M}}^*\Phi + \Phi\bar{\mathbf{M}} + \bar{\mathbf{C}}^*\mathbf{P}\bar{\mathbf{C}} - \Phi\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Phi$$

Moreover, we have $\mathscr{Q}\hat{\mathbf{x}} = \Phi\hat{\mathbf{x}} \in D(\mathscr{A}^*)$. If $\Phi(l) = 0$, then $\Phi(l)\hat{\mathbf{x}}(l) = 0$ which implies that $\Phi\hat{\mathbf{x}} \in D(\mathscr{A}^*)$. On the other hand, since Φ is the unique and non-negative solution of (4.27) on $[0, l]$, so will be $\mathscr{Q}$ of (4.23).

□

Remark 4.4.1 *Matrix Riccati differential equation (4.27) results in the following differential and algebraic equations (DAEs):*

$$\frac{d(\lambda_1\Phi_1)}{dz} = 2\bar{m}_{11}\Phi_1+\bar{c}_{11}^2 p_{11} + 2\bar{c}_{21}\bar{c}_{11}p_{12} + \bar{c}_{21}^2 p_{22} - \frac{\Phi_1^2\bar{b}_{11}^2 r_{22} - 2\Phi_1^2\bar{b}_{11}\bar{b}_{12}r_{12} + \Phi_1^2\bar{b}_{12}^2 r_{11}}{r_{11}r_{22} - r_{12}^2},\ \Phi_1(l) = 0 \tag{4.30}$$

$$\frac{d(\lambda_2\Phi_2)}{dz} = 2\bar{m}_{22}\Phi_2+\bar{c}_{12}^2 p_{11} + 2\bar{c}_{12}\bar{c}_{22}p_{12} + \bar{c}_{22}^2 p_{22} - \frac{\Phi_2^2\bar{b}_{21}^2 r_{22} - 2\Phi_2^2\bar{b}_{21}\bar{b}_{22}r_{12} + \Phi_2^2\bar{b}_{22}^2 r_{11}}{r_{11}r_{22} - r_{12}^2},\ \Phi_2(l) = 0 \tag{4.31}$$

$$0 = \bar{m}_{21}\Phi_2 + \Phi_1\bar{m}_{12} + \bar{c}_{11}\bar{c}_{12}p_{11} + \bar{c}_{21}\bar{c}_{12}p_{12} + \bar{c}_{11}\bar{c}_{22}p_{12} + \bar{c}_{21}\bar{c}_{22}p_{22} - \frac{\Phi_1\Phi_2(\bar{b}_{11}\bar{b}_{21}r_{22} - \bar{b}_{12}\bar{b}_{21}r_{12} + \bar{b}_{12}\bar{b}_{22}r_{11} - \bar{b}_{11}\bar{b}_{22}r_{12})}{r_{11}r_{22} - r_{12}^2} \tag{4.32}$$

where $\bar{b}_{ij}$, $\bar{c}_{ij}$, $\bar{m}_{ij}$, r_{ij} and $p_{ij}, i = 1, 2, j = 1, 2$ are the elements of $\bar{\mathbf{B}}$, $\bar{\mathbf{C}}$, $\bar{\mathbf{M}}$, $\mathbf{R}$ and $\mathbf{P}$, receptively. Here, there are 3 equations and 2 unknown functions Φ_1 and Φ_2. Therefore, we need one more unknown which can be selected from the entries of matrices $\mathbf{P}$ and $\mathbf{R}$.

Once $\Phi_1(z)$ and $\Phi_2(z)$ are calculated, then the optimal control variable can be found from:

$$\bar{\mathbf{u}}_{d,opt}(z,t) = \mathbf{u}_{d,opt}(z,t) - \mathbf{u}_e = -\mathbf{R}^{-1}\bar{\mathbf{B}}^*(z)\Phi(z)\hat{\mathbf{x}}(z,t) \tag{4.33}$$

4.4.2 Disturbance Rejection Problem

In order to consider the effect of change of load on the optimal control policy achieved in the previous section, here we extend the result to obtain an optimal proportional plus integral controller which compensates for the effect that these disturbances might have on the column. To this end, we penalize the rate of change of the control variable rather than the amount of control in the following objective function:

$$J(\hat{\mathbf{x}}_0, \dot{\hat{\mathbf{u}}}_d) = \int_0^\infty (\langle \mathscr{C}\hat{\mathbf{x}}(t), \mathscr{P}\mathscr{C}\hat{\mathbf{x}}(t)\rangle + \langle \dot{\hat{\mathbf{u}}}_d(t), \mathscr{R}\dot{\hat{\mathbf{u}}}_d(t)\rangle)dt \tag{4.34}$$

where $\mathscr{P}$ and $\mathscr{R}$ are defined in (4.22). In order to solve the optimal control problem, let us differentiate the state equation in (4.19):

$$\ddot{\hat{\mathbf{x}}}(t) = \mathscr{A}\dot{\hat{\mathbf{x}}}(t) + \mathscr{B}\dot{\tilde{\mathbf{u}}}_d(t) \tag{4.35}$$

and define:

$$\mathbf{x}_a = \dot{\hat{\mathbf{x}}} \in \mathscr{H}, \quad \mathbf{w} = \dot{\tilde{\mathbf{u}}}_d \in \mathscr{U}.$$

Performance index (4.34) subject to model (4.19) can now be stated in the following alternative form:

$$J(\hat{\mathbf{x}}_{a,0}, \mathbf{w}) = \int_0^\infty (\langle \mathscr{C}_a \hat{\mathbf{x}}_a(t), \mathscr{P}\mathscr{C}_a \hat{\mathbf{x}}_a(t)\rangle + \langle \mathbf{w}, \mathscr{R}\mathbf{w}\rangle) dt \tag{4.36}$$

subject to the restriction:

$$\begin{aligned} \dot{\hat{\mathbf{x}}}_a(t) &= \mathscr{A}_a \hat{\mathbf{x}}_a(t) + \mathscr{B}_a \mathbf{w} \\ \bar{\mathbf{y}}(t) &= \mathscr{C}_a \hat{\mathbf{x}}_a(t) \end{aligned} \tag{4.37}$$

where $\hat{\mathbf{x}}_a = [\hat{\mathbf{x}}, \mathbf{x}_a]^T \in L_2(0,l)^4$; $\mathscr{B}_a = [\mathbf{0}, \mathscr{B}]^T$; $\mathscr{C}_a = [\mathscr{C}, \mathbf{0}]$; and

$$\mathscr{A}_a = \begin{bmatrix} \mathbf{0} & I \\ \mathbf{0} & \mathscr{A} \end{bmatrix} \tag{4.38}$$

in which I is the identity operator.

The minimization of objective function (4.36) subject to system (4.37) requires solving the following ORE:

$$[\mathscr{A}_a^* \mathscr{Q}_a + \mathscr{Q}_a \mathscr{A}_a + \mathscr{C}_a^* \mathscr{P}\mathscr{C}_a - \mathscr{Q}_a \mathscr{B}_a \mathscr{R}^{-1} \mathscr{B}_a^* \mathscr{Q}_a] \hat{\mathbf{x}}_a = 0 \tag{4.39}$$

For ORE (4.39) to have a unique, non-negative, and self-adjoint solution $\mathscr{Q}_a \in \mathcal{L}(L_2(0,l)^4)$, system (4.37) has to be exponentially stabilizable and exponentially detectable (Curtain and Zwart, 1995, Theorem 6.2.7). The minimum cost function is given by $J(\hat{\mathbf{x}}_{a,0}, \mathbf{w}_{opt}) = \langle \hat{\mathbf{x}}_{a,0}, \mathscr{Q}_a \hat{\mathbf{x}}_{a,0}\rangle$ and for any initial condition $\hat{\mathbf{x}}_{a,0} \in L_2(0,l)^4$, the unique optimal control variable $\mathbf{w}_{opt}$, which minimizes objective function (4.36), is obtained on $t \geq 0$ as:

$$\mathbf{w}_{opt}(t) = \mathbf{K}_a \hat{\mathbf{x}}_a(t) \tag{4.40}$$

where

$$\mathbf{K}_a = -\mathscr{R}^{-1}\mathscr{B}_a^*\mathscr{Q}_a \tag{4.41}$$

In addition, $\mathscr{A}_a + \mathscr{B}_a\mathbf{K}_a$ generates an exponentially stable C_0-semigroup (Curtain and Zwart, 1995). In order to show the existence and uniqueness of solution to ORE (4.39), in the following Theorem we deal with the stabilizability and detectability properties of system (4.37).

Theorem 4.4.2 *Operator $\mathscr{A}_a$ defined in (4.38) is the infinitesimal generator of an exponentially stable C_0-semigroup.*

Proof: Operator $\mathscr{A}$ defined by (4.20) and (4.21) is the infinitesimal generator of an exponentially stable C_0-semigroup on $\mathscr{H}$ (Moghadam, 2013). Let $S(t)$ be the C_0-semigroup on $\mathscr{H}$ generated by $\mathscr{A}$. Therefore, there exist $m_1, \alpha_1 > 0$ such that $\|S(t)\| \leq m_1 e^{-\alpha_1 t}$. On the other hand, there exist $m_2, \alpha_2 > 0$ such that $\|0\| \leq m_2 e^{-\alpha_2 t}$. Since the identity operator is bounded, i.e., $\|I\| \leq \beta$, $\beta > 0$, by using (Curtain and Zwart, 1995, Lemma 3.2.2), it can be shown that $\mathscr{A}_a$ is the infinitesimal generator of a C_0-semigroup and moreover, $\mathscr{A}_a \leq me^{-\alpha t}$, $m, \alpha > 0$.

□

Since $\mathscr{A}_a$ is the infinitesimal generator of an exponentially stable C_0-semigroup, system (4.37) is exponentially stabilizable and exponentially detectable on $L_2(0,l)^4$, and therefore, ORE (4.39) has a unique, non-negative, and self-adjoint solution $\mathscr{Q}_a \in \mathcal{L}(L_2(0,l)^4)$. Let us solve the optimal control problem in the following Theorem.

Theorem 4.4.3 *The optimal proportional plus integral controller for PDAE system (4.3) to (4.11) and its infinite-dimensional state-space representation (4.19) can be achieved by:*

$$\begin{aligned}\bar{\mathbf{u}}_{d,opt}(z,t) = \mathbf{u}_{d,opt}(z,t) - \mathbf{u}_e = &-\mathbf{R}^{-1}\bar{\mathbf{B}}(z)\Psi_3(z)\hat{\mathbf{x}}(z,t) \\ &- \mathbf{R}^{-1}\bar{\mathbf{B}}(z)\Psi_2(z)\int_0^t \hat{\mathbf{x}}(z,t)dt\end{aligned} \tag{4.42}$$

where $\Psi_2 \in \mathbb{R}^{2\times 2}$ is obtained through solving the following algebraic matrix Riccati equation:

$$\bar{\mathbf{C}}^*\mathbf{P}\bar{\mathbf{C}} - \Psi_2\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Psi_2^* = 0 \tag{4.43}$$

and $\Psi_3 \in \mathbb{R}^{2\times 2}$ is a diagonal matrix which is obtained through solving the following matrix Riccati differential equation:

$$\begin{aligned} &\frac{d(\bar{\mathbf{V}}\Psi_3)}{dz} = \bar{\mathbf{M}}^*\Psi_3 + \Psi_3\bar{\mathbf{M}} + \Psi_2 + \Psi_2^* - \Psi_3\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Psi_3 \\ &\Psi_3(l) = 0 \end{aligned} \tag{4.44}$$

Proof: Let us consider the following solution to ORE (4.39):

$$\mathscr{Q}_a = \begin{bmatrix} \Psi_1 & \Psi_2 \\ \Psi_2^* & \Psi_3 \end{bmatrix} = \begin{bmatrix} \Psi_1(z) & \Psi_2(z) \\ \Psi_2^*(z) & \Psi_3(z) \end{bmatrix} I \tag{4.45}$$

where $\Psi_1, \Psi_3 \in \mathbb{R}^{2\times 2}$ are non-negative symmetric and non-negative diagonal matrices, respectively, and I is the identity operator. By substituting for $\mathscr{B}_a$ and $\mathscr{Q}_a$ into (4.41), we have:

$$\mathbf{K}_a = \begin{bmatrix} -\mathscr{R}^{-1}\mathscr{B}^*\Psi_2 & -\mathscr{R}^{-1}\mathscr{B}^*\Psi_3 \end{bmatrix}$$

and then from (4.40) we obtain:

$$\mathbf{w}_{opt}(t) = -\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Psi_2\hat{\mathbf{x}} - \mathbf{R}^{-1}\bar{\mathbf{B}}^*\Psi_3\dot{\hat{\mathbf{x}}}$$

which can be integrated to yield (4.42). In order to find Ψ_2 and Ψ_3, let us substitute for $\mathscr{A}_a$, $\mathscr{B}_a$, $\mathscr{C}_a$ and $\mathscr{Q}_a$ into (4.39), which yields:

$$\mathscr{C}^*\mathscr{P}\mathscr{C} - \Psi_2\mathscr{B}\mathscr{R}^{-1}\mathscr{B}^*\Psi_2^* = 0 \tag{4.46}$$

$$\Psi_1 + \Psi_2\mathscr{A} - \Psi_2\mathscr{B}\mathscr{R}^{-1}\mathscr{B}^*\Psi_3^* = 0 \tag{4.47}$$

$$\Psi_1 + \mathscr{A}^*\Psi_2^* - \Psi_3\mathscr{B}\mathscr{R}^{-1}\mathscr{B}^*\Psi_2^* = 0 \tag{4.48}$$

$$\Psi_2 + \mathscr{A}^*\Psi_3 + \Psi_2^* + \Psi_3\mathscr{A} - \Psi_3\mathscr{B}\mathscr{R}^{-1}\mathscr{B}^*\Psi_3 = 0 \tag{4.49}$$

ORE (4.46) can be converted to the following algebraic matrix Riccati equation:

$$\bar{\mathbf{C}}^*\mathbf{P}\bar{\mathbf{C}} - \Psi_2\bar{\mathbf{B}}\mathbf{R}^{-1}\bar{\mathbf{B}}^*\Psi_2^* = 0 \tag{4.50}$$

which can be solved to obtain Ψ_2. By the same argument used in Theorem 4.4.1, ORE (4.49) can be converted to matrix Riccati differential equation (4.44).

□

4.5 Simulation Results

In this section, a set of numerical simulations is performed to assess the performance of the LQ controller developed in Section 4.4. The control objective is to regulate the mole fraction profiles along the catalytic distillation column described by model equations (4.3) to (4.11). In the first part of the simulation study, we deal with a regulation problem in which the controller designed in Section 4.4.1 is tested against rejecting the effect of a non-zero initial condition (impulse disturbance). As it was discussed in Section 4.4.1, the LQ controller can be calculated through solving DAEs (4.30) to (4.32) and using control law (4.33). Since we are interested in controlling both state variables, the observation matrix $\mathbf{C}(z)$ is set to be the identity matrix. The weighting matrices are chosen such that $\mathbf{P} = diag(1 \times 10^{-3}, 1 \times 10^{-3})$ and $\mathbf{R} = diag(350, 350)$. We solve DAEs (4.30) to (4.32) along with nonlinear model equations (4.3) to (4.11) in gPROMS. It should be noted that gPROMS uses the method of lines (MOL) family of numerical methods to solve PDAE system (4.3) to (4.11). This involves discretization of the spatial derivatives in the PDEs to obtain a set of time-dependent ODEs. This set of ODEs along with the algebraic equations result in a set of mixed DAEs. The DAE system is then solved using a DAE solver (see (Oh and Pantelides, 1996) for more details). We choose 40 discretization points and backward finite-difference method for discretizing the spatial derivatives. The time step is then determined by gPROMS through a variable step-size method to achieve the numerical stability. An arbitrary initial condition $x_1(z, 0) = 0.2$ and $x_2(z, 0) = 0.8$ is chosen and the controller is implemented on the original nonlinear model equations (4.3) to (4.11) through 20 discretization points. The control error profiles for DME and methanol

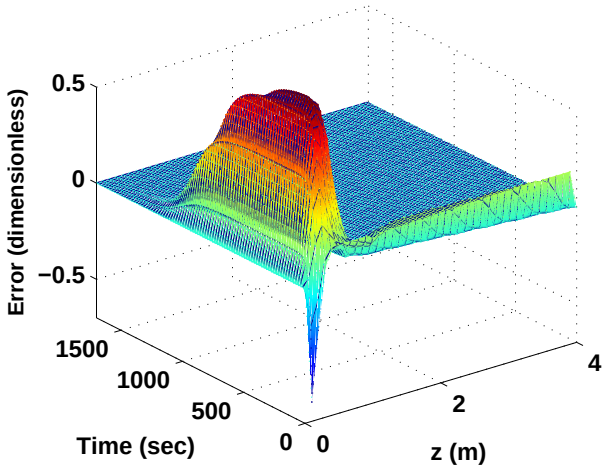
liquid mole fractions, $err_1(z,t) = x_1(z,t) - x_{1,e}(z)$ and $err_2(z,t) = x_2(z,t) - x_{2,e}(z)$, are shown in Figures 4.6(a) and 4.6(b). These figures show how the LQ controller is able to bring the mole fraction profiles to their desired equilibrium profiles shown in Figure 4.2. This is the ideal control and gives us the best achievable performance; however, this control variable is distributed throughout the domain and may not be realizable in practice. The following averaged value may be used instead, which results in the best suboptimal controller:

$$\mathbf{u}_{sub}(t) - \mathbf{u}_e = -\frac{1}{l}\int_0^l \mathbf{R}^{-1}\bar{\mathbf{B}}^*(z)\Phi(z)\hat{\mathbf{x}}(z,t)dz \tag{4.51}$$

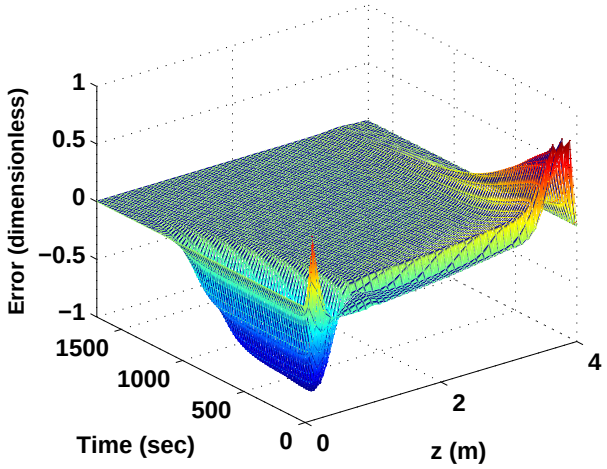
In order to have a measure of how much the control performance is deteriorated by using the suboptimal controller, and also to show the effectiveness of the designed controller, we make a comparison between the designed infinite-dimensional LQ controller and a finite-dimensional LQ controller which is obtained by using a discretized model. For the finite-dimensional LQ controller design, we approximate model (4.18) through discretizing the spatial derivatives using 20 discretization points. This number of discretization points is equal to the one we use to implement the infinite-dimensional controller. Since we have two state variables, the dimension of the resulting ODE model is 40×40. We employ finite-difference (centered finite-difference) scheme which gives us a stabilizable ODE system that provides guarantee of the existence and uniqueness of the solution to the resulting algebraic matrix Riccati equation. We choose the same state and input weights as used in designing the infinite-dimensional LQ controller and solve the resulting algebraic matrix Riccati equation in gPROMS. In order to compare the performance of the controllers, we use the spatially averaged control error given as:

$$err_{i,ave} = \frac{1}{l}\int_0^l [x_i(z,t) - x_{i,e}(z)]dz \tag{4.52}$$

The spatially averaged error for the optimal and suboptimal infinite-dimensional LQ



(a) DME



(b) Methanol

Figure 4.6: Optimal control error profiles

and optimal and suboptimal finite-dimensional LQ controllers are compared in Figure 4.7. The normalized settling times and integral of absolute errors (IAE) for responses are given in Table 4.2. In this table t_s is the settling time and τ is the residence time of the column. As it can be observed from comparing the response specifications, the infinite-dimensional LQ controller outperforms the finite-dimensional LQ controller, considerably. The performance of the suboptimal controllers are slightly poorer than the optimal controllers because of the averaging used in calculating the suboptimal control

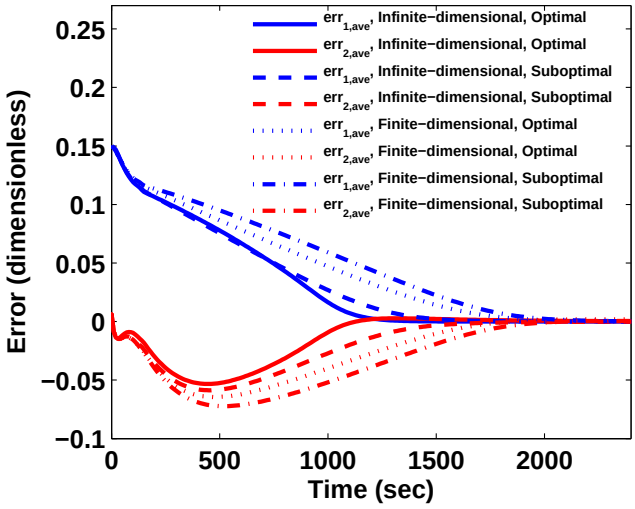


Figure 4.7: Spatially averaged error

Table 4.2: Response specifications for Figure 4.7

System	$\frac{t_s}{\tau}$	$\frac{\int_0^{5000} \lvert err_{1,ave} \rvert dt}{\tau}$	$\frac{\int_0^{5000} \lvert err_{2,ave} \rvert dt}{\tau}$
Infinite-dimensional, Optimal	$\frac{1130}{335.8} = 3.36$	$\frac{78.45}{335.8} = 0.234$	$\frac{36.70}{335.8} = 0.109$
Infinite-dimensional, Suboptimal	$\frac{1330}{335.8} = 3.96$	$\frac{83.15}{335.8} = 0.248$	$\frac{48.93}{335.8} = 0.146$
Finite-dimensional, Optimal	$\frac{1810}{335.8} = 5.39$	$\frac{105.92}{335.8} = 0.315$	$\frac{65.57}{335.8} = 0.195$
Finite-dimensional, Suboptimal	$\frac{1910}{335.8} = 5.69$	$\frac{120.92}{335.8} = 0.360$	$\frac{77.02}{335.8} = 0.229$

inputs, yet the suboptimal infinite-dimensional LQ controller outperforms the optimal finite-dimensional LQ controller. The suboptimal control input profiles for infinite and finite-dimensional controllers are also compared in Figure 4.8. The integral of absolute suboptimal control inputs are compared in Table 4.3, which indicates that the infinite-dimensional LQ controller requires less control effort than the finite-dimensional LQ controller.

In addition to comparing the controllers' accuracy which is discussed above, we also make comments on the computational effort required for each controller realization. For calculating the infinite-dimensional LQ controller, set of DAEs (4.30) to (4.32) has

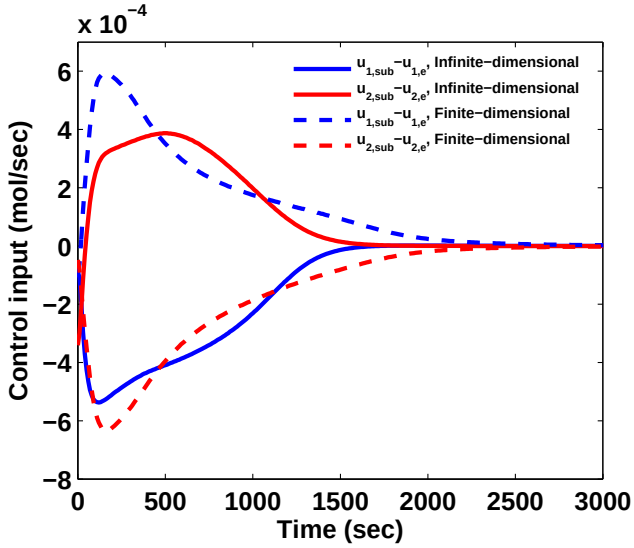


Figure 4.8: Suboptimal control input profiles

Table 4.3: Response specifications for Figure 4.8

System	$\int_0^{5000} \lvert u_{1,sub} - u_{1,e} \rvert dt$	$\int_0^{5000} \lvert u_{2,sub} - u_{2,e} \rvert \rvert dt$
Infinite-dimensional, Suboptimal	0.44	0.36
Finite-dimensional, Suboptimal	0.45	0.48

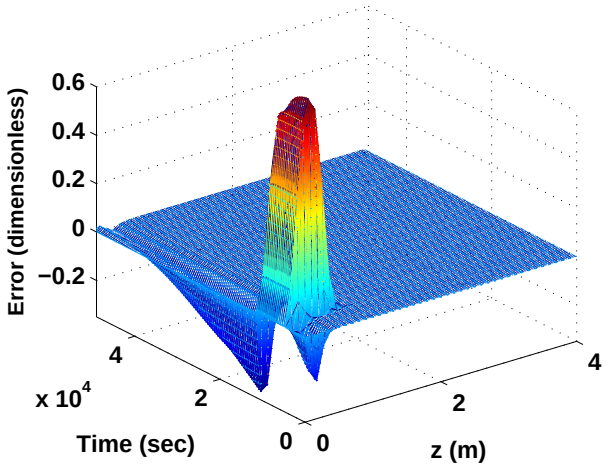
to be solved which involves two boundary value problems and one algebraic equation and this is independent of the number of discretization points chosen for the late implementation; however, depending on the number of discretization points, calculating the finite-dimensional controller requires solving a high-dimensional matrix Riccati equation. In this case a system of 40×40 matrix Riccati equations has to be solved which is computationally difficult to realize. Moreover, because of the matrix algebra calculations, the amount of online computational effort required by the finite-dimensional controller is much more than what is needed by the infinite-dimensional controller. Indeed, for the infinite-dimensional design once DAE system (4.30) to (4.32) is solved, computing the control inputs at each point requires a 2×2 matrix multiplication; however, calculating the control inputs for the finite-dimensional design involves a 40×40 matrix multiplication.

The simulation time required for testing the finite-dimensional controller is more than two times of the time required for the infinite-dimensional controller.

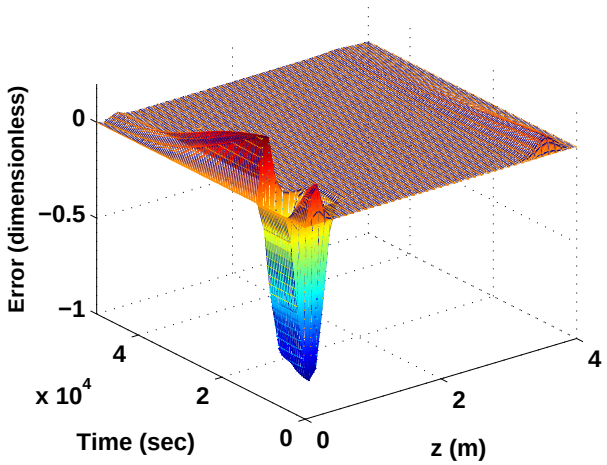
In the second part of the simulation study, we consider a disturbance rejection problem and evaluate the performance of the controller designed in Section 4.4.2. To this end, we assume that a step disturbance with the magnitude of 10% occurs at the feed flowrate. The optimal proportional plus integral controller can be achieved by solving matrix Riccati differential equation (4.44) along with algebraic matrix Riccati equation (4.43) and using control law (4.42). The observation matrix $\mathbf{C}(z)$ is set to be the identity matrix and the weighting matrices are chosen such that $\mathbf{P} = diag(1 \times 10^{-6}, 1 \times 10^{-6})$ and $\mathbf{R} = diag(8000, 8000)$. The controller is implemented on the original nonlinear model (4.3) to (4.11) and the control error profiles for DME and methanol liquid mole fractions, $err_1(z,t) = x_1(z,t) - x_{1,e}(z)$ and $err_2(z,t) = x_2(z,t) - x_{2,e}(z)$, are shown in Figures 4.9(a) and 4.9(b). As it can be observed, the optimal controller is able to reject the effect of the disturbance and bring the mole fraction profiles to their desired equilibrium profiles. The spatially averaged error for the optimal and suboptimal LQ controllers for DME and methanol liquid mole fractions are also shown in Figure 4.10. The performance of the suboptimal controller is poorer than the optimal controller, nevertheless, it also rejects the effect of such a severe disturbance. The suboptimal control input profiles are also shown in Figure 4.11, which indicates that the control efforts are not particularly aggressive and are physically realizable.

4.6 Conclusions

In this work an ORE-based infinite-dimensional LQ control policy is developed to control the mole fraction profiles along a packed catalytic distillation column. The column is modelled by a set of coupled hyperbolic PDAEs. By solving the algebraic equations for the algebraic variables and substituting them into the PDEs, a model consisting of a set of



(a) DME



(b) Methanol

Figure 4.9: Optimal control error profiles for disturbance rejection

pure hyperbolic PDEs is obtained. The resulting infinite-dimensional system, involves a hyperbolic operator in which the velocity matrix is spatially varying, non-diagonal, and not necessarily negative through of the domain. After diagonalizing the hyperbolic operator, the unique and non-negative solution to the ORE is found by converting it to an equivalent matrix Riccati differential equation which can be solved numerically. The result is then extended to obtain an optimal proportional plus integral controller which can reject the effect of load losses. In order to assess the performance of the designed controller, a

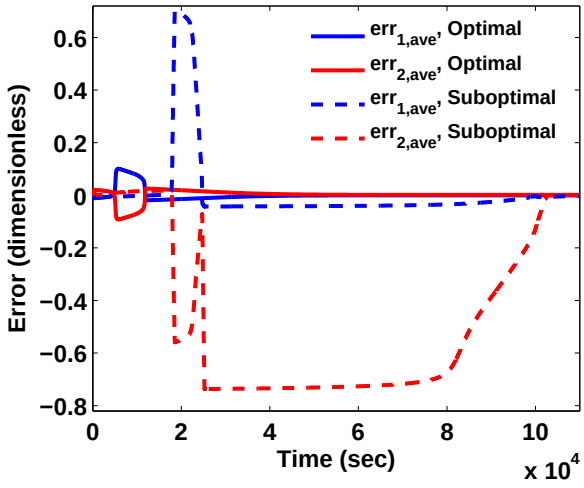


Figure 4.10: Spatially averaged error for disturbance rejection

numerical study is performed and the controller is successfully implemented on the column model.

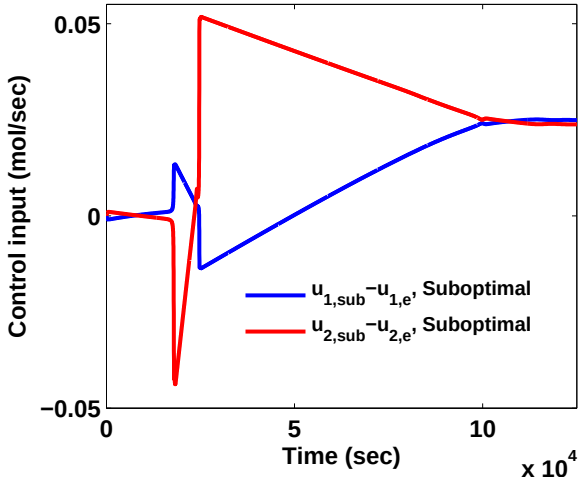


Figure 4.11: Suboptimal control input profiles for disturbance rejection

Appendix

This section includes a detailed description of the terms involved in the linear model (4.16). It should be noted that in all the expressions, subscript "e" denotes the equilibrium or the steady-state condition. Before defining matrix functions $\mathbf{V}(z)$, $\mathbf{B}(z)$ and $\mathbf{M}(z)$, let us define some useful terms.

$$\frac{K_W}{K_{M,e}} = exp(-k_3 + \frac{k_4}{T_e}), \quad k_{s,e} = k_1 exp(\frac{-k_2}{RT_e})$$

$$\theta_1 = \alpha_1 x_{1,in}(1+\tilde{x}_{1,e}) + \alpha_2 x_{2,in}(1+\tilde{x}_{2,e}) + \alpha_3[1 - x_{1,in}(1+\tilde{x}_{1,e}) - x_{2,in}(1+\tilde{x}_{2,e})]$$

$$\theta_2 = \alpha_1 x_{1,in}(1+\tilde{x}_{1,e}) + \alpha_3[1 - x_{1,in}(1+\tilde{x}_{1,e})]$$

$$\theta_3 = \alpha_2 x_{2,in}(1+\tilde{x}_{2,e}) + \alpha_3[1 - x_{2,in}(1+\tilde{x}_{2,e})]$$

$$\theta_4 = (\alpha_3 - \alpha_2)x_{1,in}(1+\tilde{x}_{1,e}), \quad \theta_5 = (\alpha_3 - \alpha_1)x_{2,in}(1+\tilde{x}_{2,e})$$

$$\theta_6 = 1 - x_{1,in}(1+\tilde{x}_{1,e}) - x_{2,in}(1+\tilde{x}_{2,e})$$

$$\theta_7 = x_{2,in}(1+\tilde{x}_{2,e}) + \frac{K_W}{K_{M,e}}[1 - x_{1,in}(1+\tilde{x}_{1,e}) - x_{2,in}(1+\tilde{x}_{2,e})]$$

$$\theta_8 = A_{vp,D} - \log_{10}(\frac{\alpha_1 P}{\theta_1})$$

$\mathbf{V}(z)$ is given by:

$$\begin{aligned}\mathbf{V}(z) = \tilde{F}(\tilde{\mathbf{x}}_e, \mathbf{u}_e) &= \begin{bmatrix} \tilde{f}_{11}(\tilde{\mathbf{x}}_e, \mathbf{u}_e) & \tilde{f}_{12}(\tilde{\mathbf{x}}_e, \mathbf{u}_e) \\ \tilde{f}_{21}(\tilde{\mathbf{x}}_e, \mathbf{u}_e) & \tilde{f}_{22}(\tilde{\mathbf{x}}_e, \mathbf{u}_e) \end{bmatrix} \\ &= \frac{1}{U_L}\begin{bmatrix} \frac{u_{2,e}\alpha_1\theta_3}{\theta_1^2} - u_{1,e} & \frac{u_{2,e}\alpha_1\theta_4 x_{2,in}}{\theta_1^2 x_{1,in}} \\ \frac{u_{2,e}\alpha_2\theta_5 x_{1,in}}{\theta_1^2 x_{2,in}} & \frac{u_{2,e}\alpha_2\theta_2}{\theta_1^2} - u_{1,e} \end{bmatrix}\end{aligned} \tag{4.53}$$

$\mathbf{B}(z)$ is given by:

$$\mathbf{B}(z) = \begin{bmatrix} -\frac{1}{U_L}\frac{\partial \tilde{x}_{1,e}}{\partial z} & (\frac{\tilde{f}_{11}(\tilde{\mathbf{x}}_e, \mathbf{u}_e)}{u_{2,e}} + \frac{u_{1,e}}{U_L u_{2,e}})\frac{\partial \tilde{x}_{1,e}}{\partial z} + \frac{\tilde{f}_{12}(\tilde{\mathbf{x}}_e, \mathbf{u}_e)}{u_{2,e}}\frac{\partial \tilde{x}_{2,e}}{\partial z} \\ -\frac{1}{U_L}\frac{\partial \tilde{x}_{2,e}}{\partial z} & \frac{\tilde{f}_{21}(\tilde{\mathbf{x}}_e, \mathbf{u}_e)}{u_{2,e}}\frac{\partial \tilde{x}_{1,e}}{\partial z} + (\frac{\tilde{f}_{22}(\tilde{\mathbf{x}}_e, \mathbf{u}_e)}{u_{2,e}} + \frac{u_{1,e}}{U_L u_{2,e}})\frac{\partial \tilde{x}_{2,e}}{\partial z} \end{bmatrix} \tag{4.54}$$

where $\tilde{f}_{11}(\tilde{\mathbf{x}}_e, \mathbf{u}_e)$, $\tilde{f}_{12}(\tilde{\mathbf{x}}_e, \mathbf{u}_e)$, $\tilde{f}_{21}(\tilde{\mathbf{x}}_e, \mathbf{u}_e)$ and $\tilde{f}_{22}(\tilde{\mathbf{x}}_e, \mathbf{u}_e)$ are given in (4.53).

$\mathbf{M}(z)$ is given by:

$$\mathbf{M}(z) = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \tag{4.55}$$

where

$$\begin{aligned} m_{11} =& \frac{u_{2,e}\alpha_1}{U_L\theta_1^3}\{-2x_{1,in}(\alpha_1-\alpha_3)\theta_3\frac{\partial\tilde{x}_{1,e}}{\partial z} + [x_{2,in}(\alpha_3-\alpha_2)\theta_1 \\ & - 2x_{2,in}(\alpha_1-\alpha_3)\theta_4]\frac{\partial\tilde{x}_{2,e}}{\partial z}\} \\ & - \frac{k_2k_{s,e}\phi x_{2,in}^2(1+\tilde{x}_{2,e})^2(\alpha_1-\alpha_3)B_{vp,D}}{U_L(\theta_7\theta_8)^2\theta_1RT_e^2\ln(10)} \\ & - \frac{2\phi k_{s,e}x_{2,in}^2(1+\tilde{x}_{2,e})^2\frac{K_W}{K_{M,e}}}{U_L\theta_7^3}[\frac{k_4(\alpha_1-\alpha_3)\theta_6B_{vp,D}}{T_e^2\theta_8^2\theta_1\ln(10)} - 1] \end{aligned} \tag{4.56}$$

$$\begin{aligned} m_{12} =& \frac{u_{2,e}\alpha_1}{U_L\theta_1^3}[x_{2,in}(\alpha_2-\alpha_3)(\theta_1-2\theta_3)\frac{\partial\tilde{x}_{1,e}}{\partial z} - \frac{2x_{2,in}^2(\alpha_2-\alpha_3)\theta_4}{x_{1,in}}\frac{\partial\tilde{x}_{2,e}}{\partial z}] \\ & - \frac{k_2k_{s,e}\phi x_{2,in}^3(1+\tilde{x}_{2,e})^2(\alpha_2-\alpha_3)B_{vp,D}}{U_L(\theta_7\theta_8)^2x_{1,in}\theta_1RT_e^2\ln(10)} \\ & + \frac{2\phi k_{s,e}x_{2,in}(1+\tilde{x}_{2,e})}{U_Lx_{1,in}\theta_7^3}\{\theta_7 - x_{2,in}^2(1+\tilde{x}_{2,e}) \\ & - x_{2,in}^2(1+\tilde{x}_{2,e})\frac{K_W}{K_{M,e}}[\frac{k_4(\alpha_2-\alpha_3)\theta_6B_{vp,D}}{T_e^2\theta_8^2\theta_1\ln(10)} + 1]\} \end{aligned} \tag{4.57}$$

$$\begin{aligned} m_{21} =& \frac{u_{2,e}\alpha_2}{U_L\theta_1^3}[\frac{-2x_{1,in}^2(\alpha_1-\alpha_3)\theta_5}{x_{2,in}}\frac{\partial\tilde{x}_{1,e}}{\partial z} + x_{1,in}(\alpha_1-\alpha_3)(\theta_1-2\theta_2)\frac{\partial\tilde{x}_{2,e}}{\partial z}] \\ & + \frac{2k_2k_{s,e}\phi x_{2,in}x_{1,in}(1+\tilde{x}_{2,e})^2(\alpha_1-\alpha_3)B_{vp,D}}{U_L(\theta_7\theta_8)^2\theta_1RT_e^2\ln(10)} \\ & + \frac{4\phi k_{s,e}x_{2,in}x_{1,in}(1+\tilde{x}_{2,e})^2\frac{K_W}{K_{M,e}}}{U_L\theta_7^3}[\frac{k_4(\alpha_1-\alpha_3)\theta_6B_{vp,D}}{T_e^2\theta_8^2\theta_1\ln(10)} - 1] \end{aligned} \tag{4.58}$$

$$\begin{aligned} m_{22} =& \frac{u_{2,e}\alpha_2}{U_L\theta_1^3}\{[x_{1,in}(\alpha_3-\alpha_1)\theta_1 - 2x_{1,in}(\alpha_2-\alpha_3)\theta_5]\frac{\partial\tilde{x}_{1,e}}{\partial z} \\ & -2x_{2,in}(\alpha_2-\alpha_3)\theta_2\frac{\partial\tilde{x}_{2,e}}{\partial z}\} + \frac{2k_2k_{s,e}\phi x_{2,in}^2(1+\tilde{x}_{2,e})^2(\alpha_2-\alpha_3)B_{vp,D}}{U_L(\theta_7\theta_8)^2\theta_1RT_e^2\ln(10)} \\ & - \frac{4\phi k_{s,e}(1+\tilde{x}_{2,e})}{U_L\theta_7^3}\{\theta_7 - x_{2,in}^2(1+\tilde{x}_{2,e}) \\ & - x_{2,in}^2(1+\tilde{x}_{2,e})\frac{K_W}{K_{M,e}}[\frac{k_4(\alpha_2-\alpha_3)\theta_6B_{vp,D}}{T_e^2\theta_8^2\theta_1\ln(10)} + 1]\} \end{aligned} \tag{4.59}$$

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Chapter 5

Conclusions and Future Work

Transport-reaction processes are quite common in chemical and biochemical engineering practice. Typically, these processes involve phase equilibria and/or are combined with well-mixed processes. The mathematical description of such systems involves combinations of PDEs, ODEs and algebraic equations. The accurate analysis and control synthesis for these systems require the development of new methods in the control theory of infinite-dimensional systems. Recently, linear quadratic (LQ) control has been of particular interest in the control theory of infinite-dimensional systems in chemical processes. This is mainly motivated by the explicit controller design that LQ method provides, which allows deriving the controller by solving an operator Riccati equation (ORE) (Aksikas *et al.*, 2009). The present thesis has been devoted to the development of ORE-based LQ control methods for combinations of hyperbolic PDEs, ODEs and algebraic equations that arise from mathematical modelling of distributed parameter systems in chemical processes.

5.1 Conclusions

The initial work focused on designing an LQ controller for coupled hyperbolic PDEs-ODEs. These systems describe transport-reaction processes combined with well-mixed processes. Coupled CSTR-PFR systems are an example. In such systems, the boundary control actuation of the transport-reaction process involves finite-dimensional dynamics,

i.e., the control variable acts through a lumped system on the boundaries of the distributed system. While the boundary control problems for PDE systems are considered hard to solve (due to the unbounded input and output operators (Krstic and Smyshlyaev, 2008)), the presence of the finite-dimensional dynamics in the control input makes the control problem of coupled PDE-ODE systems even more challenging.

Chapter 2 dealt with the development of an LQ controller for these systems. In order to solve the optimal control problem, first, the coupled PDE-ODE system was represented in an infinite-dimensional state-space setting by using the boundary control transformation method. This is required to prove the exponential stabilizability and exponential detectability properties of the system and also to solve the resulting ORE. Subsequently, the exponential stabilizability and exponential detectability properties of the coupled system were proved, which provide guarantees of the existence and uniqueness of the solution to the resulting ORE. The explicit optimal control design was then formulated by considering an infinite-time horizon and quadratic objective function for the linear infinite-dimensional state-space model. The minimization of such an objective function requires solving an ORE. The most challenging part of the problem lies in solving the ORE. This was addressed by considering a block-diagonal form of solution for the underlying ORE. This form of the solution helps to convert the ORE into an equivalent set of coupled differential and algebraic matrix equations and permits the use of a numerical scheme to solve the control design equations. It was proved that this form of the solution exists and the resulting differential and algebraic matrix equations lead to a solution. Next, an iterative algorithm was proposed to solve the set of coupled differential and algebraic matrix equations. Finally, in order to demonstrate the theory, an illustrative numerical study was performed and the developed method was successfully implemented on an interconnected CSTR-PFR process model.

Another problem treated in this thesis was the LQ control for coupled hyperbolic PDEs-

Algebraic equations. These systems describe two-phase transport-reaction processes, which are quite common in chemical engineering practice. Two-phase counter-current contactors are an example. In such systems, two transport-reaction processes are exchanging mass and energy through a direct contact. The PDEs describe the transport-reaction phenomena and the algebraic equations represent the equilibrium condition. The presence of the algebraic equations makes the velocity matrix in the transport operator spatially varying, non-diagonal, and not necessarily negative through of the domain. In contrast to transport operators with a constant, negative and diagonal velocity matrix (which is the case for single-phase systems), dealing with the well-posedness (existence and uniqueness of the solution for the open-loop system) of such systems is not a standard argument (Russell, 1978). Moreover, solving the optimal control problem (proving the existence and uniqueness of the solution to the resulting ORE and finding the unique solution) for systems involving such a transport operator is a challenging issue (Aksikas *et al.*, 2009).

These challenges were addressed in Chapter 3. After proving the closedness of the underlying transport operator, its C_0-semigroup generation property was shown by using the Hille-Yosida Theorem. Subsequently, by using the spectral analysis, it was shown that the C_0-semigroup generated by the transport operator is exponentially stable. This indicates that the underlying linear system is exponentially stabilizable and exponentially detectable and whence, the resulting ORE has a unique and non-negative solution. Such a solution was then found by converting the ORE into an equivalent matrix Riccati differential equation, which can be solved numerically. Finally, the theory was demonstrated by studying a continuous counter-current adsorption process of two interacting components in a moving-bed adsorber and the designed controller was successfully implemented on the process model through a numerical simulation.

One of the key transport-reaction processes described by coupled PDEs-Algebraic

equations is (reactive) distillation. Although the LQ controller designed in Chapter 3 may be used for regulating the (reactive) distillation processes, more theoretical development is required to address some practical issues such as rejecting the effect of load losses. This problem was addressed in Chapter 4 through the development of an optimal infinite-dimensional proportional plus integral LQ controller for the detailed dynamic model of a catalytic distillation process. Before dealing with the development of the proportional plus integral LQ controller, in the first part of the chapter, the controller obtained in Chapter 3 was applied to the column model to investigate the developed method further by studying a more challenging example. The performance of the designed infinite-dimensional LQ controller was compared with the performance of a finite-dimensional LQ controller, which was obtained by using a discretized model, through a numerical study. The simulation results showed that the infinite-dimensional controller outperforms the finite-dimensional controller, considerably.

The proportional plus integral LQ control design was then developed by considering an infinite-time horizon and quadratic objective function in which the rate of change of the control variable is penalized rather than the amount of control. This results in an augmented system with extended transport operator. It was proved that this extended transport operator is a generator of an exponentially stable C_0-semigroup, which shows that the resulting ORE for the extended system has a unique and non-negative solution. This solution was found by converting the ORE for the extended system into an equivalent set of coupled differential and algebraic matrix equations, which can be solved numerically to obtain the proportional plus integral LQ controller.

In the context of infinite-dimensional control system theory, the above results are very important as they address the LQ control problem for a wide range of transport-reaction processes. The main limitation of the methods lies in the state estimation problem. Although the exponential detectability properties of the systems under study were proved,

no results were obtained regarding observer design. Furthermore, the methods cannot address linear time-variant transport-reaction processes or those suffering from some diffusion phenomenon.

5.2 Future Work and Recommendations

This thesis was devoted to the LQ control development for combinations of hyperbolic PDEs, ODEs and algebraic equations that arise from mathematical modelling of distributed parameter systems in chemical processes. The thesis addressed some of the challenges in this subject. Further research in this area has a theoretical and practical significance.

The thesis developed LQ control for coupled hyperbolic PDEs-ODEs and also coupled hyperbolic PDEs-Algebraic equations. Some applications such as (reactive) distillation columns, in which the dynamics of the condenser-reflux drum system and reboiler are not negligible, are described by systems of coupled PDEs-ODEs-Algebraic equations. In order to address the LQ control problem for these systems, new method that combines the results from Chapter 2 and 3 should be developed. An effort has been made by the author in this regard (Moghadam *et al.*, 2012); however, this work requires more investigation in terms of the theoretical development.

In this thesis, it was assumed that the full state information for the systems considered is available. Development of an infinite-dimensional state observer for coupled PDE-ODE-Algebraic equation systems is important but challenging in the control theory of infinite-dimensional systems.

The thesis only dealt with the transport-reaction systems with time-invariant characteristics. Typically, chemical operations have time-varying properties, due to the phenomena such as catalyst deactivation and heat-exchanger fouling. Further study is required to extend the results to time-varying systems. An effort has been made by the author to tackle the LQ problem for time-varying PDE-ODE systems (Moghadam *et*

al., 2011); however, more study is required to improve the method developed for solving the resulting operator Riccati differential equation.

The developed control theory for infinite-dimensional systems in the literature cannot address many applications of transport-reaction processes in chemical and biochemical engineering. This is because of the fact that these processes involve particular complexities such as boundary actuation, multivariate nature, multiple phases and equilibrium condition. The objective of the present thesis was to address some of the challenges in this area; however, there are many other problems yet to be explored. For instance, the boundary control problem for transport-reaction processes described by systems of parabolic PDEs is required to be addressed. In (Mohammadi *et al.*, 2012) an effort has been made to develop an LQ control method for these systems; however, this work is limited to a particular class of reaction kinetics.

Another class of transport-reaction processes that can be studied, are two-phase systems described by coupled hyperbolic and parabolic PDEs. An example of such processes can be found in (Tavazzi *et al.*, 2006). These systems involve many interesting challenges regarding the infinite-dimensional control system theory and research in this area is very scarce.

Furthermore, a few transport-reaction processes, such as slurry bubble column reactor (Sehabiague *et al.*, 2008), involve three phases. The PDE models that describe such processes are truly complicated and their analysis and control synthesis require new theoretical and practical development.

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