University of Alberta

Optimal Control of Fixed-Bed Reactors with Catalyst Deactivation

by

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To my beloved parents $\cdots$

Bu tezi sevgili annem ve babama ithaf ediyorum $\cdots$

Abstract

Catalytic reactors have widespread applications in chemical and petrochemical industries. The most well known type of catalytic reactors are fixed-bed or packed-bed reactors where the reaction takes place on the surface of the catalyst.

One of the most important phenomena that takes place in a catalytic fixed-bed reactor is catalyst deactivation. Catalyst deactivation can have variety of consequences. It can have negative effects on the conversion and selectivity of the desired reaction. Consequently, it will affect the productivity and energy efficiency of the plant. It is therefore important to design efficient controllers that are able to track the optimal pre-defined trajectories of the operating conditions to ensure optimal operation of the plant.

Depending on the transport and reaction phenomena occuring in a fixed-bed reactor, it can be modelled by a set of partial differential equations (PDEs) or a mixed set of PDEs and ordinary differential equations (ODEs). Moreover, the governing transport phenomena (i.e. diffusion or convection) dictates the type of PDEs involved in the model of the reactor (i.e. parabolic or hyperbolic).

In this work, infinite dimensional optimal control of a fixed-bed reactor with catalyst deactivation is studied. Since dynamical properties of hyperbolic PDEs and parabolic PDEs are completely different, they are discussed as different topics. The thesis begins with optimal control of a class of fixed bed reactors with catalyst deactivation modelled by time-varying hyperbolic equations. Then the model predictive control of this class of distributed parameter systems under parameter

uncertainty is explored. The optimal control of reactors modelled by parabolic PDEs is first explored for the case of reactors without catalyst deactivation. Then the proposed controller is extended to a more general class of distributed parameter systems modelled by coupled parabolic PDE-ODE systems which can represent fixed-bed reactors with the rate of deactivation modelled by a set of ODEs.

Numerical simulations are performed for formulated optimal controllers and their performance is studied.

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Introduction

Catalytic reactors have widespread applications in chemical and petrochemical industries. They can be regarded as the heart of a chemical plant. The most well known type of catalytic reactors are fixed-bed or packed-bed reactors, where the reaction takes place on the surface of the catalyst.

In a chemical plant, commonly the reactors are followed by other unit operations such as separation processes. Thus, the operation of the downstream processes strongly depends on the quality of the products from the reactors. Hence, optimal operation of reactors in each plant is of key economical and operational importance.

One important phenomena that takes place in a catalytic fixed-bed reactor is catalyst deactivation. Chemical reactions occur on the active sites of the catalyst. These active sites may be lost for a variety of reasons like coking, poisoning or sintering. The loss of active sites results in decrease in the activity of the catalyst, as the activity is proportional to the number of available active sites.

Catalyst deactivation can have variety of consequences. It can have negative

effects on the conversion and selectivity of the desired reaction. Consequently, it will affect the productivity and energy efficiency of the plant. In order to compensate for the effect of catalyst deactivation, the operating conditions of the reactor are gradually changed to maintain the selectivity and conversion, which is equivalent to maintaining the overall quality and rate of production. This is commonly performed by calculation of optimal trajectories for operating conditions through an off-line dynamic optimization problem. These trajectories are used as the set-point variables for the controllers. It is therefore important to design efficient controllers that are able to track the pre-defined trajectories of the operating conditions.

Temperature is one of the key parameters affecting the reaction rate and selectivity. An important issue in control of a fixed-bed reactor is to ensure that the reactor temperature does not exceed the maximum allowable temperature for the catalyst. In addition to effects on selectivity and conversion, catalyst deactivation may cause thermal instability of the reactor. Dependence of catalyst activity on concentration and temperature results in non-uniform catalyst activity in fixed-bed reactors. If temperature disturbances occur upstream of the reactor, variation in catalyst activity can result in temperature excursions that are much larger than those in beds of uniform activity (Jaree *et al.*, 2001; Jaree *et al.*, 2008). The best approach for temperature control of the fixed-bed reactors is to control the temperature profile along the length of the reactor. This requires availability of multiple thermocouples along the length of the reactor and an efficient controller.

With growing development of advanced control technologies at the industrial scale, application of model based controllers has become possible. A high-fidelity model of the process is a key factor for successful implementation of model-based controllers. Therefore, in the last few decades extensive studies have been performed to develop controllers using accurate models of the processes.

Modelling and control of fixed-bed reactors have been the topic of many researches since early 70's. The earliest models of the fixed-bed reactors were developed by approximation of a fixed-bed reactor by a sequence of continuous flow stirred tank

reactors (CSTR). In this approach the reactor is modelled by a finite number of well-mixed reactors in series. As the number of the reactors increases, the accuracy of the model increases, but only an infinite number of interacting CSTRs would be able to provide an accurate model of a simple fixed-bed reactor.

More sophisticated models of a fixed-bed reactor can be obtained by solving mass and energy balance equations for the reactor. In order to capture all of the main "macroscopic" phenomena (i.e., reactions, diffusion, convection, and so forth), the model of a fixed-bed reactor takes the form of a set of partial differential equations. The rate of catalyst deactivation can be modelled by time-varying algebraic equations or in more complex cases by ordinary differential equations; hence, integration of catalyst deactivation dynamics into the model of the system results in a set of time-varying PDEs or a set of coupled PDE-ODE equations. Depending on the governing transport phenomena in a chemical process, i.e. diffusion or convection, the partial differential equations modelling the process may be a set of hyperbolic or parabolic equations.

In control theory, systems similar to a fixed-bed reactor are regarded as distributed parameter systems where the dependent variables are functions of time and space; as opposed to lumped parameter systems where the dependent variables are only functions of time (e.g., a well-mixed reactor). Other examples of distributed parameter systems in chemical engineering are fluidized bed reactors, heat exchangers and reactive distillation columns.

Traditionally, the majority of control methods have been developed for lumped parameter systems. Thus, the distributed parameter systems are commonly approximated with lumped parameter systems and controlled using algorithms for such lumped systems. Due to the widespread existence of DPS and economic benefits of precise control of these systems, developing controllers that use the most accurate model of these systems can have substantial performance benefit. Motivated by this, this thesis is focused on formulation of high performance controllers for distributed parameter systems with special emphasis on fixed-bed catalytic reactors. In the

following sections the available studies on the topic of distributed parameter systems and the outline of the thesis will be summarized.

1.1 Control of distributed parameter systems

As mentioned before, the most conventional approaches for control of DPS use lumping techniques to approximate the PDE model of the system by a set of coupled ODEs. Methods such as finite differences may be used for spatial discretization, resulting in approximations that consist of ordinary differential equations; however, such approximations may not be suitable for high performance control schemes, as the dimensionality of the produced sets of ODEs can be very high when trying to ensure high performance control. Also controllability and observability of the system will depend on the number and location of the discretization points (Christofides, 2001). Another approach for control of DPS is to develop the control algorithm based on the PDEs and discretize the resulting controller during the implementation. The advantage of this approach is that the controller synthesis is based on the original model of the system which represent all the dynamical properties of the system without any approximation. Over the recent years, research on the control of DPS is oriented towards development of algorithms that deal with infinite dimensional nature of these systems.

Mathematical theory of optimal control of distributed parameter systems began in late 1960s in the work of Lions (1971) and followed by other researchers (e.g., Banks and Kunisch (1984), Kappel and Salamon (1990) and Curtain and Zwart (1995)).

In a functional analysis framework, systems modelled by PDEs can be formulated in a state space form similar to that for lumped parameter systems by introducing a suitable infinite-dimensional space and operators instead of usual matrices in lumped parameter systems. The type of PDE system (e.g. hyperbolic, parabolic or elliptic) determines the approach followed for the solution of the control problem (Christofides, 2001). Based on the governing phenomenon in a chemical process, convection or diffusion, the model equations can be hyperbolic or parabolic.

For hyperbolic systems, Callier and J.Winkin (1990)-(1992) studied the LQ control problem using spectral factorization for the case of finite rank bounded observation and control operators. Aksikas (2005) extended this approach for the more general case of exponentially stable linear systems with bounded observation and control operators. In his work, this method was applied to a nonisothermal plug flow reactor to regulate the temperature and the reactant concentration in the reactor. The optimal control problem for a particular class of hyperbolic PDEs is solved via the well-known Riccati equation, which is developed in a series of papers by Aksikas and co-workers. (e.g., Aksikas and Forbes (2007), Aksikas *et al.* (2008*a*), Aksikas *et al.* (2008*b*), etc). The approach taken in this body of work does not address the case of time-varying and two time-scale hyperbolic systems, which can model many chemical engineering processes, including fixed-bed reactors with catalyst deactivation.

In the framework of model predictive control, Shang *et al.* (2004) studied characteristic-based model predictive control of hyperbolic systems. The proposed MPC is shown to have high computation efficiency without any approximation; however, input and output constraints are not addressed in this work.

The conventional approach for dealing with parabolic systems is modal decomposition (Ray, 1981). The main characteristic of parabolic systems is that their spectrum can be partitioned into a finite slow part and an infinite fast complement. This feature has been used by many researchers to perform model reduction and synthesize finite dimensional models representing the distributed parameter system with arbitrary accuracy (See Christofides (2001), Dubljevic *et al.* (2005) and references therein). The low dimensional model is used to formulate predictive controllers for the infinite dimensional system. Although the model reduction method is computationally efficient for diffusion dominant systems, it can result in a high dimensional system for convection dominant parabolic systems. Moreover, control of time-varying infinite dimensional systems as well as coupled systems have not been explored.

The control action in a DPS can be distributed over the spatial domain of the

system, or can be applied at the boundary. For example, in the case of a fixed-bed reactor, the manipulated variable can be inlet temperature (i.e., boundary control) or the temperature profile of the cooling jacket (i.e., distributed control). Boundary control systems are mathematically more challenging than systems with distributed control actions. Boundary control of DPS has been explored by few studies. Curtain and Zwart (1995) and Emirsjlow and Townley (2000) address the transformation of the boundary control problem into a well-posed abstract control problem. Recently, Byrnes *et al.* (2006) studied the boundary feedback control of parabolic systems using zero dynamics. The proposed algorithm is limited to parabolic systems with self-adjoint operator A, therefore cannot be used for chemical reactors that are modelled by multiple PDEs with non-symmetric coupling.

Although the topic of optimal control of infinite dimensional systems is explored by many researchers, the more complicated case of distributed parameter systems modelled by a set of coupled PDEs has not been as well studied. Dynamics of a fixed-bed reactor and most of other chemical processes are modelled by more than one equation (e.g., mass and energy balances) and these equations are coupled. Available infinite dimensional controllers are not able to address coupling in the modelling equations.

As mentioned before, integration of deactivation kinetics into the model of the reactor leads to a set of time-varying PDEs or a set of coupled PDEs-ODEs. The research in the area of coupled PDE-ODE systems is relatively scarce and will be addressed in this thesis.

Motivated by the fact that the precise control of fixed-bed catalytic reactors is of key importance in chemical industry, the focus of this thesis is infinite dimensional control of fixed-bed reactors. Each chapter addresses a class of distributed parameter systems that can represent an industrial fixed-bed reactor. Although the emphasis is on fixed-bed reactors, the developed controllers are capable of controlling any system that is modelled by the studied class of distributed parameter systems in each chapter.

1.2 Scope and outline

As mentioned before, catalytic reactors are the most important part of chemical plants and the optimal control of them has significant economic importance. Integration of catalyst deactivation in the modelling of the fixed-bed reactor introduces some complications to the system. The objective of this thesis is to study optimal control of fixed-bed reactors modelled by a set of partial differential equations. The main goal is to formulate optimal controllers that are able to mitigate or ameliorate the effect of catalyst deactivation on reactor performance using the distributed parameter model of the reactor with no or minimal approximation to directly formulate the controller. Since hyperbolic and parabolic systems have completely different dynamical behaviour and require different approaches to solve the control problem, the thesis is divided to two parts. Hyperbolic systems that model reactors with negligible diffusion are studied in chapters 2-3 and parabolic systems modelling diffusion-convection-reaction systems are discussed in chapters 4-5. The thesis begins with a simple case of a catalytic reactor with negligible diffusion and simple exponentially decaying deactivation kinetics and ends with a complicated case of diffusion-convection-reaction system where the catalyst deactivation is represented by a set of ODEs.

In Chapter 2, it is assumed that the effect of diffusion is negligible and the system can be modelled by a set of hyperbolic equations. It is further assumed that the effect of catalyst deactivation appears as time-varying reactive terms in the PDEs, resulting in a time-varying infinite dimensional system. This chapter is extension of the work of Aksikas *et al.* (2008*a*), which addresses a less complex case of plug flow reactors. Conditions on the stabilizability of these systems are studied and an infinite dimensional LQ controller is formulated to regulate the trajectory of the output variables around the steady state profile of the system and eliminate the effect of catalyst deactivation.

Motivated by the fact that the mathematical model of a system always has some uncertainty, as well as existence of input and output constraints in a plant, in Chapter

3 robust constrained model predictive control of uncertain coupled hyperbolic systems is studied. It is assumed that the uncertainty in the reactor model arises from unknown kinetic coefficients and uncertainty in the inlet flow measurements. In this work, the system has polytopic uncertainties and a robust MPC using method of characteristics is developed to ensure satisfaction of input and output constraints under parameter uncertainty.

Chapter 4 focuses on development of an LQ controller for coupled parabolic systems modelling a fixed-bed reactor, where both diffusion and convection phenomena are significant. An innovative approach is proposed to solve the eigenvalue problem for coupled parabolic systems with spatially varying coefficients resulting from linearization around the steady state profile of the system. Stabilizability of the system is studied using its spectral properties. Finally, an LQ controller is formulated and solved using the spectral properties of the system. This chapter is a significant step in the formulation of a more complicated case for catalytic reactors with catalyst deactivation modelled by a set of ODEs (i.e., infinite dimensional systems modelled by coupled PDE-ODE systems), which is developed in Chapter 5.

In Chapter 5, stabilizability and optimal controller formulation for systems modelled by coupled PDE-ODE systems with in-domain coupling are studied. Such systems represent fixed-bed reactors with significant diffusion and convection, where catalyst deactivation is represented by a set of ODEs. Using several exact transformations, the set of coupled PDE-ODE system is decoupled and represented as a Riesz Spectral system. Then, the LQ controller formulated in Chapter 4 is extended to this form of infinite dimensional systems.

Chapter 6 is the conclusion of the thesis and summarizes the contributions of this work and possibilities for future work.

2

LQ Control of Time-Varying Hyperbolic Systems

In this chapter the issue of the optimal control of a fixed-bed reactor with negligible diffusion and catalyst deactivation is studied. The system is modelled by a set of coupled time-varying hyperbolic partial differential equations and it is assumed that the catalyst deactivation is captured through time-varying reaction rates. An infinite dimensional LQ optimal controller is formulated by solving the corresponding operator Riccati equation[1].

[1]Portions of this chapter have been published in "Mohammadi, L., I. Aksikas and J. F. Forbes (2009), Optimal Control of a Catalytic Fixed-Bed Reactor with Catalyst Deactivation. Proceedings of the American Control Conference"; and submitted to "Mohammadi, L., I. Aksikas, S. Dubljevic, J. F. Forbes and Y. Belhamadia, Optimal Control of a Catalytic Fixed-Bed Reactor With Catalyst Deactivation. Journal of Process Control"

In a catalytic reactor, the catalyst may deactivate during the operation for a variety of reasons (e.g., poisoning by impurities in feed, formation of coke on catalyst surface, and so forth). Deactivation of the catalyst can significantly affect the performance of the reactor. Due to the economic importance of effective operation of catalytic reactors in chemical plants, formulation of high performance controllers that can maintain the process at optimal conditions is of crucial importance.

Incorporation of the catalyst deactivation in kinetic modelling of the reaction results in a time-varying reaction rate. A simplifying assumption in modelling of a catalytic reactor is existence of negligible diffusion. Therefore, a catalytic reactor with negligible diffusion and decaying catalyst can be modelled by a set of time-varying hyperbolic PDEs. Many other chemical processes can also be modelled by this class of infinite dimensional systems (e.g., a counter current heat exchanger with time-varying heat transfer coefficient).

The objective of this chapter is to formulate an infinite dimensional state-feedback LQ controller for systems that are described by a set of time-varying hyperbolic PDEs. This chapter establishes a baseline for the development of controllers for more complicated infinite dimensional systems with mixed diffusion and convection transport phenomena.

In the recent years, much work has been published on infinite dimensional control of hyperbolic systems. In the framework of functional analysis, Aksikas *et al.* (2009) studied the solution of LQ control problem for hyperbolic systems by solving an operator Riccati equation. Spectral factorization, which is based on frequency-domain description, is an alternative method for solving the LQ problem (Callier and J.Winkin (1990) and Callier and Winkin (1992)). These approaches address only optimal control of time-invariant hyperbolic systems.

Control of time-varying hyperbolic systems is studied by Aksikas *et al.* (2008*a*), but the approach is limited to plug flow reactors. Models of plug flow reactors consist of a set of hyperbolic equations with identical convective term. In these systems, mass and energy balances both have the same time scale. Generally, the model of a

catalytic reactor consists of multiple PDEs with distinct convective terms and as a result, the PDEs are multi-time scale set of equations.

The scope of this chapter is time-varying hyperbolic systems with specific focus on fixed-bed catalytic reactors. A case study of a fixed-bed hydrotreating reactor is chosen. The goal is to formulate an infinite dimensional LQ controller to regulate the temperature profile around the desired steady state trajectory and eliminate the effect of catalyst deactivation.

In this chapter, the approach proposed by Aksikas *et al.* (2008*a*) is extended to the general form of time-varying hyperbolic systems. Also, stability of these systems is studied using a Lyapunov approach. After formulation of the LQ controller, the effect of rate of catalyst deactivation on the closed loop performance of the controller has been investigated through numerical simulations.

The contributions of this chapter are:

- Stability analysis of a general form of linear time-varying hyperbolic systems;
- Solution of LQ optimal control problem for a general form of linear time-varying hyperbolic systems;
- Implementation of the formulated controller on a fixed-bed reactor.

2.1 Time-Varying Hyperbolic DPS: Background

In this section, we will provide some background information on the infinite dimensional representation of time-varying hyperbolic systems. These concepts will be used throughout this chapter to formulate the infinite dimensional controller and also analyze the stability of the time-varying infinite dimensional systems. As an example, we will begin with a simple homogeneous hyperbolic equation. It will be shown, how a system of PDEs can be formulated as an infinite dimensional system and the fundamental properties of time-varying infinite dimensional systems will be presented. Consider the initial value problem given by the following hyperbolic equation:

$$\begin{aligned} &\frac{\partial x}{\partial t} = -\frac{\partial x}{\partial z} + k(t)x \\ &x(s,z) = x_s(z) \\ &x(t,0) = 0 \end{aligned} \tag{2.1}$$

where x denotes the dependent variable, t is time and z denotes space. s is the initial time. The solution of PDE (2.1) is given by

$$x(t,z) = \begin{cases} x_s(z-t)\exp(\int_{z-t}^{z} k(\nu)d\nu) \\ 0 \end{cases} \tag{2.2}$$

By introducing $X = L^2(0,1)$ as the state space and $x(.,t) = \{x(z,t), 0 \leq z \leq 1\}$ as state variable, and the operator A

$$A(t)h = \frac{dh}{dz} \tag{2.3}$$

with the domain

$$D(A(t)) = \{h \in L^2(0,1) | h \text{ is absolutely continuous (a.c.), } \frac{dh}{dz} \in L^2(0,1) \text{ and } h(0) = 0\} \tag{2.4}$$

Equation (2.1) can be represented as an abstract infinite dimensional system

$$\begin{aligned} &\dot{x}(t) = A(t)x(t) \\ &x(s) = x_s \end{aligned} \tag{2.5}$$

The infinite dimensional representation of the solution (2.2) can be written as

$$x(t,z) = (U(t,s)x_s)(z) = \exp(\int_{z-t}^{z} k(\nu)d\nu)x_s(z-t) \tag{2.6}$$

$U(t,s)$ is the solution operator of the initial value problem (2.1) and is a two parameter family of operators. If the operator $A(t)$ is independent of t, then the two parameter family of operators $U(t,s)$ reduces to a one parameter family $U(t)$, which is the semigroup generated by A.

Evolution system theory is the generalization of the concept of the semigroup for autonomous operators to the non-autonomous operators, where operator A is a function of t. For the rest of this section fundamental concepts related to evolution systems will be introduced.

Definition 2.1.1. (Pazy, 1983, Definition 5.3, p. 129) A two parameter family of bounded linear operators $U(t,s), 0 \leq s \leq t \leq T$, on X is called an evolution system if the following two conditions are satisfied:

i) $U(s,s) = I$, $U(t,r)U(r,s) = U(t,s) \quad \text{for}\, 0 \leq s \leq r \leq t \leq T$

ii) $(t,s) \to U(t,s)$ is strongly continous for $0 \leq s \leq t \leq T$

Definition 2.1.2. (Schnaubelt and Weiss, 2010, Definition 2.2) Let $\{A(t) : D(A(t)) \to X | t \in [0,\infty\}$ be a family of densely defined linear operators on X. We say that $A(.)$ generates the evolution family U if $U(t,s)D(A(t)) \subset D(A(t))$ for all $t, s \in [0,\infty]$ and for every $s \in [0,\infty]$ and every $x_0 \in D(A(t))$ the function $x(.) = T(.,s)x_0$ is continuously differentiable and is the unique solution of the Cauchy problem

$$\dot{x}(t) = A(t)x(t), x(s) = x_0, s \leq t < \infty \tag{2.7}$$

Definition 2.1.3. (Pazy, 1983, Definition 2.1, p. 130) A family of infinitesimal generators of C_0-semigroups on a Banach space X is called stable if there are constants $M \geq 1$ and ω such that

$$\rho(A(t)) \supset (\omega, \infty) \quad \text{for} \quad t \in [0,T] \tag{2.8}$$

and

$$\left\| \prod_{j=1}^{k} R(\lambda : A(t_j)) \right\| \leq M(\lambda - \omega)^{-k} \quad \text{for} \quad \lambda > \omega \tag{2.9}$$

for every finite sequence $0 \leq t_1 \leq t_2, \cdots, t_k \leq T$. In the equations above, $\rho(A(t))$ is the resolvent set of operator $A(t)$ and $R(\lambda : A(t_j))$ is the resolvent operator defined by

$$R(\lambda : A(t_j))x = \int_0^\infty e^{-\lambda_j s} S_{t_j}(s)x ds \quad \text{for} \quad \lambda_j > \omega \tag{2.10}$$

and $\rho(A(t))$ is the resolvent set of the operator $A(t)$.

Theorem 2.1.1. *(Pazy, 1983, Theorem 2.3, p. 132) Let $\{A(t)\}_{t\in[0,T]}$ be a stable family of infinitesimal generators with stability constants M and ω. Let $B(t), 0 <$*

$t < T$ be bounded linear operators on X. If $\|B(t)\| \leq K$ for all $0 \leq T$, then $\{A(t)+B(t)\}_{t\in[0,T]}$ is a stable family of infinitesimal generators with stability constants $\omega + KM$.

Theorem 2.1.2. *(Pazy, 1983, Theorem 4.8, p. 145) Let $\{A(t)\}_{t\in[0,T]}$ be a stable family of infinitesimal generators of C_0-semigroups on X. If $D(A(t)) = D$ is independent of t and for $v \in D$, $A(t)v$ is continuously differentiable in X then there exsits a unique evolution system $U(t,s), 0 \leq s \leq t \leq T$, satisfying the following conditions*

i) $\|U(t,s)\| \leq Me^{\omega(t-s)} \quad for \quad 0 \leq s \leq t \leq T$

ii) $\frac{\partial}{\partial t}U(t,s)v|_{t=s} = A(s)v \; for \quad v \in D, 0 \leq s \leq T$

iii) $U(t,s)D \subset D \quad for \quad 0 \leq s \leq t \leq T$

2.2 Problem Statement: Time-Varying Hyperbolic PDEs

The problem of interest in this chapter is a system that can be modelled by a set of coupled first-order time-varying hyperbolic PDEs in one dimensional spatial domain. Such systems can model a fixed-bed reactor with catalyst deactivation and negligible diffusion. Since the objective of this chapter is to formulate an LQ controller for such systems, it is assumed that the PDEs are linearized around the steady state profile of the system. The mathematical description of this kind of system can be given by the following equations

$$\begin{aligned} \frac{\partial x}{\partial t}(z,t) &= V\frac{\partial x}{\partial z}(z,t) + M(z,t)x(z,t) + N(z,t)u(z,t) \\ y(z,t) &= S(z,t)x(z,t) \end{aligned} \tag{2.11}$$

with boundary and initial conditions

$$\begin{aligned} x(0,t) &= x_B \quad \forall t \geq 0 \\ x(z,0) &= x_0(z) \quad \forall z \in [0,1] \end{aligned} \tag{2.12}$$

where $x(.,t) = [x_1(.,t), \cdots, x_n(.,t)]^T \in H := L^2(0,1)^n$ denotes the vector of state variables, $z \in [0,1] \in \mathbb{R}$ and $t \in [0,\infty)$ denote spatial position and time, respectively. $u(.,t) = [u_1(.,t), \cdots, u_m(.,t)] \in U := L^2(0,1)^m$ denotes the input variable; $y(.,t) = [y_1(.,t), \cdots, y_p(.,t)] \in Y := L^2(0,1)^p$ denotes the output variable. M, N and C are matrices of appropriate sizes, whose entries are functions in $L^\infty([0,1] \times [0,\infty))$. V is a constant diagonalizable non-positive matrix. x_B is a constant column vector and $x_0(z) \in H$. Since equation (2.11) is normally the result of linearization of a set of nonlinear hyperbolic PDEs, the variables are in deviation form. Therefore, without loss of generality, it is assumed that $x_B = 0$.

The infinite dimensional description of the model (2.11)-(2.12) in the Hilbert space H is:

$$\begin{aligned} \dot{x}(t) &= A(t)x(t) + B(t)u(t) \\ x(0) &= x_0 \in H \\ y(t) &= C(t)x(t) \end{aligned} \tag{2.13}$$

where $A(t)$ is the family of linear operators defined on the domain

$$D(A(t)) = \{x \in H : x \text{ is a.c.}, \frac{dx}{dz} \in H \text{ and } x(0) = 0\} \tag{2.14}$$

by

$$A(t) = V\frac{d.}{dz} + M(z,t).I \tag{2.15}$$

and the input and output operators B and C are given by

$$B(t) = N(z,t).I \qquad \text{and} \qquad C(t) = S(z,t).I \tag{2.16}$$

where I is the identity operator.

The objective is to formulate an infinite dimensional controller for the time-varying infinite dimensional system of the form (2.13). This will be discussed in the next section. Note that, here, the only assumption made for the form of matrix V is that it is diagonalizable. This assumption is true if eigenvalues of matrix V are simple. In most chemical processes, the matrix V is diagonal. The reason for diagonality of V is that the convective transport of the state variables are independent of each

other. Hence, without loss of generality it will be assumed that matrix V is a diagonal matrix.

2.3 Optimal Control Design

This section deals with the computation of an LQ-optimal feedback operator for the system (2.13) by using the corresponding operator Riccati equation. The objective of LQ-optimal control problem is to find a square integrable control $u_o \in L^2[[0,\infty); L^2(0,l)]$ which minimizes the cost functional

$$J(x_0,u) = \int_0^\infty (\langle Cx(t), PCx(t)\rangle + \langle u(t), Ru(t)\rangle)dt \tag{2.17}$$

for any initial state $x_0 \in H$. In the cost function above, $P = P_0.I \in \mathcal{L}(Y)$ is a positive operator and $R = R_0.I \in \mathcal{L}(U)$ is a self-adjoint, coercive operator in $\mathcal{L}(U)$, where P_0 and R_0 are two positive functions.

The LQ control problem is a classical optimal control problem and its solution can be obtained by finding the positive self-adjoint operator $Q \in \mathcal{L}(H)$ that solves the operator Riccati differential equation (ORE), viz.

$$[\dot{Q} + A^*Q + QA + C^*PC - QBR^{-1}B^*Q]x = 0 \tag{2.18}$$

for all $x \in D(A)$, where $Q(D(A)) \subset D(A^*)$.

Lemma 2.3.1. *(Bensoussan* et al.*, 2007, Theorem 5.2, p.507) Consider the infinite dimensional system* (2.13)*, with control and observation operators given by* (2.16)*. Assume that* $\{A(t), B\}$ *is exponentially stabilizable. Then the corresponding operator Riccati equation* (2.18) *has a nonnegative bounded solution* Q *and for any initial state* $x_0 \in H$*, the quadratic cost* (2.17) *is minimized by the unique control* u_o *given on* $t \geq 0$ *by*

$$u_o(t) = -R_0^{-1}B^*Qx(t).$$

Now we are in a position to state the main theorem of this section, which gives an expression of the optimal state feedback in terms of the solution of a matrix Riccati partial differential equation:

Theorem 2.3.1. *Consider the linear model* (2.13). *Assume that* P_0 *is a positive matrix and* R_0 *is a self-adjoint coercive matrix such that* $\Phi := diag(\phi_1, \phi_2, \cdots, \phi_n)$ *is the solution of the matrix Riccati partial differential equation:*

$$\begin{aligned} &\frac{\partial \Phi}{\partial t} = V\frac{\partial \Phi}{\partial z} - M^*\Phi - \Phi M - C_0^* P_0 C_0 + \Phi B_0 R_0^{-1} B_0^* \Phi, \\ &\Phi(t,l) = 0, \quad t \in [0,\infty] \end{aligned} \tag{2.19}$$

Then $Q_0 := \Phi(t,z)I$ *is the unique self-adjoint nonnegative solution of the operator Riccati differential equation.*

Proof. Substituting $Q_0 := \Phi(t,z)I$ in the ORE (2.18) leads to:

$$[\dot{\Phi} + A^*\Phi + \Phi A + C^*PC - \Phi B R^{-1} B^* \Phi]x = 0 \tag{2.20}$$

where $Ah = V\frac{dh}{dz} + Mh$ and A^* is the adjoint operator of A and is defined by $A^*h = -V\frac{dh}{dz} + M^*h$. Substituting A and A^* in the above equation results in:

$$\frac{\partial \Phi}{\partial t}x = V\frac{\partial \Phi x}{\partial z} - M^*\Phi x - \Phi V\frac{\partial x}{\partial z} - M\Phi - C^*PCx + \Phi B R^{-1} B\Phi x \tag{2.21}$$

Since

$$\frac{\partial \Phi x}{\partial z} = \Phi\frac{\partial x}{\partial z} + \frac{\partial \Phi}{\partial z}x \tag{2.22}$$

equation (2.21) becomes

$$\frac{\partial \Phi}{\partial t}x = V\Phi\frac{\partial x}{\partial z} + V\frac{\partial \Phi}{\partial z}x - M^*\Phi x - \Phi V\frac{\partial x}{\partial z} - M\Phi - C^*PCx + \Phi B R^{-1} B\Phi x \tag{2.23}$$

Since V and Φ are both diagonal, $V\Phi = \Phi V$ and the above equation can be simplified to:

$$\frac{\partial \Phi}{\partial t}x = V\frac{\partial \Phi}{\partial z}x - M^*\Phi x - M\Phi - C^*PCx + \Phi B R^{-1} B\Phi x \tag{2.24}$$

On the other hand, Q_o should satisfy $Q_o(D(A)) \subset D(A^*)$. This condition is only valid if $\phi(t,l) = 0$ as this implies that $\phi(t,l)x(l) = 0, \quad \forall x \in D(A)$ and consequently $Q_o(D(A)) \subset D(A^*)$. ∎

The condition for the existence and uniqueness of the solution for the Operator Riccati equation, is exponential stabilizability of infinite dimensional system (2.13). Exponential stabilizability of this system depends on parameters of the system and should be studied for each case. In the following sections, a case study will be considered and its exponential stability will be proven. Finally, the associated matrix Riccati equation will be solved to find the solution for the optimal control problem.

2.4 Case study: A Fixed-Bed Hydrotreater

The process considered in this chapter is a fixed-bed hydrotreating reactor with catalyst deactivation. The dynamics of the reactor can be described by partial differential equations derived from mass and energy balances. To model the reactor, a plug-flow pseudo-homogeneous model is considered. Moreover, we consider a one-spatial dimension model where there are no gradients in the radial direction. The schematic diagram of the process is shown in Figure 2.1

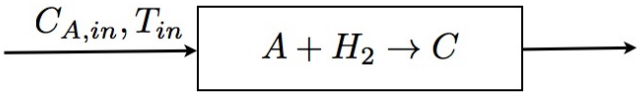


Figure 2.1: Schematic diagram of the hydrotreating reactor

In the simplified system considered here, a lumped reaction kinetics equation was assumed which has the following form (see (Chen *et al.*, 2001)):

$$\begin{aligned} &A + H_2 \rightarrow C \\ &r_A = k(t)e^{\left(-\frac{E}{RT}\right)}C_A^{n_1}C_H^{n_2} \end{aligned} \tag{2.25}$$

In the above equation, A represents Naphtha and C represents the products of the hydrotreating reaction.

Remark 2.4.1. The more accurate kinetic model of the reaction is represented by Langmuir-Hinshelwood-Hougen-Watson (LHHW) rate equations. Under the

assumption that all adsorption steps are weak, the LHHW rate equation will be simplified to a power law rate equation.

Given the modeling assumptions, the dynamics of the process are described by the following energy and mass balance partial differential equations (PDE's).

$$\begin{aligned} \epsilon\frac{\partial C_A}{\partial t} &= -\nu\frac{\partial C_A}{\partial z} - \rho_B k(t) e^{-\frac{E}{RT}} C_A^{n_1} C_H^{n_2} \\ \frac{\partial T}{\partial t} &= -\nu\frac{\partial T}{\partial z} + \frac{\rho_B \Delta H_r}{\rho C_p} k(t) e^{-\frac{E}{RT}} C_A^{n_1} C_H^{n_2} \end{aligned} \tag{2.26}$$

with the boundary conditions given, for $t \geq 0$, by:

$$\begin{aligned} C_A(0,t) &= C_{A,in}, \\ T(0,t) &= T_{in}, \end{aligned} \tag{2.27}$$

The initial conditions are assumed to be given , for $0 \leq z \leq l$, by

$$\begin{aligned} C_A(z,0) &= C_{A0}(z), \\ T(z,0) &= T_0(z) \end{aligned} \tag{2.28}$$

In the equations above, $C_A, T, \epsilon, \rho_B, \rho, C_p, E, C_H, \Delta H_r, \nu$ denote the reactant concentration, the temperature, the porosity of the reactor packing, the catalyst density, the fluid density, the activation energy, the concentration of hydrogen, the enthalpy of reaction, and the superficial velocity respectively. In addition, t, z and l denote the time and space and the length of the reactor, respectively. T_0 and C_{A0} denote the initial temperature and reactant concentration profiles, respectively, such that $T_0(0) = T_{in}$ and $C_{A0}(0) = C_{A,in}$. k is the pre-exponential factor. As a result of catalyst deactivation, this coefficient varies with time. Generally k is a function of time and operating conditions, but here we assume that the operating conditions are maintained in narrow ranges. Therefore, k is only a function of time and is assumed to be given by:

$$k = k_0 + k_1 e^{-\alpha t} \tag{2.29}$$

The above expression for kinetics of naphtha hydrotreating reaction is in agreement with the observations that after a rapid initial deactivation of the hydrotreating catalyst there is a slow deactivation phase and finally a stabilization of the catalyst activity phase (Kallinikos *et al.*, 2008).

Since temperature and concentration of the reactor can have different orders of magnitude, first we will transform the nonlinear equations to a dimensionless form. Then the nonlinear equations will be linearized around the steady state profile of the system and will be represented as an infinite dimensional system. Finally the exponential stabilizability of the system will be proven and the optimal control problem will be solved.

Dimensionless model

Let us consider the following state transformation:

$$\theta_1 = \frac{T - T_{in}}{T_{in}}, \quad \theta_2 = \frac{C_{A,in} - C_A}{C_{A,in}} \tag{2.30}$$

Then we obtain the following equivalent representation of the model (2.26).

$$\frac{\partial \theta_1}{\partial t} = -\nu \frac{\partial \theta_1}{\partial z} + \left(h_0 + h_1 e^{-\alpha t}\right)(1-\theta_2)^{n_1} e^{\frac{\mu \theta_1}{1+\theta_1}} \tag{2.31}$$

$$\frac{\partial \theta_2}{\partial t} = -\frac{\nu}{\epsilon} \frac{\partial \theta_2}{\partial z} + \left(l_0 + l_1 e^{-\alpha t}\right)(1-\theta_2)^{n_1} e^{\frac{\mu \theta_1}{1+\theta_1}} \tag{2.32}$$

with the boundary conditions:

$$\theta_1(0,t) = 0, \quad \theta_2(0,t) = 0 \tag{2.33}$$

where:

$$\mu = \frac{E}{RT_{in}}, \quad l_{0,1} = \frac{\rho_B}{\epsilon} k_{0,1} C_H^{n_2} C_{A_{in}}^{n_1} e^{-\mu}, \tag{2.34}$$

$$h_{0,1} = \frac{\rho_B(-\Delta H)}{\rho C_p T_{in}} k_{0,1} C_H^{n_2} C_{A_{in}}^{n_1} e^{-\mu} \tag{2.35}$$

Infinite-dimensional linearized model

Let us denote by θ_{ss} and u_{ss} the dimensionless steady state profile of the model (2.31)-(2.32) at the operating point. By defining the following state variables:

$$x(t) = \theta(t) - \theta_{ss} \tag{2.36}$$

and new input $u(t) = \nu(t) - \nu_{ss}$, the linearization of the system (2.31)-(2.32) around its operating profile leads to a linear time-varying infinite-dimensional system (2.13) on the Hilbert space $H := L^2(0,l) \times L^2(0,l)$. Operators $A(t), B$ and C are defined in the following.

Operator A is given by

$$A(t) = V.\frac{d.}{dz} + M(t,z).I \tag{2.37}$$

where V and M are defined by:

$$V := \begin{bmatrix} v_1 & 0 \\ 0 & v_2 \end{bmatrix} \tag{2.38}$$

where

$$v_1 = -\nu_{ss}, \quad v_2 = -\frac{\nu_{ss}}{\epsilon} \tag{2.39}$$

$$M(t,z) := \begin{bmatrix} m_{11}(t,z) & m_{12}(t,z) \\ m_{21}(t,z) & m_{22}(t,z) \end{bmatrix} \tag{2.40}$$

where the functions m_{ij} are given by:

$$\begin{aligned} m_{11} &= \mu(h_0 + h_1 e^{-\alpha t})\frac{(1-\theta_{2ss})^{n_1}}{(1+\theta_{1ss})^2} e^{\frac{\mu\theta_{1ss}}{1+\theta_{1ss}}}, \\ m_{12} &= -n_1(h_0 + h_1 e^{-\alpha t})(1-\theta_{2ss})^{n_1-1} e^{\frac{\mu\theta_{1ss}}{1+\theta_{1ss}}}, \\ m_{21} &= \mu(l_0 + l_1 e^{-\alpha t})\frac{(1-\theta_{2ss})^{n_1}}{(1+\theta_{1ss})^2} e^{\frac{\mu\theta_{1ss}}{1+\theta_{1ss}}}, \\ m_{22} &= -n_1(l_0 + l_1 e^{-\alpha t})(1-\theta_{2ss})^{n_1-1} e^{\frac{\mu\theta_{1ss}}{1+\theta_{1ss}}}. \end{aligned}$$

The input operator $B = B_0.I \in \mathcal{L}(L^2(0,l), H)$ is the linear bounded operator where:

$$\begin{aligned} B_0 &= \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \\ B_1 &= \frac{\partial\theta_{1,ss}}{\partial z}, \quad B_2 = \frac{1}{\epsilon}\frac{\partial\theta_{2,ss}}{\partial z} \end{aligned} \tag{2.41}$$

and it is assumed that the full state measurement is available along the length of the reactor, therefore, $C = I$.

2.4.1 Trajectory and stability analysis

This section is devoted to the trajectory and the exponential stability of the linearized fixed-bed reactor model described in the previous section. The following theorem shows the existence and uniqueness of an evolution system generated by the family of operators $\{A(t)\}_{0\leq t\leq T}$, for any $T > 0$.

Theorem 2.4.1. *Let $T > 0$. Consider the family of operators $\{A(t)\}_{0\leq t\leq T}$ given by (2.37) . Then, there exists a unique evolution system $U_A(\cdot,\cdot) : \{(t,s) \in R^2 : s \leq t \leq T\}$ such that*

$$\frac{\partial}{\partial t}U_A(t,s)x = A(t)U_A(t,s)x,$$
$$\forall x \in D(A(t)),\ 0 \leq s \leq t \leq T.$$

Moreover, there are constants $M \geq 1$ and ω such that

$$\|U_A(t,s)\| \leq Me^{\omega(t-s)},\ 0 \leq s \leq t \leq T.$$

Proof. The operator $A(t)$ can be written as

$$A(t) = A_0 + M(t) = \begin{bmatrix} -v_1\frac{d.}{dz} & 0 \\ 0 & -v_2\frac{d.}{dz} \end{bmatrix} + \begin{bmatrix} m_1(t,z)I & m_2(t,z)I \\ m_3(t,z)I & m_4(t,z)I \end{bmatrix} \tag{2.42}$$

In order to prove this theorem, it suffices to validate assumptions of Theorem 2.1.2. The operator A_0 is independent of t. Since $V < 0$, the operator A_0 is infinitesimal generator of an exponentially stable C_0-semigroup. $M(t)$, $t \geq 0$ is bounded linear operator, then, by using Theorem 2.1.1, $A(t)$ is a stable family of infinitesimal generators. On the other hand the domain of $A(t)$ is independent of time and for any $x \in D_0$, $A(t)x$ is differentiable. Therefore, all of the Theorem 2.1.2 assumptions are satisfied. ∎

Now we are in a position to state a theorem on the exponential stability of the linearized model.

Theorem 2.4.2. *Consider the family of operators* $\{A(t)\}_{t\geq 0}$ *as in Theorem 2.4.1. Then* $\{A(t)\}_{t\geq 0}$ *generates an exponentially stable evolution system.*

Proof. The sufficient condition for exponential stability is existence of a positive operator P that satisfies the following operator Lyapunov differential equation (Pandolfi, 1992).

$$\dot{P} + PA(t) + A(t)^*P + Q = 0 \quad \text{with} \quad P(D(A(t))) \subset D(A(t)^*) \tag{2.43}$$

where,

$$Q = Q_0 I = \begin{bmatrix} Q_1 & Q_2 \\ Q_2 & Q_3 \end{bmatrix} \tag{2.44}$$

and $Q_i, i = 1, \cdots, 3$ are arbitrary functions such that the matrix Q_0 is positive semi-definite matrix. If we assume that the solution is of the form:

$$P(t) = \begin{bmatrix} \mathcal{P}_1 I & 0 \\ 0 & \mathcal{P}_2 I \end{bmatrix} \tag{2.45}$$

where I is the identity operator and $\mathcal{P}_i$ is a real valued function, it can be shown that the following identities hold:

$$PA = \mathcal{P}A_0 + \mathcal{P}M(t)I \quad \text{and} \quad A^*P = A_0^*\mathcal{P}I + M(t)^*\mathcal{P}I \tag{2.46}$$

On the other hand it can be shown that

$$\mathcal{P}A_0 + A_0^*\mathcal{P}I = V\frac{d\mathcal{P}}{dz}I \tag{2.47}$$

Substituting Equations (2.46)-(2.47) into Equation (2.43) results in the following matrix Lyapunov partial differential equation

$$\frac{d\mathcal{P}}{dt} = -V\frac{d\mathcal{P}}{dz} - \mathcal{P}M(t) - M(t)^*\mathcal{P} - Q_0, \quad \mathcal{P}(t,1) = 0, \quad t \in [0,\infty) \tag{2.48}$$

If one can prove that the solution for matrix Lyapunov PDE (2.48) of the form $\mathcal{P}(t,z) = \begin{bmatrix} \mathcal{P}_1 & 0 \\ 0 & \mathcal{P}_2 \end{bmatrix}$ exists, the operator $P = \mathcal{P}I$ will be the solution for the operator

Lyapunov differential Equation (2.43). Positiveness on $\mathcal{P}$ implies that the operator P is positive as well.

In order to prove existence of a solution for Equation (2.48), the method of characteristics is used. In this case, there are two characteristic equations as follows

$$\frac{dt}{dr} = 1, \quad t(0) = t_0 \tag{2.49}$$

$$\frac{dz}{dr} = v_1 \quad z(0) = 0 \tag{2.50}$$

$$\frac{dz}{dr} = v_2 \quad z(0) = 0 \tag{2.51}$$

Along the characteristic equations, the following equation is equivalent to the matrix Lyapunov PDE (2.48)

$$\frac{d\mathcal{P}}{dr} = -M^*(r - t_0)\mathcal{P} - \mathcal{P}M(r - t_0) - Q_0, \quad \mathcal{P}(1) = 0 \tag{2.52}$$

By performing a change of variable: $\hat{r} = 1 - r$, the Equation (2.52) can be converted to the following Matrix Lyapunov equation:

$$\frac{d\mathcal{P}}{d\hat{r}} = M^*(\hat{r} + t_0)\mathcal{P} + \mathcal{P}M(\hat{r} + t_0) + Q_0, \quad \mathcal{P}(0) = 0 \tag{2.53}$$

Equation 2.53 can be expanded to

$$\frac{d\mathcal{P}_1}{d\hat{r}} = P_1 m_1(\hat{r} + t_0) + m_1(\hat{r} + t_0)P_1 + Q_1 \tag{2.54a}$$

$$\frac{d\mathcal{P}_2}{d\hat{r}} = P_2 m_4(\hat{r} + t_0) + m_4(\hat{r} + t_0)P_4 + Q_3 \tag{2.54b}$$

$$\mathcal{P}_1 m_2(\hat{r} + t_0) + m_3(\hat{r} + t_0)\mathcal{P}_2 + Q_2 = 0 \tag{2.54c}$$

Assuming that $Q_1, Q_3 > 0$, Equations (2.54a) and (2.54b) have positive solutions given by:

$$\mathcal{P}_1(\hat{r}) = \int_0^{\hat{r}} e^{\int_0^s m_1(\tau + t_0)d\tau} Q_1 e^{\int_0^s m_1(\tau + t_0)d\tau} ds \tag{2.55}$$

$$\mathcal{P}_2(\hat{r}) = \int_0^{\hat{r}} e^{\int_0^s m_4(\tau + t_0)d\tau} Q_3 e^{\int_0^s m_4(\tau + t_0)d\tau} ds \tag{2.56}$$

Since Q_0 is an arbitrary matrix, one can assume that it has the following form:

$$Q_0 = \begin{bmatrix} Q_1 & -(\mathcal{P}_1 m_2(\hat{r}+t_0) + m_3(\hat{r}+t_0)\mathcal{P}_2) \\ -(\mathcal{P}_1 m_2(\hat{r}+t_0) + m_3(\hat{r}+t_0)\mathcal{P}_2) & Q_3 \end{bmatrix} \tag{2.57}$$

If we can prove that the resulting matrix Q_0 is non-negative, then it can be concluded that the family of operators $\{A(t)\}_{t\geq 0}$ generates an exponential stable evolution system. For positiveness of Q_0, the following condition should hold:

$$\forall x \in D(A(t)), \langle x, Q_0 x\rangle > 0 \tag{2.58}$$

or

$$\langle \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \begin{bmatrix} Q_1 x_1 + Q_2 x_2 \\ Q_2 x_1 + Q_3 x_2 \end{bmatrix} \rangle > 0 \tag{2.59}$$

which results in

$$\langle x_1, Q_1 x_1\rangle + \langle x_1, Q_2 x_2\rangle + \langle x_2, Q_2 x_1\rangle + \langle x_2, Q_3 x_2\rangle > 0 \tag{2.60}$$

Since Q_1 and Q_3 are assumed to be positive, $\langle x_1, Q_1 x_1\rangle$ and $\langle x_2, Q_3 x_2\rangle$ are both positive. If one chooses Q_1 and Q_2 such that $Q_1 >> Q_2$ and $Q_3 >> Q_2$, the condition for positiveness of Q_0 holds. This proves that positive operators Q and P satisfying the dynamic Lyapunov equation (2.43) exist and therefore $\{A(t)\}_{t\geq 0}$ generates an exponentially stable evolution system. ■

Optimal Control Formulation

In this section the solution of the LQ controller of §2.3 is discussed for the hydrotreating reactor with infinite dimensional model given by (2.13) and operators A and B defined by equations (2.37) and (2.41). It is assumed that full state measurement is available and $C = I$.

The solution of the LQ controller can be computed by solving the equivalent matrix Riccati partial differential equation given by equation (2.19). Considering that M, V, B are given by (2.40), (2.38), (2.41), respectively, then the matrix Riccati equation (2.19) can be written as a set of partial differential and algebraic equations

given as follows (see Aksikas *et al.* (2009, Comment 3.1) and Aksikas and Forbes (2007, Comment 3.1)):

$$\begin{aligned}
&\frac{\partial \phi_1}{\partial t} = -\nu_1 \frac{d\phi_1}{dz} + 2m_{11}\phi_1 + \bar{c}_{11} - \bar{b}_{11}\phi_1^2,\\
&\frac{\partial \phi_2}{\partial t} = -\nu_2 \frac{d\phi_2}{dz} + 2m_{22}\phi_2 + \bar{c}_{22} - \bar{b}_{22}\phi_2^2,\\
&0 = m_{21}\phi_2 + \phi_1 m_{12} + \bar{c}_{12} - \phi_1 \bar{b}_{12}\phi_2,\\
&\phi_1(t,l) = 0,\\
&\phi_2(t,l) = 0
\end{aligned} \tag{2.61}$$

where the functions $m_{ij}, \bar{c}_{ij}$ and $\bar{b}_{ij}$ are the entries of the matrices $M, C_0^* P_0 C_0$ and $B_0 R_0^{-1} B_0^*$, respectively.

In the equations (2.61), there exist two unknown functions ϕ_1, ϕ_2. Note that there are three equations. In general, when there exists n state variables, the number of unknown functions is n, while the number of equations is $n(n+1)/2$. Thus the set of equations (2.61) cannot be solved to find a unique solution; however, if we assume that some entries of weighting matrices P_0 and R_0 are unknown, the number of unknown variables can be made to be equal to the number of equations and the set of equations solved to find a unique solution for the matrix Riccati eqution. In general, to complete the number of unknown variables, $n(n-1)/2$ entries of P_0 or R_0 should be assumed to be unknown. After solving the set of equations, one should validate the positive definiteness of the weighting function.

2.5 Numerical Simulations

In this section, the performance of the proposed approach is demonstrated. Values of the model parameters are given in Table 2.1.

The LQ-controller discussed in the previous section was studied via a simulation that used a nonlinear model of the reactor given in Equations (2.26)-(2.28). The performance of the proposed controller was compared to an infinite dimensional LQ controller designed by assuming constant catalyst activity. This LQ controller was

computed using the method proposed in (Aksikas *et al.*, 2009). The solution of LQ controller based on the time-invariant model of the reactor can be computed by solving a set of ODEs instead of PDEs given by (2.61). Therefore, it needs less computation effort than the LQ controller proposed in this work.

The control objective is to regulate the temperature trajectory at the desired steady state profile. Using the nominal operating conditions and the model given in Equations (2.26)-(2.28), the steady-state profiles of temperature and concentration were computed. Then, the nonlinear model was linearized around the stationary states and transformed to the infinite dimensional form of Equation (2.13). The feedback functions ϕ_1 and ϕ_2 are computed by solving a set of equations given by (2.61). To compute the feedback functions for the second case, it is assumed that the reaction coefficient is equal to $k_0 + k_1$ during the operation time. Both controllers are applied to the original nonlinear model of the system given by Equations (2.26)-(2.28). Simulations are performed using COMSOL ®. For handling possible numerical instability resulting from discontinuity in the boundary/initial conditions of the hyperbolic equations, the artificial diffusion option of the solver is enabled. In order to investigate the effect of deactivation rate, two different values of α are considered. In the first case, $\alpha = 1 \times 10^{-2}$ the deactivation time has the same order of magnitude as the residence time of the system, but in the second case, $\alpha = 1 \times 10^{-4}$, the deactivation time is much longer than the residence time of the reactor. The feedback functions ϕ_1 and ϕ_2 of two controllers for $\alpha = 1 \times 10^{-2}$ are shown in Figures 2.2-2.3. For $\alpha = 1 \times 10^{-4}$, the feedback functions of time-varying controller have the similar trend but different values; however, the feedback functions of time-invariant controller are not functions of α, as the deactivation is ignored for developing this controller.

To assess the performance of two controllers, it is assumed that the system is initially at steady state and we are interested in maintaining the temperature profile at that steady state and eliminate the effect of catalyst deactivation. The integral average of the temperature error is calculated for each case and is shown in Figure 2.4. From Figure 2.4, one can observe that for $\alpha = 1 \times 10^{-2}$, the performance of the time-

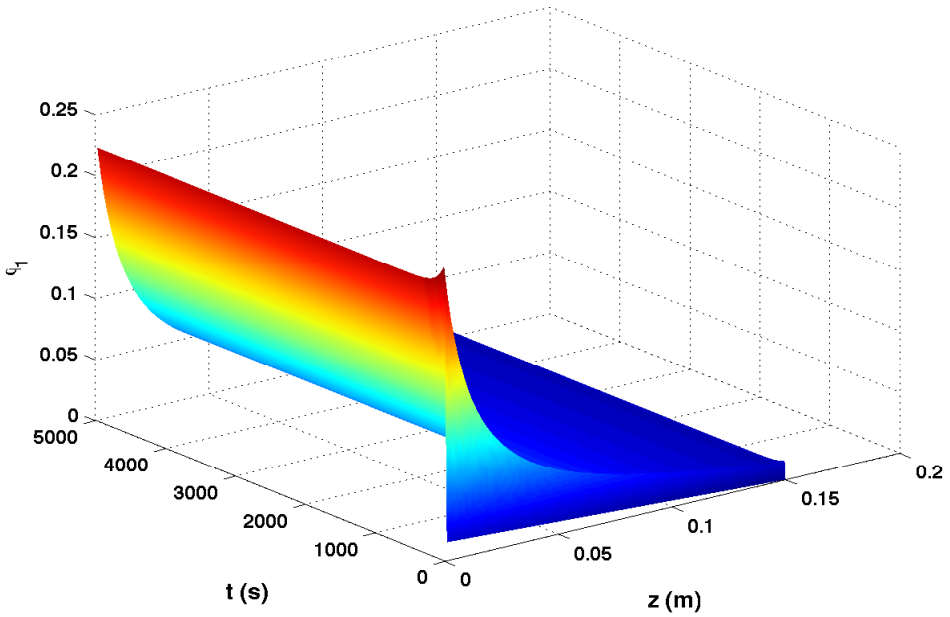
Table 2.1: Model Parameters

Parameter	Values	unit
ϵ	0.4	
ρ_B	700	$\mathrm{kg_{cat}/m^3}$
C_H	587.4437	$\mathrm{mol/m^3}$
n_1	1.12	
n_2	0.85	
E	81000	J/mol
R	8.314	J/mol K
C_{A0}	0.419344	$\mathrm{mol/m^3}$
C_{Ain}	0.419344	$\mathrm{mol/m^3}$
T_0	523	K
T_{in}	523	K
ρ	2.7	$\mathrm{Kg/m^3}$
C_p	147.49	J/Kg K
ΔH	101.3×10^3	J/mol
k_0	1.2384	
k_1	2.8896	
L	0.15	m

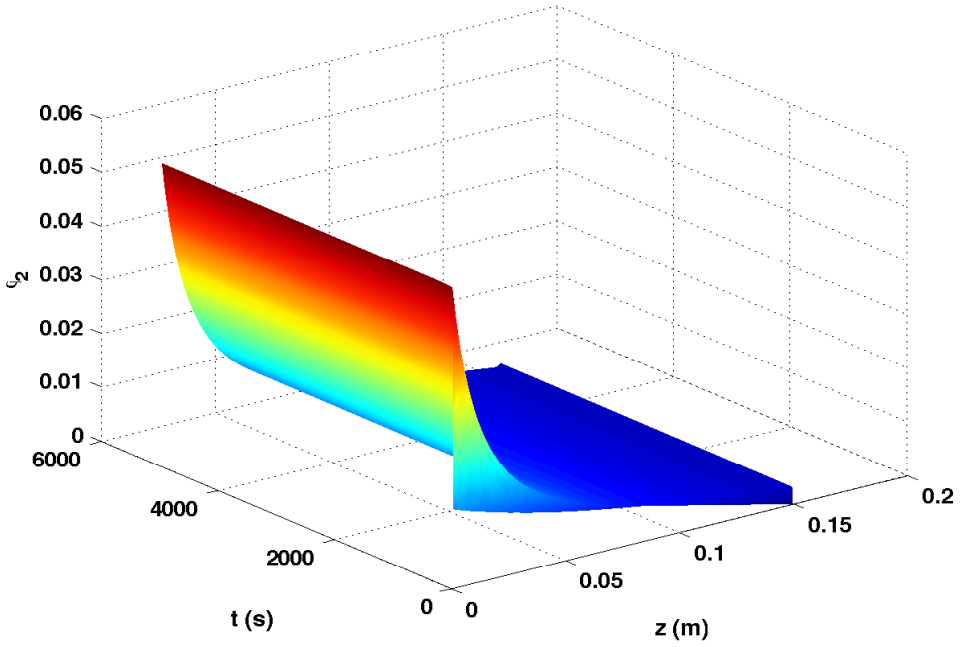
varying controller is much better than the time-invariant controller. The time-varying controller, regulates the temperature at the desired steady state profile with almost no error; however, the time-invariant controller results in oscillatory response with significant error. As the catalyst deactivation rate decreases the difference between performance of two controllers decreases. For $\alpha = 1\times10^{-4}$, the time-varying controller is still better than time invariant one, but the maximum temperature error is less than 1K which is not significant. In Figure 2.5, the trajectory of manipulated variable for two controllers are compared. It can be observed that, although the time-varying controller has significantly better performance for $\alpha = 1 \times 10^{-2}$, it does not require an aggressive input change.

2.6 Summary

In this chapter, an LQ-optimal controller for a time-varying set of two time-scale coupled hyperbolic equations was formulated. Exponential stability of these systems was analyzed using Lyapunov equation. It was shown that the solution of the optimal control problem can be found by solving an equivalent matrix Riccati partial differential equation. Numerical simulations were performed to evaluate the closed loop performance of the formulated controller on a hydrotrating fixed-bed reactor. The performance of the proposed controller was compared to the performance of an infinite dimensional controller formulated by ignoring the catalyst deactivation. Simulation results showed that the performance of the proposed controller is better than the controller ignoring the catalyst deactivation, when the deactivation time is comparable with resident time of the reactor.



(a) ϕ_1



(b) ϕ_2

Figure 2.2: Time-varying LQ-feedback functions ϕ_1 and ϕ_2, $\alpha = 1 \times 10^{-2}$

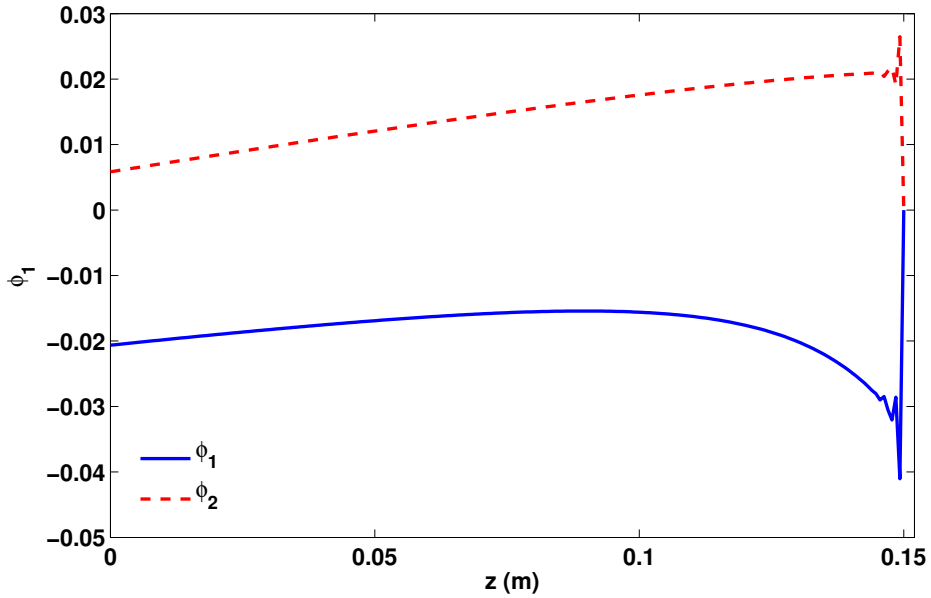
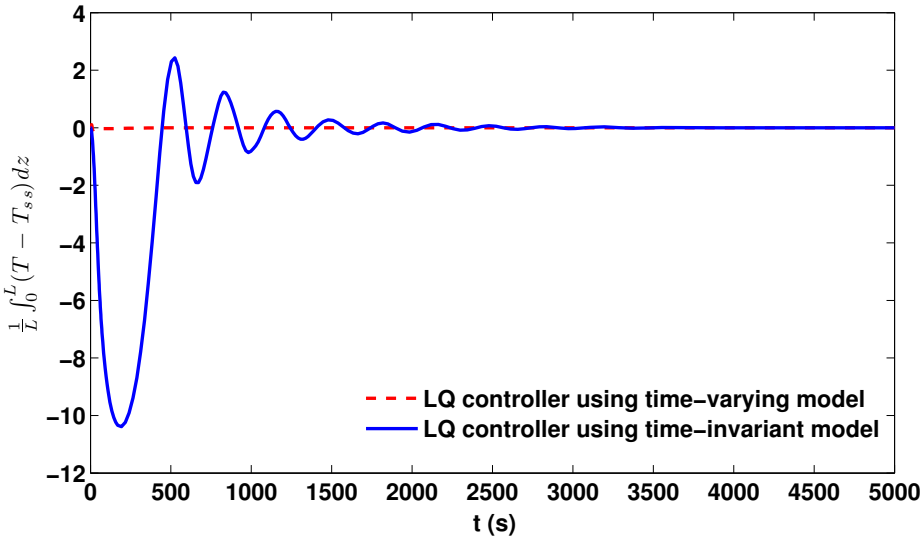
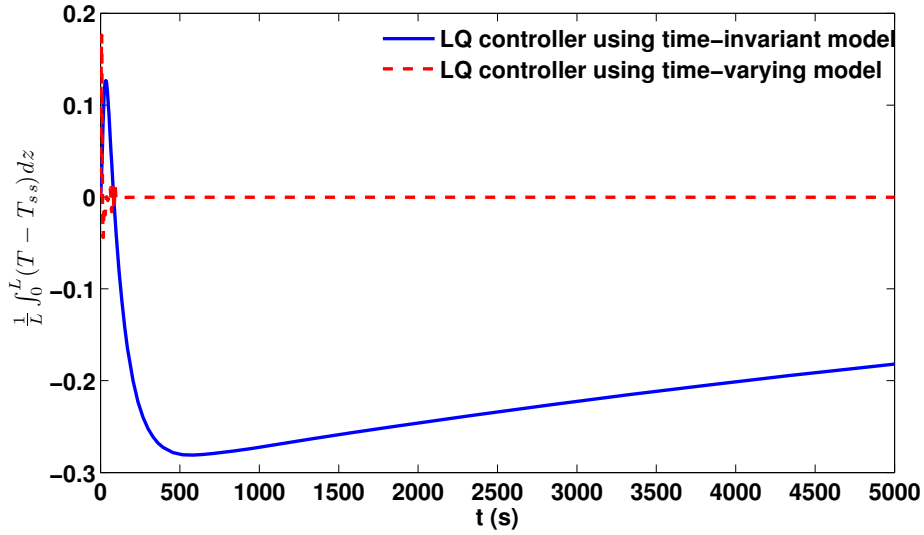


Figure 2.3: Time-invariant LQ-feedback functions ϕ_1 and ϕ_2, $\alpha = 1 \times 10^{-2}$



(a) $\alpha = 1 \times 10^{-2}$



(b) $\alpha = 1 \times 10^{-4}$

Figure 2.4: Integral average of the error

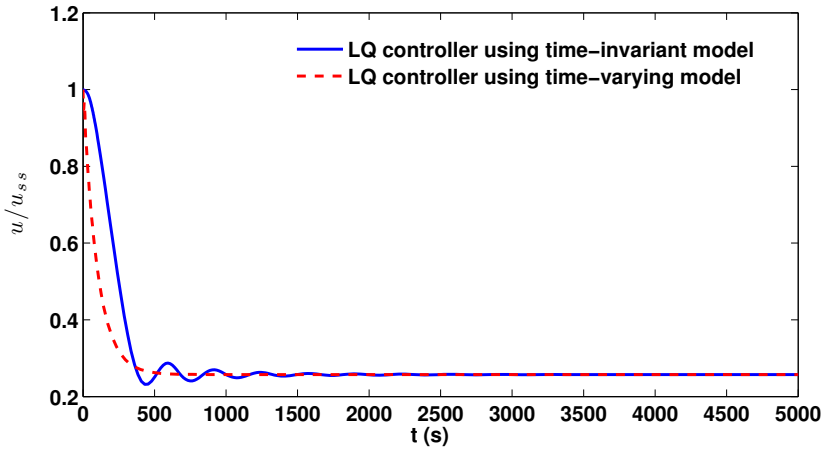


Figure 2.5: Manipulated variable, $\alpha = 1 \times 10^{-2}$

3

Robust Constrained MPC of Coupled Hyperbolic Systems

In this chapter Model Predictive Control of the fixed-bed hydrotreating reactor introduced in Chapter 2 is studied. LQ optimal controller introduced in Chapter 2 is not suitable to control processes with input/output constraints. Moreover, LQ controller's performance may deteriorate under parameter uncertainty. The robust constrained characteristic MPC is formulated for the general case of two time-scale hyperbolic system and then its performance is studied for the case of the hydrotreating reactor. The formulated MPC controller ensures that the input and output constraints are satisfied under parameter uncertainty[1]

[1]Portiones of this chapter have been published in "Mohammadi, L., S. Dubljevic and J. F. Forbes (2010), Robust Characteristic- Based MPC of a Fixed-Bed Reactor. Proceedings of the American Control Conference".

A mathematical model of a process can never represent dynamical aspects of the process completely. There is always some sort of uncertainty involved in modelling a system. A typical source of model uncertainty in a chemical process is unknown or partially known parameters like reaction rate. Presence of uncertain variables and unmodeled dynamics, if not taken into account in the controller design, may lead to poor performance of the controller or even to closed-loop instability. Another important issue, which should be considered when designing a controller, is existence of input and/or output constraints. The constraints can represent actuator limitation or safety requirements. For example, catalytic reactors are very sensitive to changes in temperature. High temperatures can accelerate the rate of catalyst deactivation; on the other hand, there is normally a minimum temperature required for the reactor to operate. When constraints on states and controls are present, in addition to robust stability, it is necessary to ensure the constraint satisfaction under model parameter uncertainty

Model Predictive Control is a class of model based controllers, which make explicit use of a model of the process to obtain the control action by minimizing an objective function (Camacho, 1999). It is a very well known approach for dealing with parameter uncertainty and constraints. The objective function in MPC is a measure of predicted performance of the system over prediction horizon. In other words, by using a model of the process, MPC predicts the future behavior of the process and determines the current control action. The control input is updated at every sampling time (Rossiter, 2003). One of the major advantages of MPC is its ability to do on-line constraint handling in a systematic way. Another advantage of MPC is that it can be easily applied to multivariable systems (Camacho, 1999). Since the essence of MPC is to optimize the prediction of the process behaviour based on a process model over values for the manipulated variables, the model is a critical element of a MPC controller (Rawlings, 2000).

Motivated by the fact that robustness of the controller and constraint handling are very important aspects of controller design, this chapter goes beyond the infinite

dimensional LQ controller introduced in Chapter 2 with the objective of development of a robust MPC controller, which is able to handle input and output constraints under parameter uncertainty.

Unfortunately, model predictive control algorithms for distributed parameter systems are relatively scarce. For Diffusion reaction systems, which are described by parabolic PDEs, Dubljevic *et al.* (2005) used modal decomposition to derive finite-dimensional systems that capture the dominant dynamics of the original PDE. The low dimensional model is subsequently used for controller design. For convection dominated parabolic PDE modal decomposition methods result in high-order finite dimensional systems. Model predictive control for high-order systems is computational demanding and cannot be applied on-line.

For hyperbolic systems, the eigenvalues of the spatial differential operator cluster along vertical or nearly vertical asymptotes in the complex plane (Christofides, 2001), and modal decomposition methods may not be used. Then, Dubljevic et al.(Dubljevic *et al.*, 2005) used finite difference method to convert the hyperbolic equations to a set of ODEs and Model Predictive Controller is designed for the resulting model. As discussed previously, using discretization methods ignores the distributed nature of the system and dynamics of the system may not be captured properly. One of the features of hyperbolic systems is that any discontinuity in the initial or boundary conditions can propagate and finite difference or finite element algorithms may become numerically unstable, and therefore are not suitable to use as a model for controller design. Moreover, hyperbolic systems have finite impulse response (FIR) behavior (Choi and Lee, 2005) and the discretization algorithms do not preserve this property. The method of characteristic is a classical algorithm for solution of a hyperbolic equation that can preserve the FIR property of the hyperbolic systems.

Characteristic-based model predictive control is an approach for model predictive control of DPS that uses method of characteristics combined with model predictive controller and is proposed by Shang *et al.* (2004). The characteristic-based MPC allows controller design for linear, quasilinear, and nonlinear low dimensional PDEs.

In this method, partial differential equations are transformed to a set of ordinary differential equations along characteristic curves, which exactly describe the original DPS. Then the controller design can be performed on ODEs instead of PDEs without approximation. Unfortunately, the model predictive control for hyperbolic systems investigated by Shang *et al.* (2004) or Shang *et al.* (2007) did not consider constraints.

In this work the problem of characteristic-based robust constrained MPC of two time-scale hyperbolic systems is studied. For designing the robust controller, the plant is assumed to lie in a polytopic set resulting from possible parameter uncertainties. The objective of robust control design is to ensure that some performance specification is met by the designed controller, as long as the plant remains within the polytopic set (Maciejowski (2002) and Kothare *et al.* (1996)).

In the original characteristic-based MPC proposed by Shang *et al.* (2004), the system is realized as an input-output system. In this work, we have reformulated the prediction method such that the resulting system is state space system that can handle state constraints. It has been shown that the resulting state space system has a certain structural features that can be exploited in the formulation of the robust model predictive controller.

To formulate the robust MPC, we assume that the uncertainties are polytopic. The robust model predictive controller is realized as a quadratic optimization problem. It is assumed that the objective of robust controller is to ensure that the constraints are satisfied as long as the plant lies inside the polytope. Therefore, the quadratic objective function is defined based on the nominal model of the system. To ensure constraint satisfaction under parameter uncertainty, the evolution of the constraints over the prediction horizon under possible parameter uncertainties is used as the constraint for the quadratic problem.

The case study considered in this chapter is the hydrotreating reactor introduced in Chapter 2; however, in this chapter it is assumed that the rate of deactivation is unknown and therefore the pre-exponential factor in the kinetic term is uncertain. Another uncertainty arises from fluctuations in the inlet flowrate. The proposed

robust constrained MPC is applied to the process and the closed loop performance is analyzed.

The contributions of this chapter can be summarized as:

- State Space realization of two time-scale hyperbolic systems using the method of characteristics;
- Formulation of stability guaranteed robust model predictive controller that ensures constraint satisfaction under parameter uncertainty.

3.1 Characteristics-Based MPC

The method of characteristics is a technique for solving hyperbolic partial differential equations (Shang *et al.*, 2004). The idea behind the method of characteristics is that every hyperbolic PDE has a characteristic curve associated with it, along which dynamics evolve, and as a result, the hyperbolic PDE can be represented as an equivalent system of ODEs.

Consider a quasilinear system of first-order equations with two dependent variables ν_1, ν_2 and two independent variables t and z.

$$\begin{aligned} \frac{\partial \nu_1}{\partial t} + a_1 \frac{\partial \nu_1}{\partial z} &= f_1(\nu_1, \nu_2, u) \\ \frac{\partial \nu_2}{\partial t} + a_2 \frac{\partial \nu_2}{\partial z} &= f_2(\nu_1, \nu_2, u) \end{aligned} \tag{3.1}$$

If coefficients $a_1 \neq a_2$, the system has two different characteristics determined by:

$$\begin{aligned} \text{Characteristic C}_1 : \quad & \frac{dz}{dt} = a_1 \\ \text{Characteristic C}_2 : \quad & \frac{dz}{dt} = a_2 \end{aligned} \tag{3.2}$$

along these characteristics dynamic of the system is described by the following set of ODEs:

$$\begin{aligned} \frac{d\nu_1}{dt} &= f_1(\nu_1, \nu_2, u) \quad \text{along characteristic C}_1 \\ \frac{d\nu_2}{dt} &= f_2(\nu_1, \nu_2, u) \quad \text{along characteristic C}_2 \end{aligned} \tag{3.3}$$

Then, by using the method of characteristics, the set of partial differential equations (3.1) is transformed to a set of ODEs along the characteristic curves. This set of ODEs can be used to predict the system's evolution. The characteristic ODEs are coupled with respect to the two characteristic curves, and the values of state variables at any point in time and space should be determined by simultaneous integration of both characteristic ODEs along two nonparallel characteristic curves passing through that point. This can be used for evaluation of the future values of state variables. In Fig. 3.1 the calculation of the future output variables using the method of characteristics is illustrated. This method for prediction of the future behaviour is proposed in (Shang *et al.*, 2004). The idea is that each point in space and time (e.g. P) has a *domain of dependence*. The domain of dependence for point P in Figure 3.1 is the area enclosed by characteristic curves passing through point P. The solution at P depends on the values of state variables within its domain of dependence. In other words, the solution at P can be calculated by integration of characteristic equations along characteristic curves $P-Q$ and $P-R$. Values of state variables at Q and R are used as initial conditions for integration. The mathematical description is

$$\nu_1(P) = \int_{t(Q)}^{t(P)} f_1(Q)dt \tag{3.4}$$

$$\nu_2(P) = \int_{t(R)}^{t(P)} f_2(R)dt \tag{3.5}$$

where:

$$t(P) = \frac{a_1 t(Q) - 2a_2 t(Q) + a_2 t(R) + Z(R) - Z(Q)}{a_1 - a_2} \tag{3.6}$$

The position of the point P is calculated by:

$$Z(P) = \frac{a_1 Z(R) - a_2 Z(Q) + a_1 a_2 [t(R) - t(Q)]}{a_1 - a_2} \tag{3.7}$$

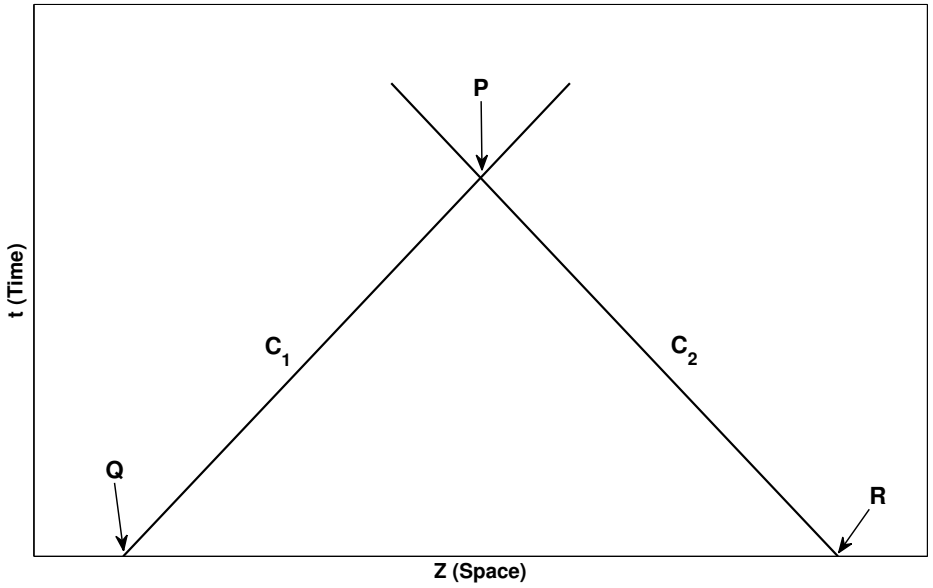


Figure 3.1: Calculation of the state variable along the characteristic curves

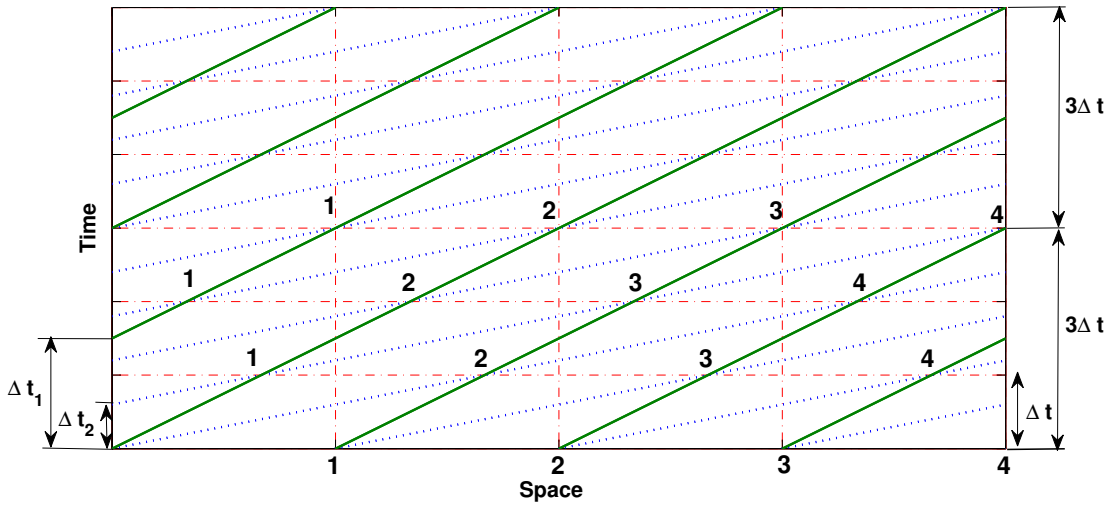


Figure 3.2: Prediction of state variables for $a_1/a_2 = 0.4$

State Space Representation

In this chapter we are interested in robust model predictive control of linear systems, therefore before attempting to derive the state space model of the system, assume that the model equations (3.1) are linearized about the steady state profile of the reactor. The linearized model can be represented by:

$$\begin{aligned}\frac{\partial \nu_1'}{\partial t} &= -a_1\frac{\partial \nu_1'}{\partial z} + M_{11}(z)\nu_1' + M_{12}(z)\nu_2' + \mathcal{B}_1(z)u' \\ \frac{\partial \nu_2'}{\partial t} &= -a_2\frac{\partial \nu_2'}{\partial z} + M_{21}(z)\nu_1' + M_{22}(z)\nu_2' + \mathcal{B}_2(z)u'\end{aligned} \tag{3.8}$$

where $'$ indicates that the variables are in deviation form.

The characteristic curves for the linearized model (3.8) are:

$$\mathrm{C}_1 = \frac{dz}{dt} = a_1 \tag{3.9}$$

$$\mathrm{C}_2 = \frac{dz}{dt} = a_2 \tag{3.10}$$

and the characteristic equations are:

$$\frac{d\nu_1'}{dt} = M_{11}\nu_1' + M_{12}\nu_2' + \mathcal{B}_1u' \tag{3.11}$$

$$\frac{d\nu_2'}{dt} = M_{21}\nu_1' + M_{22}\nu_2' + \mathcal{B}_2u' \tag{3.12}$$

Using the prediction method discussed in the previous section, values of ν_1' and ν_2' can be calculated along the length of the reactor. At any time $t = t_k$, the length of the reactor can be discretized using a finite number of discretization point. By defining the values of ν_1 and ν_2 at discretization points as state variables, the set of PDEs can be represented as a state space model. The idea is that at $t = t_k$ the measurements of the state variables are available at the discretization points. These measurements are used to determine the value of the state variables at the intersections of the characteristic curves passing the initial discretization points. Using the approach discussed in the previous section, the values of the state variables can be calculated at the intersection points. A graphical representation of this method is shown in Figures 3.2-3.4. The state vector is defined as:

$$x = \begin{bmatrix} \nu'_{11} & \nu'_{12} & \cdots & \nu'_{1N} & \nu'_{21} & \nu'_{22} & \cdots & \nu'_{2N} \end{bmatrix}^T$$

where N is the number of discretization points. The values of state variables at time $T = \Delta t$ can be calculated using Equations (3.4)-(3.5). This procedure will be repeated for $T = 2\Delta t, 3\Delta t, \ldots$ Since the positions of the intersection points change at each sample time, the resulting state space model is a linear time-varying discrete system represented by

$$x_{k+1} = A_k x_k + B u_k \tag{3.13}$$

$$y_k = C_k x_k \tag{3.14}$$

The positions of the intersection points are functions of the ratio of slopes of two characteristic curves, and therefore the structure of A depends on the ratio of two slopes.

Example 3.1.1. As an example, we will explore the structure of matrix A for the case that this ratio is equal to 0.4. In Figure 3.2, positions of the intersections are illustrated at different sample times. If one repeats the integration procedure for six sample times, it will be observed that the structure of the matrix A is repeated every third sample time. The reason is that the positions of the intersection points also change periodically with period of three sample times. The structure of the matrix A is given by

$$A_1 = \left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha_{11}(1) & 0 & 0 & 0 & \alpha_{12}(1) & 0 & 0 & 0 \\ 0 & \alpha_{11}(2) & 0 & 0 & 0 & \alpha_{12}(2) & 0 & 0 \\ 0 & 0 & \alpha_{11}(3) & 0 & 0 & 0 & \alpha_{12}(3) & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha_{21}(1) & 0 & 0 & 0 & \alpha_{22}(1) & 0 & 0 & 0 \\ 0 & \alpha_{21}(2) & 0 & 0 & 0 & \alpha_{22}(2) & 0 & 0 \end{array}\right]$$

$$A_3 = \left[\begin{array}{cccc|cccc} \alpha_{11}(1) & 0 & 0 & 0 & \alpha_{12}(1) & 0 & 0 & 0 \\ 0 & \alpha_{11}(2) & 0 & 0 & 0 & \alpha_{12}(2) & 0 & 0 \\ 0 & 0 & \alpha_{11}(3) & 0 & 0 & 0 & \alpha_{12}(3) & 0 \\ 0 & 0 & 0 & \alpha_{11}(4) & 0 & 0 & 0 & \alpha_{12}(4) \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha_{21}(1) & 0 & 0 & 0 & \alpha_{22}(1) & 0 & 0 & 0 \\ 0 & \alpha_{21}(2) & 0 & 0 & 0 & \alpha_{22}(2) & 0 & 0 \\ 0 & 0 & \alpha_{21}(3) & 0 & 0 & 0 & \alpha_{22}(3) & 0 \end{array}\right]$$

$$A_2 = A_1 \quad \text{and} \quad A_k = \begin{cases} A_1 & k = 3n+1 \\ A_2 & k = 3n+2 \\ A_3 & k = 3n \end{cases}$$

where $\alpha_{ij}(l)$ is the result of the integration of the characteristic equations given by:

$$\begin{aligned} \alpha_{11}(l) &= \int_{t_{k-1}}^{t_k} M_{11}(l)dt \\ \alpha_{12}(l) &= \int_{t_{k-1}}^{t_k} M_{12}(l)dt \\ \alpha_{21}(l) &= \int_{t_{k-1}}^{t_k} M_{21}(l)dt \\ \alpha_{22}(l) &= \int_{t_{k-1}}^{t_k} M_{22}(l)dt \end{aligned} \tag{3.15}$$

and l represents the spatial position of each discretization point.

The structure of the matrix B also depends on the ratio of two slopes and for the

case of 0.4 is given by

$$B_1 = \begin{bmatrix} \mathcal{B}_1(1)\Delta t \\ \mathcal{B}_1(2)\Delta t \\ \mathcal{B}_1(3)\Delta t \\ \mathcal{B}_1(4)\Delta t \\ \hline \mathcal{B}_2(1) \times (\Delta t - \Delta t_2) \\ \mathcal{B}_2(2)\Delta t \\ \mathcal{B}_2(3)\Delta t \\ \mathcal{B}_2(4)\Delta t \end{bmatrix}, \quad B_2 = \begin{bmatrix} \mathcal{B}_1(1) \times (2\Delta t - \Delta t_1) \\ \mathcal{B}_1(2)\Delta t \\ \mathcal{B}_1(3)\Delta t \\ \mathcal{B}_1(4)\Delta t \\ \hline \mathcal{B}_2(1) \times (2\Delta t - 3\Delta t_2) \\ \mathcal{B}_2(2) \times (2\Delta t - 2\Delta t_2) \\ \mathcal{B}_2(3)\Delta t \\ \mathcal{B}_2(4)\Delta t \end{bmatrix}$$

$$B_3 = \begin{bmatrix} \mathcal{B}_1(1)\Delta t \\ \mathcal{B}_1(2)\Delta t \\ \mathcal{B}_1(3)\Delta t \\ \mathcal{B}_1(4)\Delta t \\ \hline \mathcal{B}_2(1) \times (3\Delta t - 4\Delta t_2) \\ \mathcal{B}_2(2)\Delta t \\ \mathcal{B}_2(3)\Delta t \\ \mathcal{B}_2(4)\Delta t \end{bmatrix}, \quad B_k = \begin{cases} B_1 & k = 3n+1 \\ B_2 & k = 3n+2 \\ B_3 & k = 3n \end{cases} \tag{3.16}$$

Matrix C depends on the available measurements. Assuming that the only output variable is the value of ν_1 at $z = l$, output matrix C will be:

$$\begin{aligned} C_1 &= \left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 1 + M_{11}(4) \times (\Delta t_1 - \Delta t) & 0 & 0 & 0 & M_{12}(4) \times (\Delta t_1 - \Delta t) \end{array}\right] \\ C_2 &= [], \quad C_3 = \left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{array}\right] \\ C_k &= \begin{cases} C_1 & k = 3n+1 \\ C_2 & k = 3n+2 \\ C_3 & k = 3n \end{cases} \end{aligned} \tag{3.17}$$

□

As mentioned, the position of the intersection points, and therefore the structure of the state space system, is a function of the ratio of the slopes of two characteristic curves. In Figures 3.3-3.4, the intersection points are illustrated for the cases that the ratio is equal to 0.5 and 0.6, respectively. It can be observed that for the first

case, the position of intersection points are constant. Therefore, this case will result in a linear time-invariant state space system. In the second case, the period is equal to two, which means that the resulting state space system will have a period of two sample times.

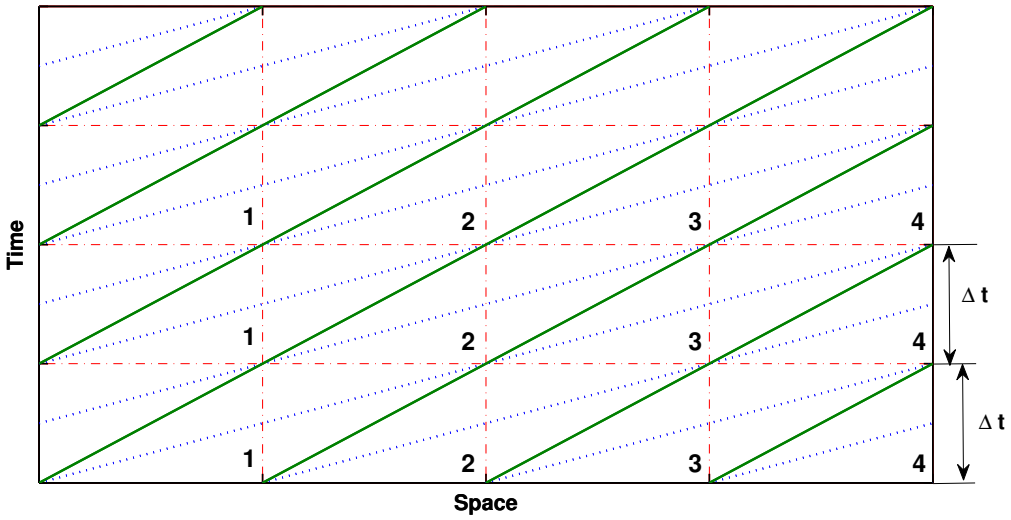


Figure 3.3: Prediction of state variables for $a_1/a_2 = 0.5$

In order to use common MPC algorithms, the periodic system should be converted to a linear time-invariant system. If the period of the system is N, this can be done by assembling N sample times to one larger sample time and defining a new state space system with larger sample time. For the case that the period is equal to 3, the system can be converted to a linear time-invariant system by defining

$$\bar{A} = A_3A_2A_1 \tag{3.18}$$

$$\bar{B} = \begin{bmatrix} A_3A_2B_1 & A_3B_2 & B_3 \end{bmatrix} \tag{3.19}$$

$$\bar{C} = [C_1,\, C_2A_1,\, C_3A_2A_1]^T \tag{3.20}$$

Finally, the LTI representation suitable for the design of MPC controller is given as:

$$\begin{aligned} x_{k+1} &= \bar{A}x_k + \bar{B}u_k, \\ y_k &= \bar{C}x_k, \end{aligned} \tag{3.21}$$

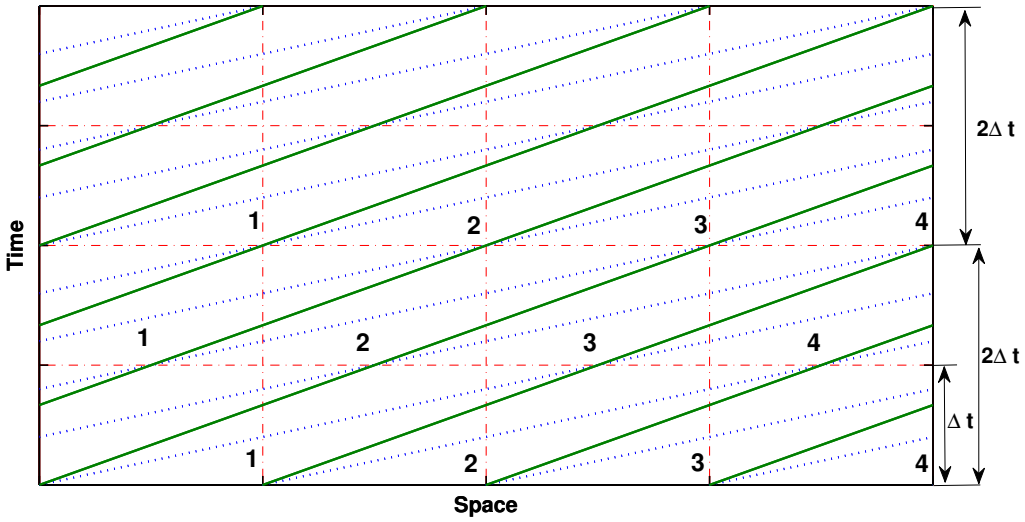


Figure 3.4: Prediction of state variables for $a_1/a_2 = 0.6$

Now that we successfully derived a linear time-invariant state space system, we can proceed with designing a robust model predictive controller that will be addressed in the next section.

3.2 Robust Characteristic-Based MPC

In order to include the parametric uncertainty of the plant, it is assumed that the small variations in the uncertain parameters of the system generate a family of the linear systems given by Equation (3.21). It is assumed that the set of uncertain models generated by the uncertain parameters, $[\bar{A}_i \quad \bar{B}_i]$ build a polytopic set $\Omega\{[\bar{A}_i \quad \bar{B}_i]\}$ and the real model of the system lies within or on the convex hull of the polytopic set. Thus the system can be described by a polytopic uncertain system. Polytope Ω is defined by

$$\Omega = \text{Co}\{[\bar{A}_1 \quad \bar{B}_1], [\bar{A}_2 \quad \bar{B}_2], \cdots, [\bar{A}_L \quad \bar{B}_L]\} \tag{3.22}$$

So if $[\bar{A}, \quad \bar{B}] \in \Omega$ then, for some nonnegative $\lambda_1, \lambda_2, \cdots, \lambda_L$ summing to one, we

have

$$[\bar{A} \quad \bar{B}] = \sum_{i=1}^{L} \lambda_i [\bar{A}_i \quad \bar{B}_i]$$

which means that there is a convex hull of uncertain plants, which is generated by considering all possible combinations of uncertain parameters.

In this work the model predictive control algorithm proposed by Muske and Rawlings (1993) is modified to consider parameter uncertainty. It is assumed that the objective of the robust controller is only to ensure constraint satisfaction under any possible parameter uncertainty. Hence, the quadratic performance index is constructed based on the nominal model of the system, while the construction of the constraints captures the dynamics of all possible parametric uncertain models. Matrix $\bar{A}$ in Equation (3.21) is a nilpotent matrix, which implies that the system has an FIR property. This FIR property is a natural feature of co-current hyperbolic systems and implies that the system is always stable and all eigenvalues of $\bar{A}$ are inside the unit circle. In the case of a tubular reactor, the reason for the FIR property is that each species is processed in a limited time in the reactor and leaves out of the reactor in finite time. Therefore, an impulse change in reactor input will propagate only for finite time.

For stable systems, Muske and Rawlings (1993) proposed the following stability guaranteed MPC formulation for a LTI state space system $\sum(A, B, C)$ at time k

$$\min_{u^N} y_{k+N}^T \bar{Q} y_{k+N} + \sum_{j=0}^{N-1} (y_{k+j}^T Q y_{k+j} + u_{k+j}^T R u_{k+j} + \Delta u_{k+j}^T S \Delta u_{k+j}) \tag{3.23}$$

Subject to:

$$x(k+1) = Ax(k) + Bu(k) \tag{3.24}$$

$$y(k) = Cx(k) \tag{3.25}$$

$$u_{min} \leq u_{k+j} \leq u_{max}, \quad j = 0, 1, \ldots, N-1 \tag{3.26}$$

$$y_{min} \leq y_{k+j} \leq y_{max}, \quad j = 0, 1, \ldots, N-1 \tag{3.27}$$

$$\Delta u_{min} \leq \Delta u_{k+j} \leq \Delta u_{max}, \quad j = 0, 1, \ldots, N-1 \tag{3.28}$$

In the cost function (3.23), $\bar{Q}$ is the weighting on the final value of the state variables. In order to ensure the stability of the closed loop system, $\bar{Q}$ should be the solution of the following Lyapunov equation (Muske and Rawlings, 1993)

$$\bar{Q} = C^T Q C + A^T \bar{Q} A \tag{3.29}$$

Since we are interested in the robust constraint satisfaction, the objective function used in this work is similar to Equation (3.23), but the constraints should change to consider all the possible realizations of the system. The constraints that should be included in the MPC problem are

$$x(k+1) = \bar{A}_i x(k) + \bar{B}_i u(k) \tag{3.30}$$

$$y(k) = \bar{C}_i x(k) \quad i = 1, 2, ..., L \tag{3.31}$$

$$u_{min} \leq u_{k+j} \leq u_{max}, \quad {}_{j=0,1,...,N-1} \tag{3.32}$$

$$y_{min} \leq y_{k+j} \leq y_{max}, \quad j = 0, 1, \ldots, N-1 \tag{3.33}$$

$$\Delta u_{min} \leq \Delta u_{k+j} \leq \Delta u_{max}, \quad j = 0, 1, \ldots, N-1 \tag{3.34}$$

The MPC problem can be converted to the following convex quadratic problem that can be solved by any quadratic programming algorithm (Muske and Rawlings, 1993).

$$\min_{u^N} \Phi_k = (u^N)^T H u^N + 2(u^N)^T (G x_k - F u_{k-1}) \tag{3.35}$$

Subject to:

$$\begin{bmatrix} I \\ -I \\ \mathcal{A}_1 \\ \mathcal{A}_2 \\ \vdots \\ \mathcal{A}_L \\ -\mathcal{A}_1 \\ -\mathcal{A}_2 \\ \vdots \\ -\mathcal{A}_L \\ W \\ -W \end{bmatrix} u^N \leq \begin{bmatrix} i_1 \\ i_2 \\ \mathcal{B}_1 \\ \mathcal{B}_2 \\ \vdots \\ \mathcal{B}_L \\ \mathcal{D}_1 \\ \mathcal{D}_2 \\ \vdots \\ \mathcal{D}_L \\ w_1 \\ w_2 \end{bmatrix}$$

Matrices, H, G and F are calculated by determining the prediction of the output variable as a function of the input variable and are given by

$$H = \begin{bmatrix} B^T\bar{Q}B + R + 2S & B^TA^T\bar{Q}B - S & \cdots & B^TA^{T^{N-1}}\bar{Q}B \\ B^T\bar{Q}AB - S & B^T\bar{Q}B + R + 2S & \cdots & B^TA^{T^{N-2}}\bar{Q}B \\ \vdots & \vdots & \ddots & \cdots \\ B^T\bar{Q}A^{N-1}B & B^T\bar{Q}A^{N-2}B & \cdots & B^T\bar{Q}B + R + 2S \end{bmatrix} \tag{3.36}$$

$$G = \begin{bmatrix} B^T\bar{Q}A \\ B^T\bar{Q}A^2 \\ \vdots \\ B^T\bar{Q}A^N \end{bmatrix}, \quad F = \begin{bmatrix} S \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{3.37}$$

Matrices $\mathcal{A}_i, W, i_1, i_2, \mathcal{B}_i$ are defined to consider the constraints over the prediction horizon and under possible realizations of the system and are defined as

$$\mathcal{A}_i = \begin{bmatrix} C_iB_i & 0 & 0 & 0 \\ C_iA_iB_i & C_iB_i & 0 & 0 \\ C_iA_i^2B_i & C_iA_iB_i & C_iB_i & 0 \\ \vdots & \vdots & \vdots & \vdots \\ C_iA_i^{N-1}B_i & C_iA_i^{N-2}B_i & C_iA_ii^{N-3}B_i & C_iB_i \end{bmatrix}, \quad i = 1, \ldots, L \tag{3.38}$$

$$\mathcal{B}_i = \begin{bmatrix} y_{max} - C_iA_i \\ y_{max} - C_iA_i^2 \\ y_{max} - C_iA_i^3 \\ \vdots \\ y_{max} - C_iA_i^N \end{bmatrix}, \quad \mathcal{D}_i = \begin{bmatrix} -y_{min} + C_iA_i \\ -y_{min} + C_iA_i^2 \\ -y_{min} + C_iA_i^3 \\ \vdots \\ -y_{min} + C_iA_i^N \end{bmatrix} \tag{3.39}$$

$$W = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & -1 & 1 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{3.40}$$

$$w_1 = \begin{bmatrix} \Delta u_{max} + u_{k-1} \\ \Delta u_{max} \\ \Delta u_{max} \\ \Delta u_{max} \\ \Delta u_{max} \end{bmatrix}, \quad w_1 = \begin{bmatrix} \Delta u_{min} - u_{k-1} \\ \Delta u_{min} \\ \Delta u_{min} \\ \Delta u_{min} \\ \Delta u_{min} \end{bmatrix} \tag{3.41}$$

The resulting quadratic problem can be solved with any quadratic programming algorithm, and as long as the real plant lies inside the polytope (3.22) the formulated MPC is able to handle constraints.

3.3 Case Study

In this section, the proposed characteristic based MPC is applied to the hydrotreating reactor that was introduced in Chapter 2, and its closed loop performance is analyzed. The objective is to control the reactor's outlet temperature at a specified setpoint by manipulating the superficial velocity of the reactor. It is assumed that the parameters k and v_{ss} are uncertain variables. Therefore, the linearized real model of the system lies in the convex hull of a polytopic set with four vertices. It is assumed that the pre-exponential factor, k, can have 40% uncertainty and v_{ss} can have 20% uncertainty. It is also assumed that the manipulating and output variables have lower and upper constraints that shall not be violated.

The state space model that is used for formulating the controller is constructed using the proposed method in §3.1. In order to develop the model for controller formulation, 20 discretization points are used. For simulation of the real plant 60 discretization points are used to construct the model and the controller is applied to this model.

The prediction horizon is assumed to be 20 sample times. It should be mentioned that the resulting state space system is a FIR system, so increasing the prediction horizon to more than resident time of the reactor will not improve the performance of the controller.

To evaluate the closed loop performance of the controller, it is assumed that the system is not initially at steady state and the initial temperature and concentrations are: $T_0 = 0.95T_{in}, C_{A_0} = C_{A_{in}}$. A random model which lies inside the polytopic set is chosen as the real model of the system. Numerical simulations are performed to evaluate the performance of the controller. To solve the quadratic problem, Matlab's quadratic programming tool is used.

Figures 3.5 and 3.6 illustrate the profiles of the reactor temperature and concentration respectively. Figure 3.7 shows the profile of the manipulated variable and Figure 3.8 is the trajectory of the control variable.

As Figures 3.7-3.8 show the constraints on input and output trajectories are satisfied even if the real model of the system is not one of the models considered during the controller formulation.

Note that the chosen initial and boundary conditions have discontinuity (See Figures 3.5 and 3.6), however, the proposed proposed algorithm is numerically stable and the discontinuity only propagates along the characteristic curve.

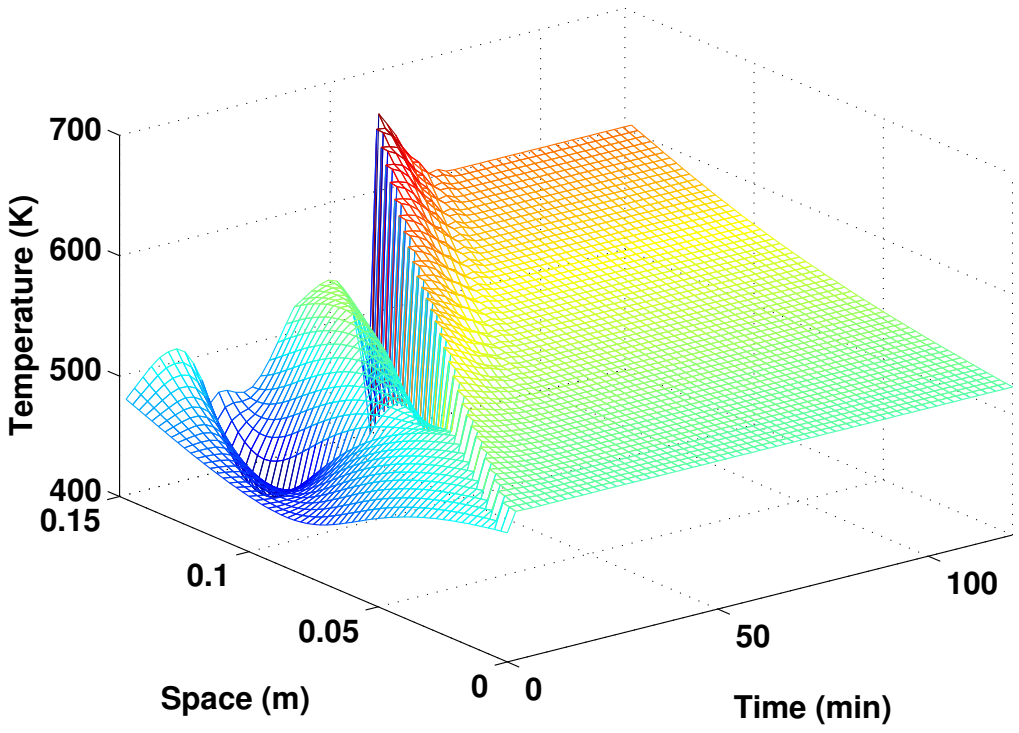


Figure 3.5: Temperature trajectory under the robust controller

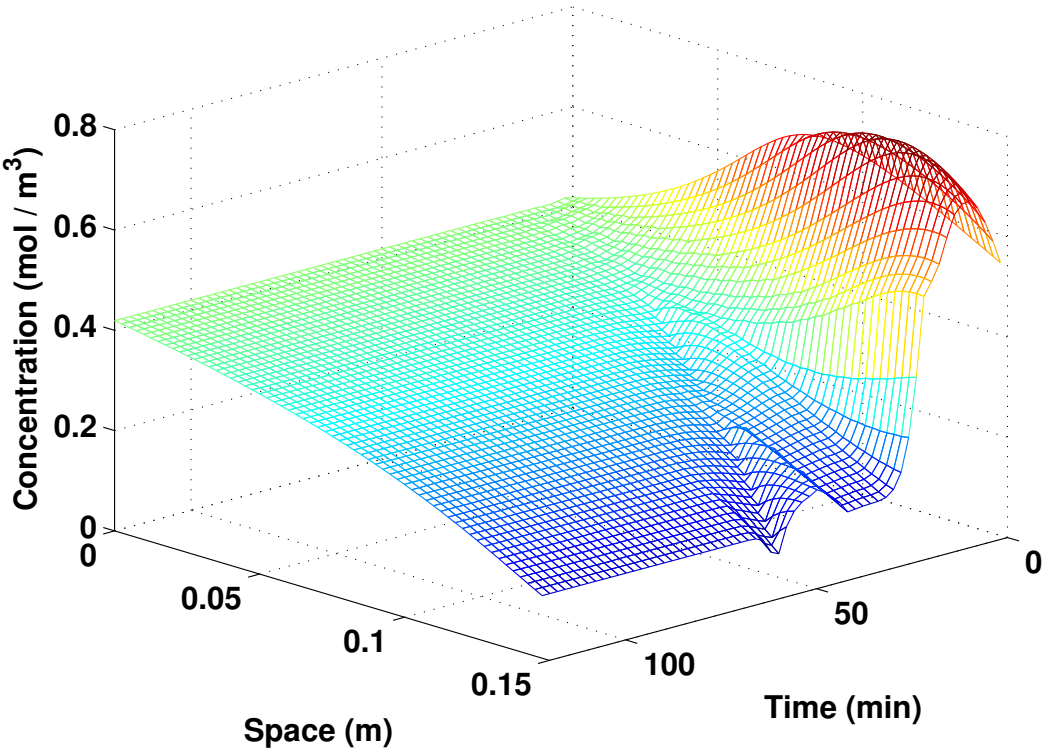


Figure 3.6: Concentration trajectory under the robust controller

3.4 Summary

In this chapter a characteristic based robust model predictive control algorithm was developed for systems modelled by two time-scale coupled hyperbolic partial differential equations. The set of partial differential equations was transformed to a set of ODEs using the method of characteristics. In order to construct the state space model of the system, the spatial domain was discretized to a finite number of intervals. The structure of the resulting state space model was explored. It was shown that the resulting state space system has certain periodic features depending on the ratio of slopes of two characteristic curves. It was also shown that the proposed method preserved the finite impulse response property of the co-current hyperbolic system. This ensures that the dynamics of the system is captured properly, unlike other discretization algorithms that cannot preserve this property and may result in

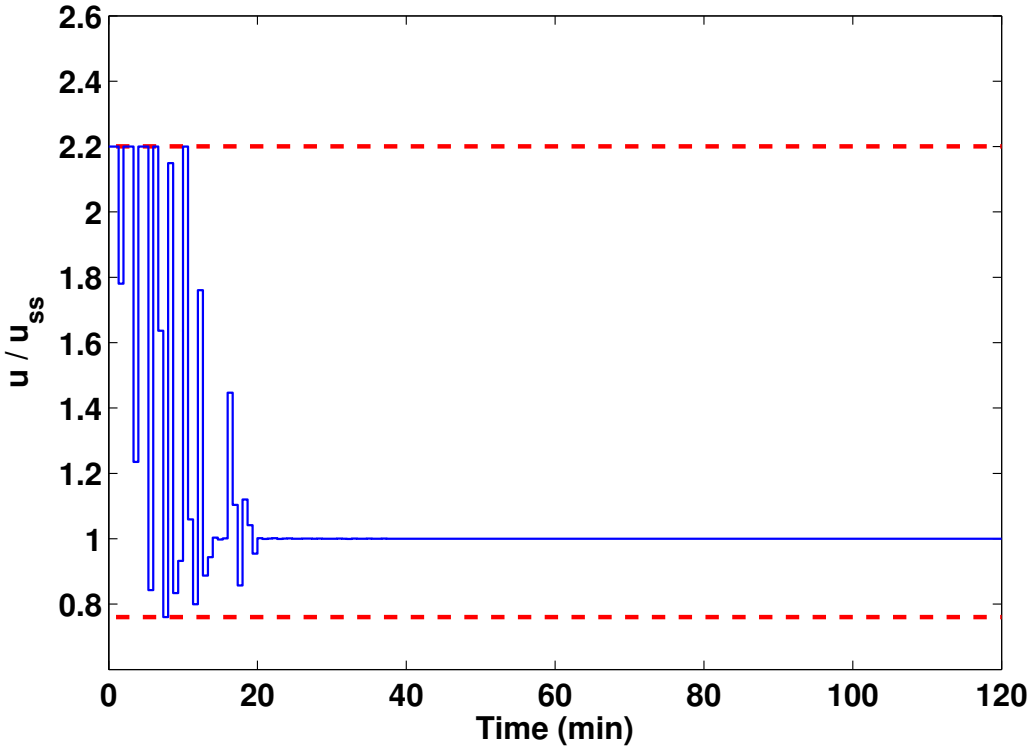


Figure 3.7: Input trajectory under the robust controller

numerical instability of the model if any discontinuity exists.

In order to deal with parameter uncertainty, it was assumed that the uncertain models of the system generate a polytopic set and the real model of the system lies in the polytope Ω. The MPC problem was defined by nominal performance index, but the evolution of the constraints over the prediction horizon was considered for all polytopic models. This formulation of robust controller ensures that constraints are satisfied as long as the real model of the plant lies inside the polytope; however, the performance of the controller may deteriorate as only the nominal model on the system is considered in the performance index.

A case study involving a hydrotreating reactor was used to evaluate the closed loop response of the controller. In this case study two uncertain parameters existed which lead to four polytopic models. Simulation results indicated that this algorithm is able to satisfy input and output constraints under parameter uncertainty.

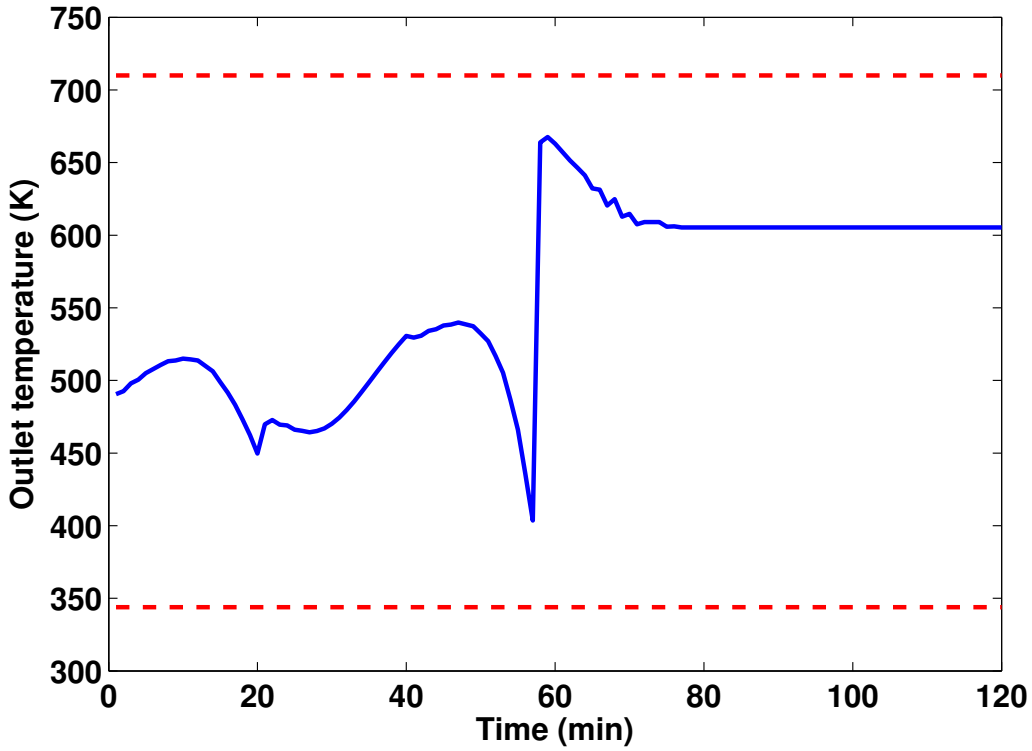


Figure 3.8: Output trajectory under the robust controller

4

LQ Control of Diffusion-Convection-Reaction Systems

This chapter addresses the optimal control of fixed-bed reactors modelled by a set of coupled parabolic PDEs. This chapter takes the first step in solution of the optimal control problem for coupled parabolic PDE-ODE systems, which can represent fixed-bed reactors with catalyst deactivation modelled by a set of ODEs. In this chapter an innovative approach is proposed to solve the eigenvalue problem for a set of coupled parabolic PDEs with spatially varying coefficients. This class of parabolic PDEs is the result of linearization of the nonlinear model of the system around the steady state profile of the system. Using the spectral properties of the system stability of the system is studied and the optimal control problem is solved[1].

[1]Portions of this chapter have been published in "Mohammadi, L., I. Aksikas, S. Dubljevic and J. F. Forbes (2012a). LQ-boundary control of a diffusion-convection-reaction system. International Journal of Control 85, 171-181" and "Mohammadi, L., I. Aksikas, S. Dubljevic and J. F. Forbes (2011), Linear Quadratic Optimal Boundary Control of a Diffusion-Convection-Reaction System. Proceedings of the 18th IFAC World Conference"

The focus of the previous two chapters was on the optimal control of systems modelled by a set of hyperbolic PDEs (i.e. catalytic reactors with negligible diffusion). In the real world, pure hyperbolic systems are rare. Normally, hyperbolic equations result from ignoring the effect of diffusion phenomenon within the system. In most chemical engineering processes, more specifically in most fixed-bed reactors, diffusion may not be ignored and as a result, the model of the system should be represented by a set of parabolic PDEs.

Motivated by this, the current chapter focuses on the infinite dimensional control of systems described by a set of parabolic PDEs, which can be used to represent a fixed-bed reactor with both diffusion and convection phenomena. The only difference between a first order hyperbolic PDE and a parabolic PDE is presence of the second order derivative with respect to the space variable. This difference results in completely different dynamical behaviour and mathematical properties. Unlike hyperbolic systems, for parabolic systems the operator Riccati equation cannot be converted to a matrix Riccati equation. Therefore, we need an alternative method to solve the operator Riccati equation. Parabolic systems can be characterized by their set of eigenvalues and eigenfunctions. The spectral property of these systems is the tool that is generally used to deal with parabolic systems.

Chemical processes are normally modelled by a set of nonlinear equations and in order to apply linear controllers, one needs to linearize the system of equations around the steady state profile of the system. By linearizing the nonlinear equations about the steady state profile of the system, a set of linear parabolic PDEs with spatially varying coefficients is produced. Solution of the eigenvalue problem for a single parabolic PDE with constant coefficients is very well known in the mathematical literature, but there is no general algorithm to solve the eigenvalue problem for a parabolic PDE with spatially varying coefficients. In this work, an innovative idea is proposed to solve the eigenvalue problem of parabolic PDEs with spatially varying coefficients. The proposed approach uses the techniques for the solution of the heat equation for composite media.

Control of diffusion-reaction systems, which are described by parabolic PDEs has studied by many researchers (e.g., Christofides (2001), Dubljevic *et al.* (2005) and and references therein). In these works, modal decomposition is used to derive finite-dimensional system that captures the dominant dynamics of the original PDE and is subsequently used for low dimensional model predictive controller design. The potential drawback of this approach is that for diffusion-convection-reaction systems the number of modes that should be used to derive the ODE system may be very large, which leads to computationally demanding controllers. Additionally, the control problem for coupled parabolic systems has not been addressed in these studies.

Boundary control of parabolic systems have been explored in few studies. Curtain and Zwart (1995) and Emirsjlow and Townley (2000) introduced transformation of the boundary control problem to a well-posed abstract control problem using an exact transformation. Recently, Byrnes *et al.* (2006) studied the boundary feedback control of parabolic systems using zero dynamics. The proposed algorithm is limited to parabolic systems with self-adjoint operator A, therefore cannot be used for chemical reactors that are modelled by multiple PDEs with non-symmetric coupling. Moreover, the proposed controller is not optimal and may result in aggressive control actions. Model predictive boundary control of parabolic systems is studied by Dubljevic and Christofides (2006). This work uses the exact transformation introduced by Curtain and Zwart (1995) along with modal decomposition to solve the boundary control problem for a parabolic PDE, but it is also limited to systems described by a single parabolic PDE. To the best of the author's knowledge, there is no detailed study that addresses optimal boundary control of spatially varying coupled parabolic PDEs in general.

In this chapter, we are interested in the boundary control of systems modelled by coupled parabolic PDEs with spatially varying coefficients. The boundary control problem is transformed into a well-posed abstract boundary control problem by applying an exact transformation similar to the transformation introduced by (Curtain and Zwart, 1995). The stabilizability of the resulting systems is also

investigated. Stability of linear parabolic systems with constant coefficients is studied by Winkin *et al.* (2000), Delattre *et al.* (2003) for the special case of a tubular reactor with two state variables. In this chapter, we extend this work for the more general case of coupled parabolic systems with spatially varying coefficients and arbitrary number of state variables. Finally, by using the spectral properties of the system, the operator Riccati equation is converted into a set of coupled algebraic equations, which can be solved numerically. In this work, our focus is on parabolic systems defined on one-dimensional spatial domain, but the approach can easily be extended to a more general form of parabolic systems with 2D or 3D spatial domain.

The majority of the previous work on infinite dimensional systems modelled by parabolic PDEs concentrated on cases that are described by a single spatially invariant parabolic PDE. This work is a first step in investigation of the control techniques for systems that are described by a set of PDEs with spatially varying coefficients, which would model many chemical engineering processes. A case study involving a tubular reactor, wherein the catalytic cracking of gas oil takes place is used to illustrate our method.

The main contributions of this chapter can be summarized as:

- Solution of eigenvalue problem for a set of coupled parabolic PDEs with spatially varying coefficients;
- Formulation and solution of an optimal boundary control problem for systems modelled by a set of coupled parabolic PDEs;
- Stability analysis of coupled parabolic systems.

4.1 Parabolic DPS: Background

In this section, we will provide some background for infinite dimensional representation of parabolic partial differential equations. The introduced concepts will be used throughout this chapter to formulate the infinite dimensional controller and analyze the stabilizabily of the parabolic systems. We will use the following heat

equation for illustration

$$\begin{aligned} &\frac{\partial x}{\partial t}(x,t) = \frac{\partial^2 x}{\partial z^2}(x,t),\ x(z,t) = x_0(z) \\ &\frac{\partial x}{\partial z}(0,t) = 0 \\ &\frac{\partial x}{\partial z}(1,t) = 0 \end{aligned} \tag{4.1}$$

By introducing $X = \mathbf{L}_2(0,1)$ as the state space and $x(.,t) = \{x(z,t), 0 \leq z \leq 1\}$ as the state variable, and the operator A

$$\begin{aligned} Ah &= \frac{d^2h}{dz^2} \text{ with} \\ D(A) &= \{h \in \mathbf{L}_2(0,1) | h, \frac{dh}{dx} \text{ are absolutely continuous,} \\ &\quad \frac{d^2h}{dz^2} \in \mathbf{L}_2(0,1) \text{ and } \frac{dh}{dz}(0) = \frac{dh}{dz}(1) = 0\} \end{aligned} \tag{4.2}$$

the abstract formulation of (4.1) can be written as

$$\begin{aligned} \dot{x}(t) &= Ax(t) \\ x(0) &= x_0 \end{aligned} \tag{4.3}$$

The solution of the above problem is given by

$$x(z,t) = \langle x_0, 1\rangle + \sum_{n=1}^{\infty} 2e^{-n^2\pi^2 t}\langle x_0(.), \cos(n\pi.)\rangle \cos(n\pi.) \tag{4.4}$$

In (4.4), $-n^2\pi^2$, $n = 1, \cdots, \infty$ are eigenvalues of the operator A and $\cos(n\pi z)$, $n = 1, \cdots, \infty$ are the associated eigenfunctions. In general, eigenfunctions and eigenvalues of an operator $\mathcal{A}$ are found by solving the following eigenvalue problem

$$\mathcal{A}V = \lambda V \tag{4.5}$$

where λ and V are the eigenvalues and corresponding eigenfunctions of the operator $\mathcal{A}$.

By defining the following operator

$$T(t)x_0(z) = \langle x_0(z), 1\rangle + \sum_{n=1}^{\infty} 2e^{-n^2\pi^2 t}\langle x_0(z), \cos(n\pi z)\rangle \cos(n\pi z) \tag{4.6}$$

the abstract formulation of (4.4) can be written as

$$x(t) = T(t)x_0 \tag{4.7}$$

$T(t)$, maps the initial condition x_0 to the state of the dynamical system x at time t, and is the generalization of e^{At} in finite dimensional systems.

The operator A is an example of Riesz-Spectral operators. In the following, definitions of Riesz- Spectral operator, Resolvent Set and a special case of Riesz-Spectral operators (i.e. Sturm-Liouville Operator) will be provided.

Definition 4.1.1. (Curtain and Zwart, 1995) A sequence of vectors $\{\phi_n, n \geq 1\}$ in a Hilbert space Z forms a Riesz basis for Z if the following conditions hold:

(a) $\overline{span}\{\phi_n\} = Z$;

(b) There exist positive constants m and M such that for arbitrary $N \in \mathbb{N}$ and arbitrary scalars $\alpha_n, n = 1, \cdots, N$ such that

$$m \sum_{n=1}^{N} |\alpha_n|^2 \leq \| \sum_{n=1}^{N} \alpha_n \phi_n \|^2 \leq M \sum_{n=1}^{N} |\alpha_n|^2 \tag{4.8}$$

Definition 4.1.2. (Guo and Zwart, 2001) Operator A is a Riesz-Spectral operator if the following conditions hold:

(a) A is closed.

(b) Its eigenvalues are isolated and have finite multiplicity.

(c) The corresponding eigenvectors $\{\phi_n, n \geq 1\}$ form a Riesz basis in Z.

(d) The closure of $\{\lambda_n, n \geq 1\}$ is totally disconnected.

Definition 4.1.3. (Curtain and Zwart, 1995) Let A be a closed linear operator on a normed linear space X. We say that λ is in the *resolvent set* $\rho(A)$ of A, if $(\lambda I - A)^{-1}$ exists and is a bounded linear operator on a dense domain of X. $(\lambda I - A)^{-1}$ is called the *Resolvent* of A.

Theorem 4.1.1. *(Curtain and Zwart, 1995) Suppose that A is a Riesz-spectral operator with distinct eigenvalues $\{\lambda_n, n \geq 1\}$ and corresponding eigenvectors $\{\phi_n, n \geq 1\}$. Also assume that $\{\psi_n, n \geq 1\}$ are the eigenvectors of A^* such that $\langle \phi_n, \psi_n \rangle = \delta_{nm}$. Then A satisfies:*

a. $\rho(A) = \{\lambda \in \mathbb{C} | \inf_{n \geq 1} |\lambda - \lambda_n| \geq 0\}$, *and for* $\lambda \in \rho(A)$, $(\lambda I - A)^{-1}$ *is given by*

$$(\lambda I - A)^{-1} = \sum_{n=1}^{\infty} \frac{1}{\lambda - \lambda_n} \langle ., \psi_n \rangle \phi_n \tag{4.9}$$

b. A has the representation

$$Az = \sum_{n=1}^{\infty} \lambda_n \langle z, \psi_n \rangle \phi_n, \quad z \in D(A) \tag{4.10}$$

c. A is the infinitesimal generator of a C_0-semigroup if and only if $\sup_{n \geq 1} Re(\lambda_n) < \infty$ *and $T(t)$ is given by*

$$T(t) = \sum_{n=1}^{\infty} e^{\lambda_n t} \langle ., \psi_n \rangle \phi_n \tag{4.11}$$

d. The growth bound of the semigroup is given by

$$\omega_0 = \inf_{t>0} \left(\frac{1}{2} \log(\|T(t)\| \right) = \sup_{n \geq 1} Re(\lambda_n) \tag{4.12}$$

Definition 4.1.4. (Winkin *et al.*, 2000) Consider the operator $\mathcal{A}$ defined on the domain

$$\begin{aligned} D(\mathcal{A}) = \{ & f \in L^2(a,b) : f, \frac{df}{dz} \text{ absolutely continuous,} \\ & \frac{d^2 f}{dz^2} \in L^2(a,b), \text{ and } \alpha_a \frac{df}{dz}(a) + \beta_a f(a) = 0, \alpha_b \frac{df}{dz}(b) + \beta_b f(b) = 0 \} \end{aligned} \tag{4.13}$$

where a and b are real numbers, $(\alpha_a, \beta_a) \neq (0,0)$ and $(\alpha_b, \beta_b) \neq (0,0)$. $\mathcal{A}$ is said to be a Sturm-Liouville operator if

$$\forall f \in D(\mathcal{A}), \mathcal{A}f = \frac{1}{\rho(z)} \left(\frac{d}{dz} \left(-p(z) \frac{df}{dz}(z) \right) + q(z) f(z) \right) \tag{4.14}$$

Definition 4.1.5. (Winkin *et al.*, 2000) A linear state space system $\sum(A, B, C, D)$ is called a Sturm-Liouville system, if and only if $-A$ is a Sturm-Liouville operator.

4.2 LQ Control of Parabolic DPS

As mentioned in Chapter 2, LQ control is a well-known optimal control algorithm for linear state space systems of the form

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx \end{aligned} \tag{4.15}$$

and assumes a performance metric of the form

$$J(x_0, u) = \int_0^\infty \langle y(s), y(s) \rangle + \langle u(s), Ru(s) \rangle ds \tag{4.16}$$

where $u(s)$ and $y(s)$ are the input and output trajectories, respectively, and R is a self-adjoint, coercive operator in $\mathcal{L}(U)$. In order to formulate the LQ optimal control problem for a parabolic system, the model of the systems should be formulated as (4.15). In the following, the formulation of the parabolic PDEs as an infinite dimensional state space system represented by (4.15) will be discussed. As discussed before, we will assume that the nonlinear model of the system is linearized around the steady space profile of the system. Therefore, the coefficients of the reactive term are spatially varying.

Consider a system described by a set of linear parabolic PDEs in one spatial dimension:

$$\frac{\partial \theta}{\partial t} = \mathbf{D}\frac{\partial^2 \theta}{\partial z^2} - \mathbf{V}\frac{\partial \theta}{\partial z} + \mathbf{N}(z)\theta \tag{4.17}$$

with the following boundary and initial conditions

$$\begin{aligned} &\mathbf{D}\frac{\partial \theta}{\partial z}|_{z=0} = \mathbf{V}(\theta_{z=0} - \theta_{in}) \\ &\frac{\partial \theta}{\partial z}|_{z=l} = 0 \\ &\theta(z, 0) = \theta_0 \end{aligned} \tag{4.18}$$

where $\theta(., t) = [\theta_1(., t), \cdots, \theta_n(., t)]^T \in \mathcal{H} := L^2(0, l)^n$ denotes the vector of state variables, $z \in [0, l] \in \mathbb{R}$ and $t \in [0, \infty)$ denote position and time, respectively. $\mathbf{D}, \mathbf{V}, \mathbf{N}$ are matrices of appropriate sizes, whose entries are functions in $L^\infty([0, l] \times [0, \infty))$. $\mathbf{D}$

and $\mathbf{V}$ are constant diagonal matrices and $\mathbf{N}$ is a spatially varying triangular matrix. We also assume that the θ_{in} is the manipulated variable.

The system of equations (4.18) is non-self adjoint in general. In order to simplify the controller synthesis, the system of equations (4.18) can be converted to a self-adjoint diffusion-reaction system by the following transformation:

$$x = \mathbf{T}\theta = \exp(-\frac{\mathbf{D^{-1}V}}{2}z)\theta \tag{4.19}$$

The resulting system is

$$\begin{aligned}
\frac{\partial x}{\partial t} =& \mathbf{D}\frac{\partial^2 x}{\partial z^2} + (\mathbf{TN}(z)\mathbf{T^{-1}} - \frac{\mathbf{VD^{-1}V}}{4})x \\
\mathbf{D}\frac{\partial x}{\partial z}|_{z=0} &= \frac{\mathbf{V}}{2}x|_{z=0} - V\theta_{in} \\
\mathbf{D}\frac{\partial x}{\partial z}|_{z=l} &= \frac{\mathbf{V}}{2}x|_{z=l} \\
x(z,0) &= \mathbf{T^{-1}}\theta(z,0)
\end{aligned} \tag{4.20}$$

The above transformation can be performed for any set of parabolic PDEs. Therefore, without loss of generality we assume that for the rest of this work the model of the system can be described by the following set of parabolic PDEs.

$$\begin{aligned}
\frac{\partial x}{\partial t} &= \mathbf{D}\frac{\partial^2 x}{\partial z^2} + \mathbf{M}(z)x \\
\mathbf{D}\frac{\partial x}{\partial z}|_{z=0} &= \frac{\mathbf{V}}{2}x|_{z=0} - u \\
\mathbf{D}\frac{\partial x}{\partial z}|_{z=l} &= \frac{\mathbf{V}}{2}x|_{z=l} \\
x(z,0) &= x_0(z)
\end{aligned} \tag{4.21}$$

The system of equations (4.21) can be formulated as an abstract boundary control problem on the Hilbert space $\mathcal{H} := L^2(0,l)^n$ (Curtain and Zwart, 1995).

$$\begin{cases}
\frac{dx(t)}{dt} = \mathfrak{A}x(t), \\
x(0) = x_0 \\
\mathfrak{B}x(t) = u(t) \\
y(t) = \mathfrak{C}x(t)
\end{cases} \tag{4.22}$$

Where $\mathfrak{A}$ is a linear operator on the domain:

$$\mathcal{D}(\mathfrak{A}) = \{x \in H : x \text{ and } \frac{dx}{dz} \text{ are a.c. }, \frac{d^2x}{dz^2} \in H, \mathbf{D}\frac{\partial x}{\partial z}|_{z=l} = \frac{\mathbf{V}}{2}x|_{z=l}\} \tag{4.23}$$

(where a.c. means that x is absolutely continuous) and is defined by

$$\mathfrak{A} = \mathbf{D}\frac{d^2.}{dz^2} + \mathbf{M}(z).I \tag{4.24}$$

$\mathfrak{B} : \mathcal{H} \to \mathbb{R}$ is the boundary operator with the domain

$$\mathcal{D}(\mathfrak{B}) = \{x \in \mathcal{H} : x \text{ is a.c. }, \frac{dx}{dz} \in \mathcal{H}\} \tag{4.25}$$

and defined by

$$\mathfrak{B}x(.) = -\mathbf{D}\frac{dx(.)}{dz}|_{z=0} + \frac{\mathbf{V}}{2}x(.)|_{z=0} \tag{4.26}$$

and the output operator, $\mathfrak{C}$, is defined by the available measurement.

The infinite dimensional system described by (4.22), is not a well-posed infinite dimensional system. In order to convert this system into a well-posed system with bounded input and output operators, the boundary condition of the system should be converted to a homogeneous boundary condition and the input variable u should appear in the dynamical equation of the system similar to system (4.15) . In order to reformulate it to a well-posed abstract Cauchy problem, a new operator $\mathcal{A}$ is defined by:

$$\begin{aligned}
\mathcal{A}x &= \mathfrak{A}x \\
\mathcal{D}(\mathcal{A}) &= \mathcal{D}(\mathfrak{A}) \cap \ker(\mathfrak{B}) \\
&= \{x \in H : x \text{ and } \frac{dx}{dz} \text{ are a.c. }, \frac{d^2x}{dz^2} \in \mathcal{H} \\
&\qquad \text{and } \mathbf{D}\frac{\partial x(0,t)}{\partial z} - \frac{\mathbf{V}}{2}x(0,t) = 0, \mathbf{D}\frac{\partial x(l,t)}{\partial z} - \frac{\mathbf{V}}{2}x(l,t) = 0\}
\end{aligned} \tag{4.27}$$

Let us assume that $\mathcal{A}$ is the infinitesimal generator of a C_0-semigroup on $\mathcal{H}$ and there exist a B such that for all u, $Bu \in \mathcal{D}(\mathfrak{A})$, and the following holds:

$$\mathfrak{B}Bu = u, \quad u \in U \tag{4.28}$$

In other words, B should satisfy the following conditions:

$$-\mathbf{D}\frac{dB(0)}{dz} + \frac{\mathbf{V}}{2}B(0) = 1 \tag{4.29a}$$

$$\mathbf{D}\frac{\partial B(l)}{\partial z} = \frac{\mathbf{V}}{2}B(l) \tag{4.29b}$$

Condition (4.29a) is equivalent to (4.28) and the condition (4.29b) is from the assumption that $Bu \in \mathcal{D}(\mathfrak{A})$. B can be any arbitrary function that satisfies these conditions.

By defining a new input $\tilde{u}(t) = \dot{u}(t)$ and a new state $x^e(t) = \begin{bmatrix} u(t) & x(t) - Bu(t) \end{bmatrix}'$, the problem can be reformulated on the extended state space $H^e = \mathcal{H} \oplus U$ as (Curtain and Zwart, 1995):

$$\begin{aligned} \dot{x}^e(t) &= A^e x^e(t) + B^e \tilde{u}(t) \\ y^e &= C^e x^e \end{aligned} \tag{4.30}$$

where

$$A^e = \begin{bmatrix} 0 & 0 \\ \mathfrak{A}B & \mathcal{A} \end{bmatrix}, \quad B^e = \begin{bmatrix} I \\ -B \end{bmatrix}, \quad C^e = \mathfrak{C}\begin{bmatrix} B & I \end{bmatrix} \tag{4.31}$$

The infinite dimensional system (4.30) is a well-posed system with bounded input and output operators, which is an exact representation of the original infinite dimensional system (4.18). Therefore, one can design the LQ controller for the well-posed system and apply it to the original system without any approximation. Additionally, the dynamical properties of the extended system are similar to the dynamical properties of the original system. Hence, it is sufficient to study the dynamical properties of the extended system.

Optimal Control Design

In this section, a linear-quadratic optimal controller is formulated for a system described by (4.30). The state-feedback controller assumes that full state measurement is available. The existence of the solution for the LQ control problem

requires that the linear system is exponentially stabilizable and detectable. These two properties will be investigated and in the following sections it will be proven that the infinite dimensional system (4.30) is a Riesz-Spectral system. In this section, we will use the spectral properties of Riesz-Spectral systems to solve the LQ control problem.

The linear quadratic control problem on an inifinite-time horizon employs the cost function:

$$J(x_0, u) = \int_0^\infty \langle y(s), y(s)\rangle + \langle u(s), Ru(s)\rangle ds \tag{4.32}$$

where $u(s)$ and $y(s)$ are the input and output trajectories, respectively, and R is a self-adjoint, coercive operator in $\mathcal{L}(U)$. The output function $y(\cdot)$ is given by Equation (4.30).

It is well-known that the solution of this optimal control problem can be obtained by solving the following algebraic Riccati equation (ARE) (Curtain and Zwart, 1995):

$$\langle A^e x_1, \Pi x_2\rangle + \langle \Pi x_1, A^e x_2\rangle + \langle C^e x_1, C^e x_2\rangle - \langle B^{e^*}\Pi x_1, R^{-1}B^{e^*}\Pi x_2\rangle = 0 \tag{4.33}$$

When (A^e, B^e) is exponentially stabilizable and (C^e, A^e) is exponentially detectable, the algebraic Riccati equation (4.33) has a unique nonnegative self-adjoint solution $\Pi \in \mathcal{L}(\mathcal{H})$ and for any initial state $x_0 \in \mathcal{H}$ the quadratic cost (4.32) is minimized by the unique control u_{opt} given by:

$$u_{opt}(s; x_0) = -R^{-1}B^{e^*}\Pi x_{opt}(s), \quad x_{opt}(s) = T_{-B^eR^{-1}B^{e^*}\Pi}(s)x(0) \tag{4.34}$$

In addition, the optimal cost is given by $J(x_0, u_{opt}) = \langle x_0, \Pi x_0\rangle$.

The ARE (4.33) is valid for any infinite dimensional system, but depending on the characteristics of the infinite dimensional system different approaches are needed to solve it. For Riesz spectral systems, the spectral properties of the system can be used to solve the ARE (4.33). Let us denote by ϕ_n, the normalized eigenfunctions of A^e. If we take $z_1 = \phi_m$ and $z_2 = \phi_n$, then the Riccati equation (4.33) becomes:

$$\langle A^e\phi_n, \Pi\phi_m\rangle + \langle \Pi\phi_n, A^e\phi_m\rangle + \langle C^e\phi_n, C^e\phi_m\rangle - \langle B^{e^*}\Pi\phi_n, R^{-1}B^{e^*}\Pi\phi_m\rangle = 0 \tag{4.35}$$

If we assume that the solution Π has the form $\Pi z = \sum_{n,m}\Pi_{nm}\langle z, \psi_m\rangle\psi_n$ where $\Pi_{nm} = \langle \phi_n, \Pi\phi_m\rangle$, then Equation (4.35) becomes the system of infinite number of

coupled scalar equations:

$$(\sigma_n + \sigma_m)\Pi_{nm} + C_{nm} - \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\Pi_{nk}\Pi_{lm}B_{nm} = 0 \tag{4.36}$$

where $C_{nm} = \langle C^e\phi_n, C^e\phi_m\rangle$, and $B_{nm} = \langle R^{-1}B^e\psi_n, B^e\psi_m\rangle$.

Using the spectral properties of the Riesz Spectral systems, the operator Riccati equation (4.33) is converted to a set of coupled algebraic equations that can be solved by any numerical algorithm. Then the main step to solve the optimal control problem for these systems is to calculate the spectrum of the operator A^e. This can be performed by solving the eigenvalue problem for the operator A^e. In the following section, the solution of the eigenvalue problem for system of Equation (4.30) will be studied.

4.2.1 Eigenvalue Problem

This section is devoted to solving the eigenvalue problem of an infinite dimensional system given by equation (4.30). The analytical solution of the eigenvalue problem for a general form of the operator A^e is not possible. In this work, it is assumed that the matrix $\mathbf{M}(z)$ of the operator $\mathfrak{A}$ has a triangular form. This assumption is true if there is only one way coupling between state variables. For example, in the case of systems with two state variables x_1 and x_2, the one way coupling means that x_1 is a function of x_2, but x_2 is independent of x_1. For most chemical engineering processes the operator A^e can be converted to a triangularized form using a transformation. Also, without loss of generality, the eigenvalue problem is solved for a case with two state variables. The extension of solution for more than two state variables is straightforward. The eigenvalue problem of interest will be:

$$A^e\phi = \lambda\phi \tag{4.37}$$

where A^e has the following form:

$$A^e = \begin{bmatrix} 0 & 0 \\ \mathfrak{A}B & \mathcal{A} \end{bmatrix} \tag{4.38}$$

and

$$\mathcal{A} = \begin{bmatrix} A_{11} & 0 \\ A_{12} & A_{22} \end{bmatrix} = \begin{bmatrix} D_{11}\frac{d^2.}{dz^2} + M_{11}(.) & 0 \\ M_{21}(.) & D_{22}\frac{d^2.}{dz^2} + M_{22}(.) \end{bmatrix} \tag{4.39}$$

Eigenvalues and eigenfunctions of A_{11} and A_{22}

A_{11} and A_{22} are both self-adjoint Sturm-Liouville operators. Assuming that the operators A_{11} and A_{22} were Sturm-Liouville operators with constant coefficients of the form

$$\begin{aligned} &\frac{\partial \vartheta}{\partial t} = D\frac{\partial^2 \vartheta}{\partial^2 z} + M\vartheta \\ &D\frac{\partial \vartheta(0,t)}{\partial z} = \frac{V}{2}\vartheta \\ &D\frac{\partial \vartheta(L,t)}{\partial z} = -\frac{V}{2}\vartheta(L,t) \end{aligned} \tag{4.40}$$

their eigenvalues would be given by:

$$\mu_n^2 = D\omega_n^2 + M \tag{4.41}$$

where ω_n is the solution to the following equation:

$$\tan(\omega l) = \frac{4D\omega V}{4D^2\omega^2 - V^2} \tag{4.42}$$

and the corresponding eigenfunctions are given by:

$$\psi_n = \cos(\omega_n z) + \frac{V}{2D\omega_n}\sin(\omega_n z) \tag{4.43}$$

Recall that the linearization of nonlinear equations around the steady state profile results in equations with spatially varying coefficients. Therefore, calculation of the spectrum of the operator A_{ii} is a challenging issue. In this work, the method of solving the heat equation for composite media (Friedman, 1976) is adopted to solve the eigenvalue problem for a Sturm-Liouville operator with spatially varying coefficients. In this approach, the length of the reactor is divided into a finite number of segments. It is assumed that within each segment, the values of coefficients are constant. Figure 4.1 illustrates the discretization method. The mathematical formulation of this approach can be given as (de. Monte, 2002):

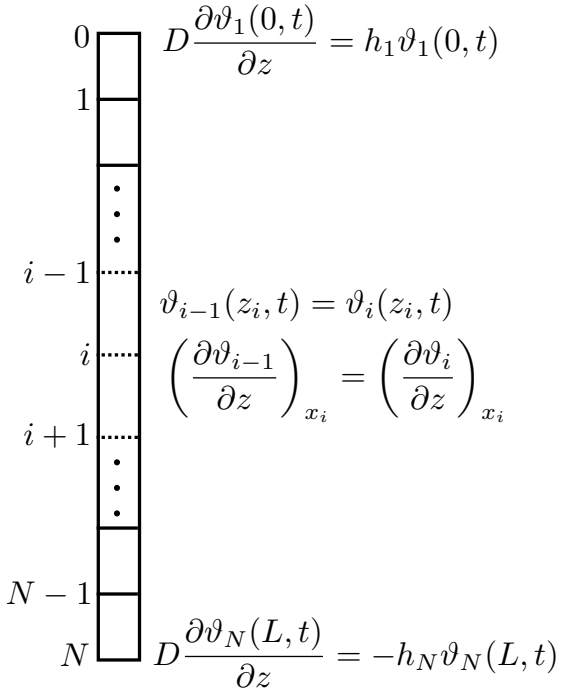


Figure 4.1: Approximation of the reactor as a composite media

$$\frac{\partial \vartheta_i}{\partial t} = D\frac{\partial^2 \vartheta_i}{\partial^2 z} + k_i\vartheta_i, \quad \vartheta_i = x_1(z), z \in [z_{i-1}, z_i],\ i = 1, \cdots, N \tag{4.44}$$

The boundary condition at $z = 0$ is:

$$D\frac{\partial \vartheta_1(0,t)}{\partial z} = h_1\vartheta_1(0,t), \quad h_1 = \frac{v}{2} \tag{4.45}$$

The continuity boundary conditions are:

$$\vartheta_{i-1}(z_i,t) = \vartheta_i(z_i,t) \quad (i = 2, 3, \cdots, N) \tag{4.46}$$

$$\left(\frac{\partial \vartheta_{i-1}}{\partial z}\right)_{x_i} = \left(\frac{\partial \vartheta_i}{\partial z}\right)_{x_i} \quad (i = 2, 3, \cdots, N) \tag{4.47}$$

The boundary condition at $x = L$ is:

$$D\frac{\partial \vartheta_N(L,t)}{\partial z} = -h_N\vartheta_N(L,t), \quad h_N = \frac{v}{2} \tag{4.48}$$

The continuity conditions at the boundary imply that, at the interfaces of the segments, the concentration and the flux are equal. This approach results in a set of N

PDEs coupled through boundaries. The PDEs should be solved for each segment with unspecified boundary data at the interfaces. Then, the solutions can be determined by applying the continuity conditions.

Equations (4.44)-(4.48) can be solved by the method of separation of variables. We will have:

$$\vartheta_i(z,t) = Z_i(z)G_i(t), \quad z \in [z_i, z_{i+1}] \tag{4.49}$$

Substituting the above equation in the original PDE, we obtain:

$$D\frac{\partial^2 Z_i}{\partial^2 z} + k_i Z_i = -\lambda_i^2 Z_i \tag{4.50}$$

which can be written as:

$$D\frac{\partial^2 Z_i}{\partial^2 z} + \varpi_i^2 Z_i = 0, \quad \varpi_i^2 = k_i + \lambda_i^2; \tag{4.51}$$

Eigenfunctions associated with Equation (4.51) have the form:

$$Z_i(z) = a_i \sin(\varpi_i x) + b_i \cos(\varpi_i x) \tag{4.52}$$

a_i and b_i are integration constants and should be calculated by the boundary conditions at each segment. Since the PDEs are coupled through boundary conditions these coefficients should be calculated simultaneously. Finally, Z_i can be obtained as (de. Monte, 2002):

$$Z_i(z) = a_1 \Phi_i(\varpi_i) \left(\sin(\varpi_i z) + \Gamma_i \cos(\varpi_i z)\right), \quad z \in [z_i,\ z_{i+1}] \tag{4.53}$$

where

$$\Phi_1 = 1; \quad \Phi_i(\varpi_1, \cdots, \varpi_i) = \Phi_{i,i-1}\Phi_{i-1,i-2}\cdots\Phi_{2,1} \tag{4.54}$$

and

$$\Phi_{i,i-1}(\varpi_1, \cdots, \varpi_i) = \frac{(\sin(\varpi_{i-1} z_i) + \Gamma_{i-1}\cos(\varpi_{i-1} z_i))}{(\sin(\varpi_i z_i) + \Gamma_i \cos(\varpi_i z_i))} \tag{4.55a}$$

$$\Phi_{M,M-1}(\varpi_1, \cdots, \varpi_M) = \frac{1}{k_M}\frac{(\cos(\varpi_{M-1} z_i) - \Gamma_{M-1}\sin(\varpi_{M-1} z_M))}{(\cos(\varpi_M z_M) - \Gamma_M \sin(\varpi_M z_M))} \tag{4.55b}$$

$$\Gamma_1 = -\frac{h_1 \sin(\varpi_1 z_1) - k_1 \varpi_1 \cos(\varpi_1 z_1)}{h_1 \cos(\varpi_1 z_1) + k_1 \varpi_1 \sin(\varpi_1 z_1)} \tag{4.56a}$$

$$\Gamma_i = \frac{\left[\begin{array}{c} \cos(\varpi_i z_i)\left(\sin(\varpi_{i-1} z_i) + \Gamma_{i-1}\cos(\varpi_{i-1} z_i)\right) \\ -\sin(\varpi_i z_i)\left(\cos(\varpi_{i-1} z_i) - \Gamma_{i-1}\sin(\varpi_{i-1} z_i)\right) \end{array}\right]}{\left[\begin{array}{c} \sin(\varpi_i z_i)\left(\sin(\varpi_{i-1} z_i) + \Gamma_{i-1}\cos(\varpi_{i-1} z_i)\right) \\ +\cos(\varpi_i z_i)\left(\cos(\varpi_{i-1} z_i) - \Gamma_{i-1}\sin(\varpi_{i-1} z_i)\right) \end{array}\right]} \tag{4.56b}$$

$$\Gamma_M = -\frac{h_{M+1} \sin(\varpi_M z_{M+1}) + k_M \varpi_M \cos(\varpi_M z_{M+1})}{h_{M+1} \cos(\varpi_M z_{M+1}) - k_M \varpi_i \sin(\varpi_M z_{M+1})} \tag{4.56c}$$

Γ_M can be evaluated by both Equation (4.56b) for $i = M$ and Equation (4.56c). Therefore, one can compute λ by comparing these equations. A solution can be obtained by using numerical or graphical methods. There are an infinite number of eigenvalues satisfying this condition and each has a corresponding eigenfunction of the form given in Equation (4.53).

Eigenvalues and eigenfunctions of the operator $\mathcal{A}$

The operator $\mathcal{A}$ is triangular and therefore, its eigenvalues consist of eigenvalues of A_{11} and A_{22}, $\sigma(\mathcal{A}) = \sigma(A_{11}) \cup \sigma(A_{22})$. Let λ_n and χ_n be eigenvalues and eigenfunctions of the operators A_{11} and μ_n and ψ_n be eigenvalues and eigenfunctions of the operator A_{22} computed by the method described in section 4.2.1. Hence, $\sigma(\mathcal{A})$ is given by:

$$\sigma_{2n+1} = \lambda_n, \quad \text{for } n \geq 0 \tag{4.57}$$

$$\sigma_{2n} = \mu_n, \quad \text{for } n \geq 1 \tag{4.58}$$

The corresponding eigenvectors can be found by solving the eigenvalue problem for the operator $\mathcal{A}$. For example, if we define $\phi_{2n+1} = \begin{bmatrix} \varsigma_{1,n} \\ \varsigma_{2,n} \end{bmatrix}$ as eigenvectors associated with σ_{2n+1} we have

$$\mathcal{A}\phi_{2n+1} = \sigma_{2n+1}\phi_{2n+1}$$

$$\begin{bmatrix} A_{11} & 0 \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} \varsigma_{1,n} \\ \varsigma_{2,n} \end{bmatrix} = \lambda_n \begin{bmatrix} \varsigma_{1,n} \\ \varsigma_{2,n} \end{bmatrix} \tag{4.59}$$

Equation (4.59) simplifies to

$$A_{11}\varsigma_{1,n} = \lambda_n \varsigma_{1,n} \tag{4.60a}$$

$$A_{21}\varsigma_{1,n} + A_{22}\varsigma_{2,n} = \lambda_n \varsigma_{2,n} \tag{4.60b}$$

Equation (4.60a) implies that $\varsigma_{1,n}$ is eigenfunction of A_{11} or $\varsigma_{1,n} = \chi_n$. Rearranging Equation (4.60b) results in

$$\varsigma_{2,n} = (\lambda_n - A_{22})^{-1} A_{21} \chi_n \tag{4.61}$$

Therefore

$$\phi_{2n+1} = \begin{bmatrix} \chi_n \\ (\lambda_n I - A_{22})^{-1} A_{21} \chi_n \end{bmatrix} \tag{4.62}$$

Following the same approach for σ_{2n} results in

$$\phi_{2n} = \begin{bmatrix} 0 \\ \psi_n \end{bmatrix} \tag{4.63}$$

The corresponding biorthonormal eigenfunctions can be computed by a similar approach and are:

$$\Psi_{2n+1} = \begin{bmatrix} \chi_n \\ 0 \end{bmatrix} \tag{4.64}$$

$$\Psi_{2n} = \begin{bmatrix} (\mu_n I - A_{11})^{-1} A_{21} \psi_n \\ \psi_n \end{bmatrix} \tag{4.65}$$

In the equations above, $(\mu_n I - A_{11})^{-1}$ and $(\lambda_n I - A_{22})^{-1}$ are the resolvents of the operators A_{11} and A_{22}, respectively, and can be calculated using Equation (4.9)

$$(\mu_n I - A_{11})^{-1} A_{21} \psi_n = \sum_{m=0}^{\infty} \frac{1}{\mu_n - \lambda_m} \langle A_{21}\psi_n, \chi_m \rangle \chi_m$$

$$(\lambda_n I - A_{22})^{-1} A_{21} \chi_n = \sum_{m=0}^{\infty} \frac{1}{\lambda_n - \mu_m} \langle A_{21}\chi_n, \psi_m \rangle \psi_m$$

Eigenvalues and eigenfunctions of the operator A^e

A^e is a triangular operator with $\mathcal{A}$ and 0 as its diagonal elements, therefore $\sigma(A^e) = \sigma(A) \cup \{0\}$. The multiplicity of $\{0\}$ is denoted by r_0 and is equal to the number

of manipulated variables. Following a similar approach to the previous section, the corresponding eigenfunctions on the extended space are given by

$$\tilde{\phi_{i0}} = \begin{bmatrix} e_i \\ -\mathcal{A}^{-1}(\mathfrak{A}B) \end{bmatrix} = \begin{bmatrix} e_i \\ \sum_{m=0}^{\infty} \frac{1}{\sigma_m} \langle \mathfrak{A}B, \Psi_m \rangle \phi_m \end{bmatrix}, \quad i = 1, \ldots, r_0 \tag{4.66}$$

and

$$\tilde{\phi_n} = \begin{bmatrix} 0 \\ \phi_n \end{bmatrix}, \quad n \geq 1 \tag{4.67}$$

where ϕ_n is the eigenfunction of the operator $\mathcal{A}$ and $e_i, i = 1, \ldots, m$ is the orthonormal basis function for U. Calculation of the associated biorthonormal eigenfunctions is straightforward and are given by:

$$\hat{\Psi}_{i0} = \begin{bmatrix} e_i \\ 0 \end{bmatrix}, \quad i = 1, \ldots, r_0$$

$$\hat{\Psi}_n = \begin{bmatrix} \frac{1}{\sigma_n} (\mathfrak{A}B)^* \Psi_n \\ \Psi_n \end{bmatrix}$$

where σ_n and Ψ_n are the eigenvalues and the corresponding eigenfunctions of A^*. In the equations above, $\tilde{\phi_{i0}}$ and $\hat{\Psi}_{i0}$ are corresponding eigenfunctions and biorthonormal eigenfunctions corresponding to eigenvalues equal to 0.

4.3 Stability Analysis

Theorem 4.3.1. *Consider the family of operators* $\{A^e(t)\}_{t \geq 0}$ *given by Equations* (4.38)-(4.39). *Then,* $\{A^e(t)\}_{t \geq 0}$ *is a stable family of infinitesimal generators of* C_0*-semigroup on* H.

Proof. Operator $\mathcal{A}$ has a lower triangular form and the diagonal elements of $-\mathcal{A}$ are Sturm-Liouville operators. Therefore, A_{11}, A_{22} are the infinitesimal generators of C_0-semigroups T_{11} and T_{22}, respectively (Winkin *et al.* (2000), Delattre *et al.* (2003)). As discussed in §4.2.1, eigenvalues of $\mathcal{A}$ consist of eigenvalues of A_{11} and A_{22}. Therefore, the operator $\mathcal{A}$ has real, countable and distinct eigenvalues. Furthermore, eigenfunctions of $\mathcal{A}$ and its adjoint are biorthogonal. Thus, the operator $\mathcal{A}$ is a Riesz

spectral operator(Delattre *et al.*, 2003). By (Curtain and Zwart, 1995), Lemma 3.2.2, the operator $\mathcal{A}$ is the infinitesimal generator of the C_0-semigroup T given by

$$T(t) = \begin{bmatrix} T_{11}(t) & 0 \\ T_{21}(t) & T_{22}(t) \end{bmatrix} \tag{4.68}$$

where

$$T_{21}(t)x_1 = \int_0^t T_{22}(t-s)A_{21}T_{11}(s)x_1 ds \tag{4.69}$$

By the same approach, one can deduce that the operator A^e is a Riesz spectral operator and generates a C_0- semigroup given by:

$$T^e(t) = \begin{bmatrix} I & 0 \\ S(t) & T(t) \end{bmatrix} \tag{4.70}$$

where $S(t)x = \int_0^t T(s)\mathfrak{A}Bxds$, and $T(t)$ is the C_0-semigroup generated by $\mathcal{A}$. ■

Theorem 4.3.2. *Consider the state linear system $\sum(A, B, -)$, where A is a Riesz-Spectral operator on the Hilbert space Z with the representation*

$$Az = \sum_{n=1}^{\infty} \lambda_n \sum_{j=1}^{r_n} \langle z, \psi_{nj}\rangle \phi_{nj} \tag{4.71}$$

$\{\lambda_n, n \geq 1\}$ are eigenvalues of A with finite multiplicity r_n, and $\{\phi_{nj}, j = 1, \cdots, r_n, n \geq 1\}$ and $\{\psi_{nj}, j = 1, \cdots, r_n, n \geq 1\}$ are generalized eigenfunctions of A and A^*, respectively. B is a finite rank operator defined by

$$Bu = \sum_{i=1}^{m} b_i u_i, \quad \text{where } b_i \in Z \tag{4.72}$$

Necessary and sufficient conditions for $\sum(A, B, -)$ to be β-exponentially stabilizable are that there exists an $\epsilon > 0$ such that $\sigma^+_{\beta-\epsilon}(A)$comprises, at most, finitely many eigenvalues and

$$rank \begin{pmatrix} \langle b_1, \psi_{n_1}\rangle & \cdots & \langle b_m, \psi_{n_1}\rangle \\ \vdots & & \vdots \\ \langle b_1, \psi_{n_{rn}}\rangle & \cdots & \langle b_m, \psi_{n_{rn}}\rangle \end{pmatrix} = r_n \tag{4.73}$$

for all n such that $\lambda_n \in \sigma^+_{\beta-\epsilon}(A)$.

Proof. Since $\sigma^+_{\beta-\epsilon}(A)$ comprises at most finitely many eigenvalues, $Z^+_{\beta-\epsilon}$ is finite dimensional. Therefore, A satisfies the spectrum decomposition assumption (Curtain and Zwart, 1995) and the corresponding spectral projection on the finite dimensional subspace $Z^+_{\beta-\epsilon}$ is given by

$$P_{\beta-\epsilon}z = \frac{1}{2\pi j}\int_{\Gamma_{\beta-\epsilon}} (\lambda I - A)^{-1} z d\lambda = \sum_{\lambda_i \in \sigma^+_{\beta-\epsilon}} \sum_{j=1}^{r_n} \langle z, \psi_{n_j}\rangle \phi_{n_j} \tag{4.74}$$

It can easily be calculated that

$$Z^+_{\beta-\epsilon} = \operatorname*{span}_{\lambda_n \in \sigma^+_{\beta-\epsilon}} \{\phi_{n_j}, j = 1, \cdots, r_n\} \tag{4.75}$$

$$Z^-_{\beta-\epsilon} = \operatorname*{\overline{span}}_{\lambda_n \in \sigma^-_{\beta-\epsilon}} \{\phi_{n_j}, j = 1, \cdots, r_n\} \tag{4.76}$$

$$T^-_{\beta-\epsilon}(t)z = \sum_{\lambda_n \in \sigma^-_{\beta-\epsilon}} e^{\lambda_n t} \sum_{j=1}^{r_n} \langle z, \psi_{n_j}\rangle \phi_{n_j} \tag{4.77}$$

$$A^+_{\beta-\epsilon}z = \sum_{\lambda_n \in \sigma^+_{\beta-\epsilon}} \lambda_n \sum_{j=1}^{r_n} \langle z, \psi_{n_j}\rangle \phi_{n_j} \tag{4.78}$$

$$B^+_{\beta-\epsilon}u = \sum_{\lambda_n \in \sigma^+_{\beta-\epsilon}} \sum_{j=1}^{r_n} \langle Bu, \psi_{n_j}\rangle \phi_{n_j} \tag{4.79}$$

$T^-_{\beta-\epsilon}(t)$ satisfies the spectrum determined growth assumption and is β-exponentially stable. Now we need to show that the finite dimensional system $\sum(A^+_{\beta-\epsilon}, B^+_{\beta-\epsilon}, -)$ is controllable, which is equivalent to proving that the reachability subspace of $\sum(A^+_{\beta-\epsilon}, B^+_{\beta-\epsilon}, -)$ is dense in $Z^+_{\beta-\epsilon}$. From Curtain and Zwart (1995, Definition A.2.29), $\mathcal{R}$ is dense in $Z^+_{\beta-\epsilon}$ if and only if $\mathcal{R}^\perp = \{0\}$ where $\mathcal{R}^\perp$ is the orthogonal complement of $\mathcal{R}$. $\mathcal{R}$ and $\mathcal{R}^\perp$ are given by

$$\begin{aligned}\mathcal{R} := \{z \in Z^+_{\beta-\epsilon} |\ &\text{there exist } \tau > 0 \text{ and } u \in L_2([0,\tau]; U) \\ &\text{such that } z = \int_0^\tau T^+_{\beta-\epsilon}(\tau - s) B^+_{\beta-\epsilon} u(s) ds\}\end{aligned} \tag{4.80}$$

$$\mathcal{R}^\perp = \{x \in Z^+_{\beta-\epsilon} | \langle x, y\rangle = 0 \text{ for all } y \in \mathcal{R}\} \tag{4.81}$$

In order to have $\mathcal{R}^{\perp} = \{0\}$, there should be no $x \in Z^{+}_{\beta-\epsilon}$ that is orthogonal to the reachability subspace $\mathcal{R}$. This means that for every $x \in Z^{+}_{\beta-\epsilon}$, there is a u such that $\langle x, \int_0^{\tau} T^{+}_{\beta-\epsilon}(\tau - s) B^{+}_{\beta-\epsilon} u(s) ds \rangle \neq 0$. It can be shown that this condition is equivalent to

$$\sum_{\lambda_n} e^{\lambda_n(\tau-s)} \sum_{j=1}^{r_n} \langle x, \phi_{n_j} \rangle \langle Bu, \psi_{n_j} \rangle \neq 0 \tag{4.82}$$

Thus for every $\lambda_n \in \sigma^{+}$ and $j = 1, \cdots, r_n$ there exists a u such that $\sum_{j=1}^{r_n} \langle x, \phi_{n_j} \rangle \langle Bu, \psi_{n_j} \rangle \neq 0$. This condition is equivalent to

$$B_n U_n \neq 0 \tag{4.83}$$

$$B_n = \begin{bmatrix} \langle b_1, \psi_{n_1} \rangle & \langle b_2, \psi_{n_1} \rangle & \cdots & \langle b_m, \psi_{n_1} \rangle \\ \langle b_1, \psi_{n_2} \rangle & \langle b_2, \psi_{n_2} \rangle & \cdots & \langle b_m, \psi_{n_2} \rangle \\ \vdots & \vdots & & \vdots \\ \langle b_1, \psi_{n_r n} \rangle & \langle b_2, \psi_{n_r n} \rangle & \cdots & \langle b_m, \psi_{n_r n} \rangle \end{bmatrix} \tag{4.84}$$

$$U_n = \begin{bmatrix} \langle u_1, \psi_{n_1} \rangle & \langle u_1, \psi_{n_r n} \rangle & \cdots & \langle u_1, \psi_{n_r n} \rangle \\ \langle u_2, \psi_{n_1} \rangle & \langle u_2, \psi_{n_2} \rangle & \cdots & \langle u_2, \psi_{n_r n} \rangle \\ \vdots & \vdots & & \vdots \\ \langle u_m, \psi_{n_1} \rangle & \langle u_m, \psi_{n_2} \rangle & \cdots & \langle u_m, \psi_{n_r n} \rangle \end{bmatrix} \tag{4.85}$$

If $\text{rank}(B_n) < r_n$, there exists a $u \neq 0$ such that $B_n U_n = 0$. Thus, the system is uncontrollable if $\text{rank}(B_n) < r_n$. If $\text{rank}(B_n) = r_n$, the only solution for $B_n U_n = 0$ is $u = 0$ and therefore $\mathcal{R}^{\perp} = \{0\}$ and the system is controllable.

By duality, $\sum(A, -, C)$ is β-exponentially detectable, if $\sum(A^*, C^*, -)$ is β-exponentially stabilizable. Similarly, the system $\sum(A^e, -, C^e)$ is β-exponentially detectable. ∎

Remark 4.3.1. Consider the infinite dimensional system $\sum(A^e, B^e, C^e)$ given by Equation (4.30). As discussed in §4.2.1, the eigenvalues of A^e consist of eigenvalues of $\mathcal{A}$ and 0 with finite multiplicity m. Since the diagonal entries of $\mathcal{A}$ are Sturm-Liouville operators, the spectrum of $\mathcal{A}$ is finitely bounded (i.e., there exists a ω such that all $\lambda \in \sigma(\mathcal{A}) < \omega$). Therefore, for any arbitraty β, $\sigma^{+}_{\beta-\epsilon}(A^e)$ comprises finitely

many eigenvalues and the first condition of Theorem (4.3.2) holds. The condition (4.73) depends on the choice of B and should be verified for each case study.

4.4 Case Study: A Fixed-Bed Reactor with Axial Dispersion

In this section, the proposed linear-quadratic optimal controller is applied to a tubular catalytic cracking reactor. This process involves axial dispersion, convection and reactions, and can be modelled by a set of parabolic equations. The controller is used to regulate the distribution of the concentration of gasoline along the length of the reactor by manipulating the inlet concentration.

4.4.1 Model Description

The model that is used to describe the catalytic cracking reactor is developed by Froment (1990). This simplified model of the system considers three lumped components: feed (gas oil), gasoline fraction and the remaining products (e.g., butanes, coke, dry gas). The reaction scheme is as following

$$\begin{aligned} A &\xrightarrow{k_1} B \xrightarrow{k_2} C \\ A &\xrightarrow{k_3} C \end{aligned} \tag{4.86}$$

where A represents gas oil, B gasoline, and C other products. The rate equations are (Weekman, 1969):

$$\begin{aligned} r_A &= -(k_1 + k_3) y_A^2 = -k_0 y_A^2 \\ r_B &= k_1 y_A^2 - k_2 y_B \end{aligned} \tag{4.87}$$

The schematic diagram of the reactor is shown in Figure 4.2. To model the reactor, an isothermal process is considered. Therefore the dynamics of the system are described by the following parabolic partial differential equations (PDEs) representing

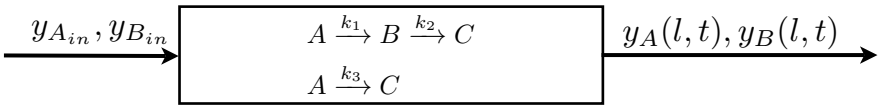


Figure 4.2: Schematic diagram of the catalytic cracking reactor

the component balances within the reactor:

$$\begin{aligned} \frac{\partial y_A}{\partial t} &= D_a \frac{\partial^2 y_A}{\partial z^2} - v\frac{\partial y_A}{\partial z} + r_A, \\ \frac{\partial y_B}{\partial t} &= D_a \frac{\partial^2 y_B}{\partial z^2} - v\frac{\partial y_B}{\partial z} + r_B \end{aligned} \tag{4.88}$$

Initial and boundary conditions are:

$$\begin{aligned} D_a \frac{\partial y_A}{\partial z}|_{z=0} &= v(y_A|_{z=0} - y_{A_{in}}), \\ D_a \frac{\partial y_B}{\partial z}|_{z=0} &= v(y_B|_{z=0} - y_{B_{in}}), \\ \frac{\partial y_A}{\partial z}|_{z=l} &= 0, \\ \frac{\partial y_B}{\partial z}|_{z=l} &= 0, \\ y_A(z,0) &= y_{A_0}(z), \\ y_B(z,0) &= y_{B_0}(z) \end{aligned} \tag{4.89}$$

In the equations above, $y_A, y_B, D_a, v, y_{A_{in}}$, and $y_{B_{in}}$ denote the weight fractions of reactant A and B, the axial dispersion coefficient, the superficial velocity, the inlet weight fraction of component A, and the inlet weight fraction of component B, respectively.

The corresponding steady-state equations of the PDE model defined by Equation (4.88) are given by the following ordinary differential equations:

$$\begin{aligned} D_a \frac{\partial^2 y_{A_{ss}}}{\partial z^2} - v\frac{\partial y_{A_{ss}}}{\partial z} - k_0 y_{A_{ss}}^2 &= 0, \\ D_a \frac{\partial^2 y_{B_{ss}}}{\partial z^2} - v\frac{\partial y_{B_{ss}}}{\partial z} + k_1 y_{A_{ss}}^2 - k_2 y_{B_{ss}} &= 0 \end{aligned} \tag{4.90}$$

Linearized model

Let us define the following state variables:

$$\theta(t) = \begin{bmatrix} y_A - y_{A_{ss}} \\ y_B - y_{B_{ss}} \end{bmatrix} \tag{4.91}$$

and assuming the inlet weight fraction of A, $y_{A_{in}}$ as the manipulated variable, the new input is:

$$u(t) = v(y_{A_{in}} - y_{A_{in,ss}}) \tag{4.92}$$

Then, the nonlinear system given in Equation (4.88) can be linearized around its steady state profile to yield:

$$\frac{\partial}{\partial t}\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} D_a\frac{\partial^2}{\partial z^2} - v\frac{\partial}{\partial z} - 2k_0 y_{A_{ss}} & 0 \\ 2k_1 y_{A_{ss}} & D_a\frac{\partial^2}{\partial z^2} - v\frac{\partial}{\partial z} - k_2 \end{bmatrix}\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \tag{4.93}$$

with the initial and boundary conditions:

$$\begin{aligned} D_a\frac{\partial}{\partial z}\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{z=0} &= v\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{z=0} - \begin{bmatrix} u \\ 0 \end{bmatrix}, \\ D_a\frac{\partial}{\partial z}\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{z=l} &= \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \\ \theta(z,0) = \theta_0 &= \begin{bmatrix} \theta_{1_0}(z) \\ \theta_{2_0}(z) \end{bmatrix} = \begin{bmatrix} y_{A_0} - y_{A_{ss}} \\ y_{A_0} - y_{A_{ss}} \end{bmatrix} \end{aligned} \tag{4.94}$$

The linearized model given by Equation (4.93) is a set of linear Sturm-Liouville equations and can be converted into a diffusion-reaction system with the transformation given in Equation (4.19). The resulting equations are:

$$\frac{\partial}{\partial t}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} D_a\frac{\partial^2}{\partial z^2} - \hat{k}_1(z) & 0 \\ 2k_1 y_{A_{ss}}(z) & D_a\frac{\partial^2}{\partial z^2} - \hat{k}_2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \tag{4.95}$$

with the following boundary and initial conditions:

$$\begin{aligned} D_a\frac{\partial}{\partial z}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{z=0} &= \frac{v}{2}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{z=0} - \begin{bmatrix} u \\ 0 \end{bmatrix} \\ D_a\frac{\partial}{\partial z}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{z=l} &= -\frac{v}{2}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{z=l} \\ x(z,0) &= x_0 \end{aligned} \tag{4.96}$$

where $x_0 = e^{-\frac{v}{2D}z}\theta_0$, $\hat{k}_1(z) = -\frac{v^2}{4D_a} - 2k_0 y_{A_{ss}}(z)$, and $\hat{k}_2 = -\frac{v^2}{4D_a} - k_2$.

Infinite-Dimensional representation

Equations (4.95)-(4.96) can be formulated as an abstract boundary control problem on the Hilbert space $H := L^2(0,l) \times L^2(0,l)$ given by (4.22),

The operator $\mathfrak{A}$ is given as follows:

$$\mathfrak{A} = \begin{bmatrix} D_a \frac{d^2}{dz^2} - \hat{k}_1(z) & 0 \\ 2k_1 y_{A_{ss}}(z) & D_a \frac{d^2}{dz^2} - \hat{k_2} \end{bmatrix} := \begin{bmatrix} A_{11} & 0 \\ A_{21} & A_{22} \end{bmatrix} \tag{4.97}$$

with the domain:

$$\mathcal{D}(\mathfrak{A}) = \{x \in H : x \text{ and } \frac{dx}{dz} \text{ are a.c. }, \frac{d^2x}{dz^2} \in H \text{ and } D_a \frac{\partial x_1(l,t)}{\partial z} + \frac{v}{2} x_1(l,t) = 0, \tag{4.98}$$

$$D_a \frac{\partial x_2(0,t)}{\partial z} - \frac{v}{2} x_2(0,t) = 0,\ D_a \frac{\partial x_2(l,t)}{\partial z} + \frac{v}{2} x_2(l,t) = 0\} \tag{4.99}$$

where a.c. means that x is absolutely continuous. The boundary operator $\mathfrak{B} : H \to R$ is given as:

$$\mathfrak{B}x(z) = \begin{bmatrix} -D_a \frac{d}{dz} + \frac{v}{2} & 0 \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} \tag{4.100}$$

with the domain:

$$\mathcal{D}(\mathfrak{B}) = \{x \in H : x \text{ is a.c. }, \frac{dx}{dz} \in H\} \tag{4.101}$$

and the output operator, $\mathfrak{C}$, is defined by the available measurement.

This abstract boundary control problem is transformed to a well-posed system as discussed in section §4.2. The new operator $\mathcal{A}$ is defined by:

$$\begin{aligned} \mathcal{A}x &= \mathfrak{A}x \\ \mathcal{D}(\mathcal{A}) &= \mathcal{D}(\mathfrak{A}) \cap \ker(\mathfrak{B}) \\ &= \{x \in H : x \text{ and } \frac{dx}{dz} \text{ are a.c. }, \frac{d^2x}{dz^2} \in H \\ &\qquad \text{and } D_a \frac{\partial x(0,t)}{\partial z} + \frac{v}{2} x(0,t) = 0,\ D_a \frac{\partial x(l,t)}{\partial z} + \frac{v}{2} x(l,t) = 0\} \end{aligned} \tag{4.102}$$

The function B in equation (4.28) is an arbitrary function satisfying the conditions (4.29a) and (4.29b). Here, it is assumed that B is a vector of two second order polynomials and the coefficients are found using the conditions (4.29a) and (4.29b)

as following

$$B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \tag{4.103}$$

$$B_1 = \frac{-2}{4D_a l + v l^2} z^2 + \frac{2}{v} \tag{4.104}$$

$$B_2 = -\frac{1}{4D_a l + v l^2} z^2 + \frac{1}{4D_a + v l} z + \frac{2D_a}{4D_a v + v^2 l} \tag{4.105}$$

Finally, the new well posed system can be formulated using the procedure given in §4.2, and the optimal control problem can be solved as discussed in section §4.2

4.4.2 Simulation Study

In this section the closed loop performance of the proposed approach is demonstrated. Values of the model parameters are given in Table 4.1 (Weekman, 1969).

The LQ-controller discussed in the previous section was studied via a simulation that used a nonlinear model of the reactor given in Equations (4.87)-(4.89). The performance of the proposed controller was compared to a finite dimensional LQ controller. The finite dimensional LQ controller was computed using the model derived by converting the PDEs to ODEs by applying central finite difference approach.

Table 4.1: Model Parameters

Parameter	Value	Unit
k_0	22.9	(hr×weight fraction)$^{-1}$
k_1	18.1	(hr×weight fraction)$^{-1}$
k_2	1.7	hr^{-1}
D_a	0.5	m^{2}hr^{-1}
v	2	m×hr^{-1}
$y_{A_{in}}$	0.7	weight fraction
$y_{B_{in}}$	0	weight fraction

The control objective is to drive the trajectory of y_B to the desired steady state profile. Using the nominal operating conditions, and the model given in Equations

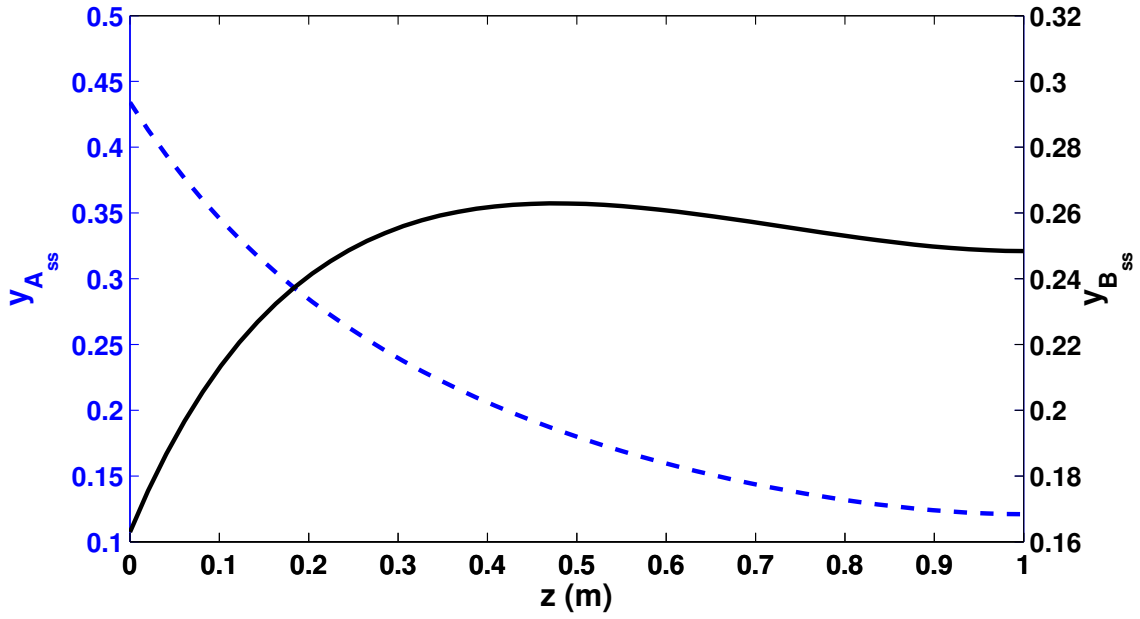


Figure 4.3: Steady state profile of y_A and y_B

(4.87)-(4.89), the steady-state profiles of y_A and y_B were computed and are shown in Figure 4.3. Then, the nonlinear model was linearized around the stationary states and transformed to the self-adjoint form of Equations (4.95)-(4.96). Spectra of operators A_{11} and A_{22} were calculated using the algorithm discussed in §4.2.1. In order to compute the spectrum of A_{11}, it was assumed that the length of the reactor is divided into 50 equally-spaced sections and the coefficient of the reaction term is constant in each section. First five eigenvalues of the operator A_{11} are:

$$\lambda = \{-2.39 \times 10^{-5}, -1.34 \times 10^{-4}, -4.46 \times 10^{-4}, -1.12 \times 10^{-3}, -2.35 \times 10^{-3}\}$$

The spectrum of A_{22} can be computed using Equations (4.41)-(4.43). First five eigenvalues of A_{22} are:

$$\lambda = \{-2.04 \times 10^{-6}, -1.096 \times 10^{-5}, -5.68 \times 10^{-5}, -2.08 \times 10^{-4}, -5.78 \times 10^{-4}\}$$

Finally, the spectrum of A^e was computed using Equations (4.66)-(4.67). The results are shown in Figures 4.4-4.5. Once the eigenvalues and eigenfunctions of

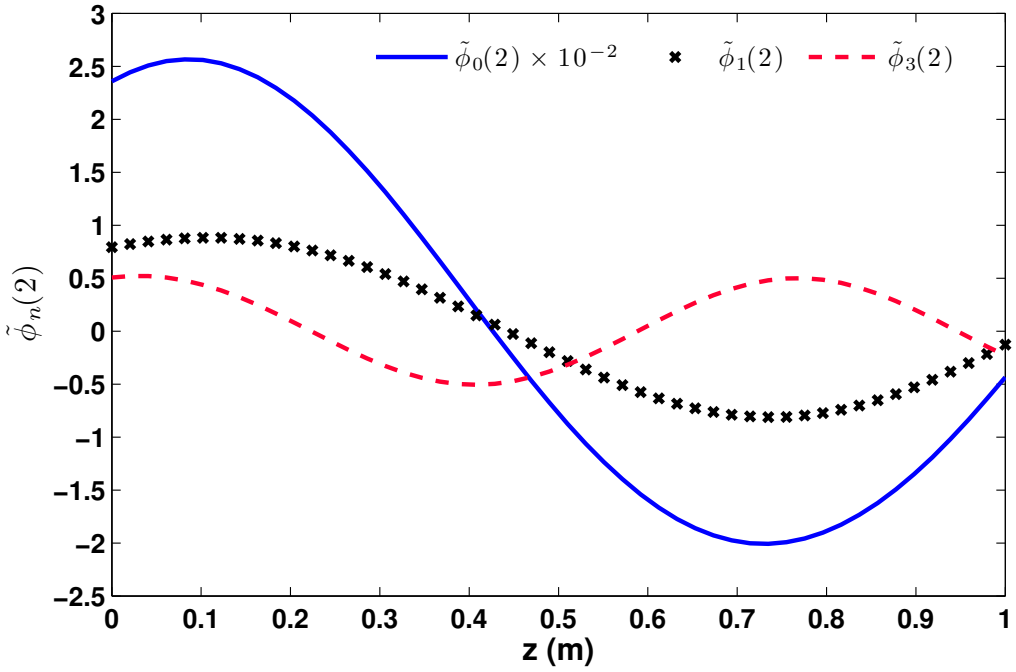


Figure 4.4: Second element of $\hat{\phi}_n$ given by Equation (4.67) and Equations (4.62)-(4.63)

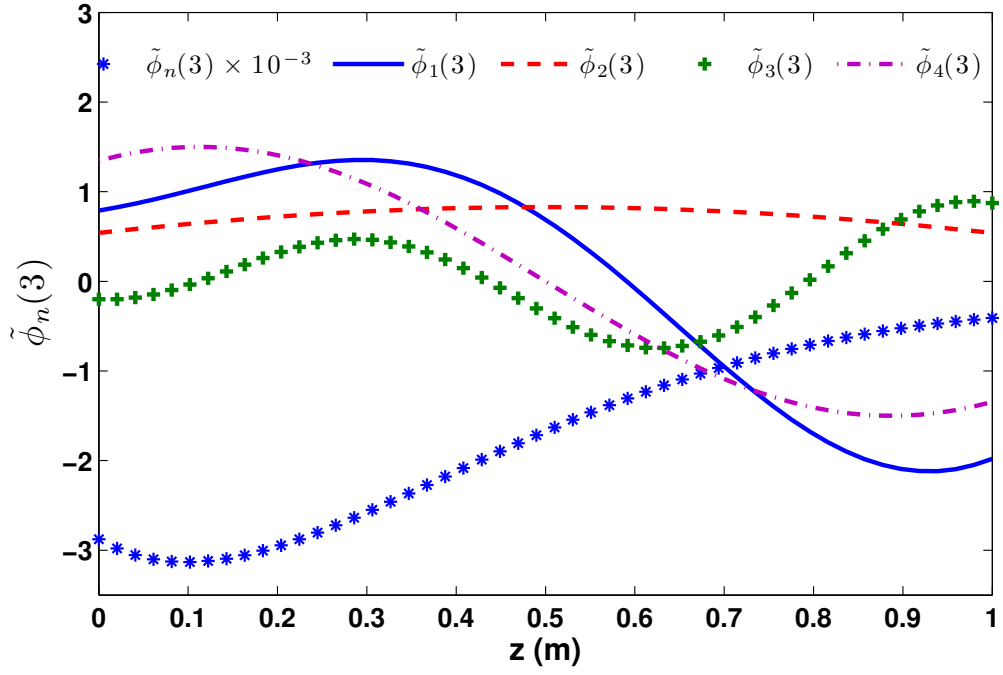


Figure 4.5: Third element of $\hat{\phi}_n$ given by Equation (4.67) and Equations (4.62)-(4.63)

the operator A^e are calculated, the LQ-feedback controller can be computed using Equation (4.36). Note that since Π is a self-adjoint operator, $\langle \phi_n, \Pi\phi_m \rangle = \langle \phi_m, \Pi\phi_n \rangle$, therefore $\Pi_{nm} = \Pi_{mn}$. As a result, Equation (4.36) gives $\frac{n(n+1)}{2}$ coupled algebraic equations that should be solved simultaneously where n is the number of modes that are used to formulate the controller. Since there are two orders of magnitude difference between the first and fifth eigenvalues of the operator A^e, the effect of higher order eigenvalues on the dynamic of the system is considered to be negligible; therefore, in this work, the first five modes were used for numerical simulation. The computed LQ controller was applied to the nonlinear model of the reactor. Simulation of the nonlinear system was performed using COMSOL®. The closed loop trajectory of y_B is shown in Figure 4.6. It should be mentioned the simulation based on first 21 modes resulted in identical results.

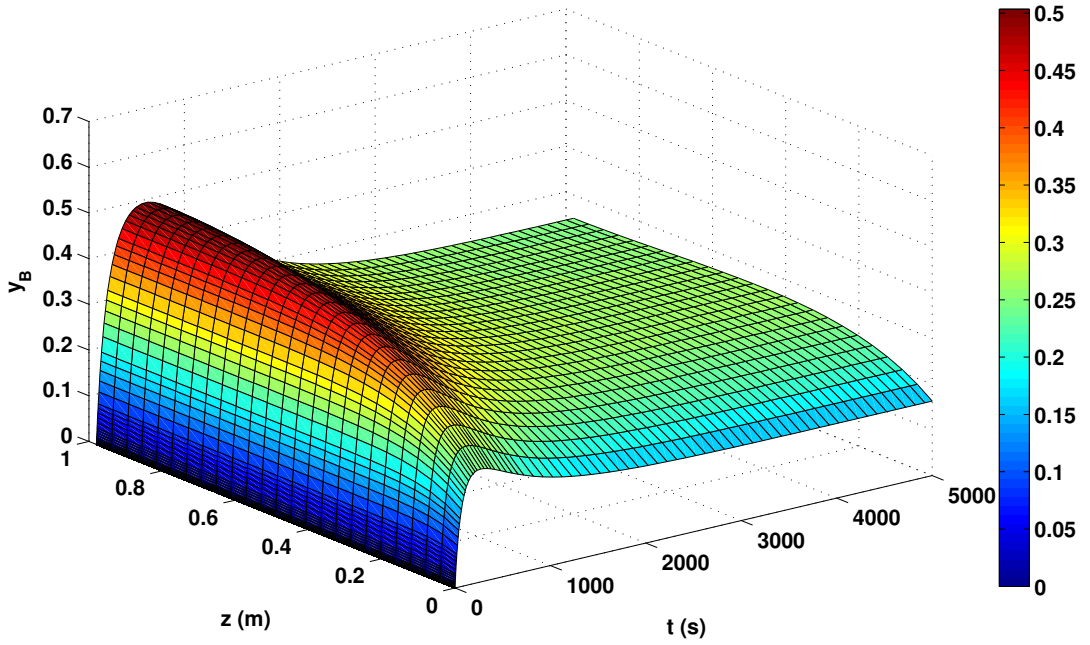


Figure 4.6: Closed loop trajectory of y_B

In order to investigate the performance of the controller, a LQ controller based on a finite difference method was designed. A very fine discretization (n=50) is used to develop the controller. Tuning of the LQ controller based on finite difference was

challenging for this case study. Small values of input weight resulted in infeasible values for manipulated variable. Since the manipulated variable is the inlet weight fraction of component A, its value should be between 0 and 1. In Figure 4.7 the trajectory of the manipulated variable is shown for three different cases. As it is illustrated for $R = 5 \times 10^5$ the value of $y_{A_{in}}$ is greater than 1. This problem can be solved by increasing the weight on the input. As it is shown in Figure 4.7, the optimal input trajectory is feasible for $R = 1 \times 10^6$.

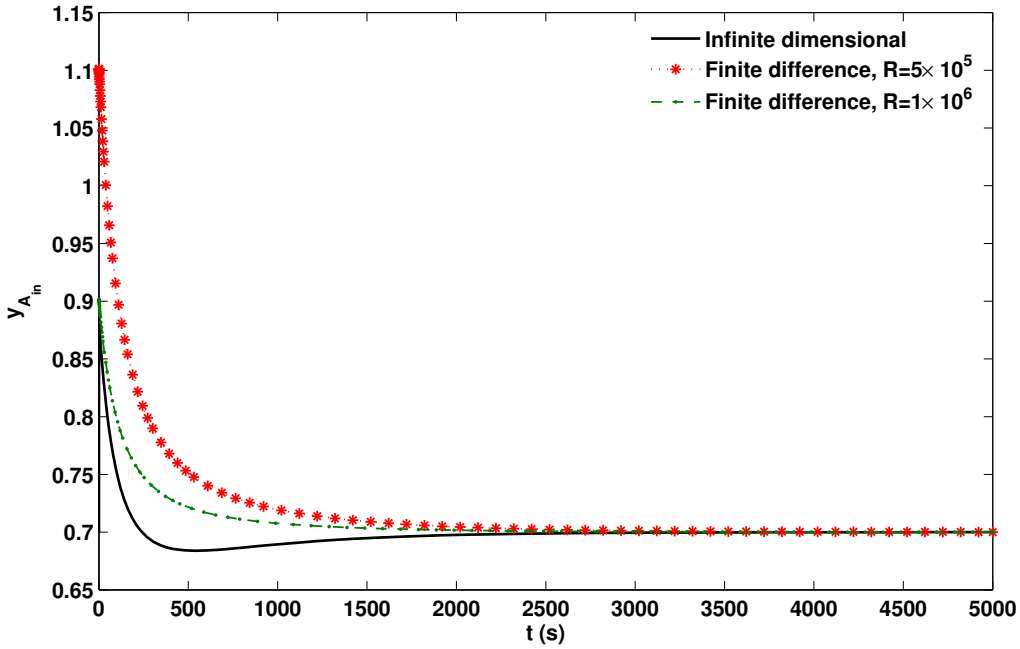


Figure 4.7: Closed loop trajectory of the input variable (Inlet Concentration)

Closed loop trajectory of y_B for $R = 1 \times 10^6$ is shown in Figure 4.8. To compare the performance of two approaches, the l^2-norm of the error between the steady-state and closed loop profiles have been calculated. The results are illustrated in Figure 4.9. It can be observed that the l^2-norm of the error for infinite dimensional case is smaller than either finite dimensional cases. By increasing the weight on the input for finite dimensional case, the performance deteriorates. The l^2-norm of the errors for finite and infinite dimensional controllers are given in Table 4.2. It can be observed that this value for infinite dimensional case is 16% better than the best

finite dimensional controller which is physically meaningful (i.e., results in values of manipulated variable between 0 and 1).

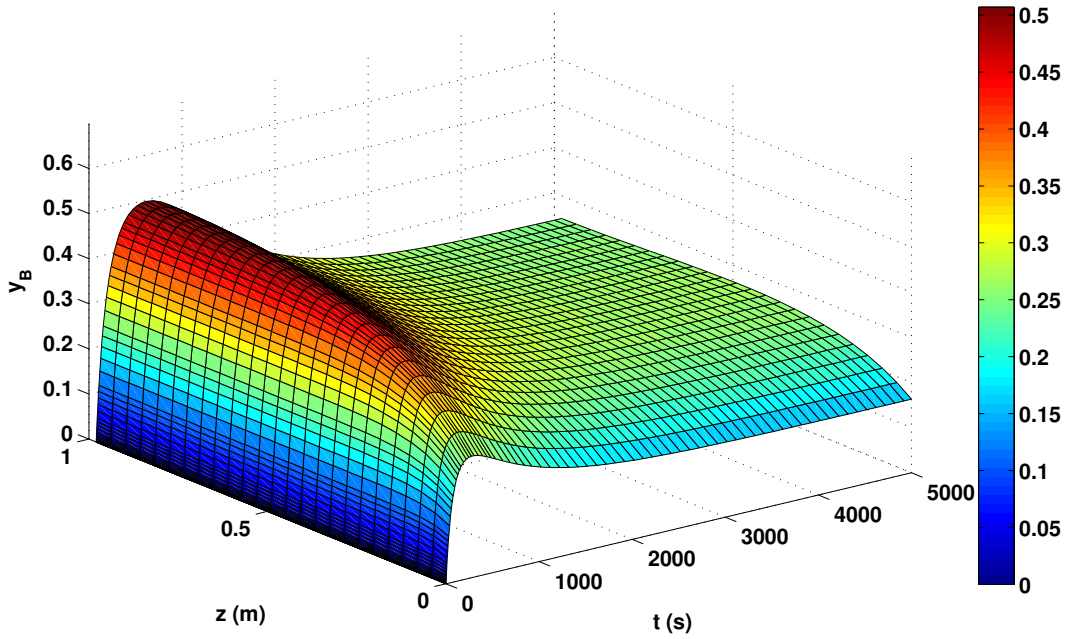


Figure 4.8: Closed loop trajectory of y_B for finite dimensional controller

Table 4.2: Comparison of the l^2-norm

Controller	l^2-norm
Infinite dimensional controller	1771
Finite dimensional controller with $R = 5 \times 10^5$	1903
Finite dimensional controller with $R = 1 \times 10^6$	2064

Designing of the infinite dimensional controller needs more effort than the finite dimensional controller, as it requires solution of eigenvalue problem given in §4.2.1. On the other hand the infinite dimensional controller results in better performance than finite dimensional one. One might claim that by increasing the number of discretization points in finite difference algorithm, the finite dimensional controller may result in better performance. Since the infinite dimensional controller involves matrix algebra, increasing the size of the matrices results in increase in online

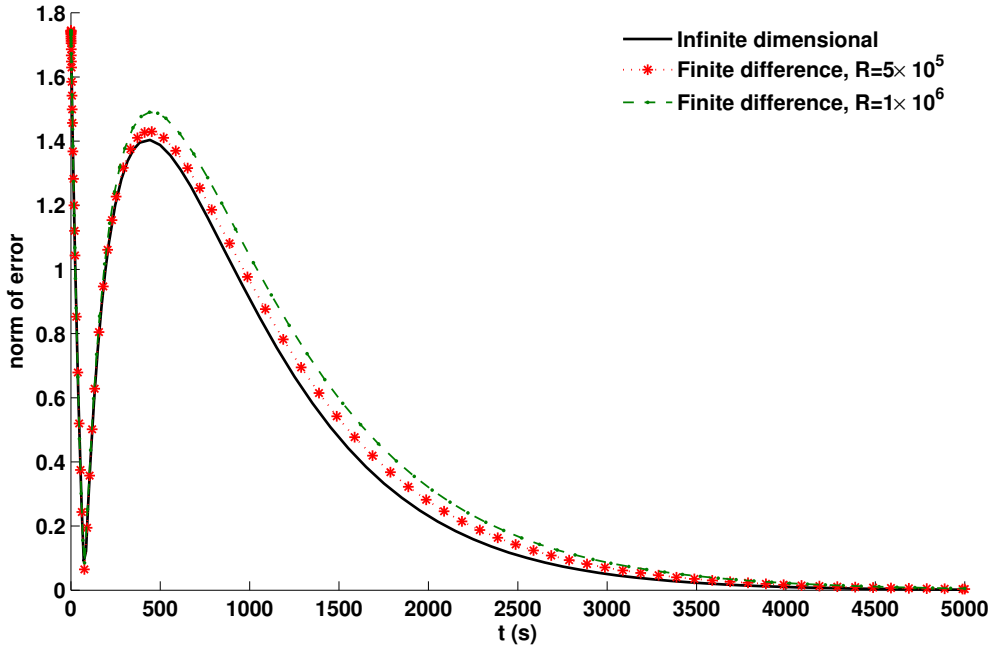


Figure 4.9: Trajectory of tracking error

computation effort: however, the infinite dimensional controller does not involve matrix algebra. Thus by increasing the number of modes the computation effort will not increase significantly. It should also be mentioned that, unlike the finite dimensional controller, the infinite dimensional controller results in feasible optimal trajectories for all values of R. Difficulty in tuning the controller, computational effort and poor performance of the finite dimensional controller justifies implementing the infinite dimensional controller. It should be noted that the infinite dimensional controller requires more effort for design but leads to a better performance.

4.5 Summary

In this chapter, optimal boundary control of infinite dimensional systems described by a set of parabolic PDEs with spatially varying coefficients was studied. Using an exact transformation, the boundary control problem was transformed to a well-posed abstract system. It was shown that the resulting system is a Riesz Spectral

system. Stabilizability of the system was investigated using the spectral properties of the system. In order to compute the spectra of the system, a method similar to solution of the heat equation for composite media was used to compute the spectrum of the system. Moreover, by using the spectral properties of the system, the operator Riccati equation was converted to a set of algebraic equations that can be solved numerically.

A tubular reactor with axial dispersion was considered as the case study. The reactor can be modelled by a set of nonlinear parabolic partial differential equations. Linearization around the steady state profile of the system resulted in a set of linear PDEs with spatially varying coefficients. Then, an LQ controller was formulated to regulate the output variable to the steady state profile. The performance of the proposed controller was compared to an LQ controller based on finite difference approximation of the PDEs. Simulation results showed that the infinite dimensional controller leads to better performance in terms of the l^2-norm of the errors.

5

LQ Control of Coupled Parabolic PDE-ODE systems

In this chapter optimal control of a diffusion-convection-reaction system with catalyst deactivation modelled by a set of ODEs is studied. The system can be described by a set of coupled parabolic PDEs and ODEs. This chapter is the extension of the optimal controller discussed in Chapter 4. Most industrial fixed-bed reactors, as well as fluidized-bed reactors, fall into this class of distributed parameter systems and therefore, the contributions of this chapter have significant industrial importance. The focus in this chapter is on catalytic reactors, but the developed theory is applicable to any distributed parameter system that can be described by the studied form of coupled PDE-ODE systems.

This chapter addresses infinite dimensional LQ control of the systems that are described by a set of coupled parabolic PDEs and ODEs. These kind of systems arise in modeling of chemical and bio-chemical processes, where part of the process is a distributed parameter system and part of it is a lumped parameter system. Examples of these systems include a tubular reactor followed by a well mixed reactor or a catalytic reactor with catalyst deactivation, where the rate of the catalyst deactivation is modelled by a set of ODEs. Two types of coupling can exist between PDEs and ODEs. One type of coupling is through the boundary condition, where the boundary condition of the distributed portion is a function of the state variables of the lumped parameter system. A tubular and a well mixed reactor in series is a simple example for this coupling. These kind of systems are called cascaded PDE-ODE systems and their control was the subject of few recent studies (Krstic, 2009; Susto and Krstic, 2010). The second type of coupling takes place in the domain of the PDE, which means the parameters of the distributed part (e.g., the coefficients) are functions of the states of the lumped parameter system. Examples of this kind of coupling include catalytic reactor with catalyst deactivation, where the deactivation kinetics is described by a set of ODEs, or a heat exchanger with a time varying heat transfer coefficient. Most biochemical processes are also modelled by a set of coupled PDE-ODE with in-domain coupling (e.g., in-situ bioremediation). To the best of authors knowledge, there is no published work on the infinite dimensional optimal control of coupled parabolic PDEs-ODEs with in-domain coupling and this work is the first step on the study of infinite dimensional optimal controller for these systems.

In this chapter, the distributed parameter part of the system is assumed to be similar to the infinite dimensional system studied in Chapter 4 and it is assumed that the parameters of the reactive term are modelled by a set of ODEs which represent the deactivation kinetics. Similar to Chapter 4, we are interested in the boundary control of the system.

By introducing a transformation, the coupled PDE-ODE system is converted to decoupled subsystems. Conditions on the existence of this transformation is studied.

Then, by using the transformation introduced in Chapter 4, the boundary control system is converted to a well-posed infinite dimensional system with bounded input and output operators. The method of computing the spectrum of the operator introduced in Chapter 4 is extended to address the PDE-ODE system. It is shown that the resulting infinite dimensional system is a Riesz spectral system and its stability condition is investigated. Finally, the state feedback LQ controller is formulated for this system and its performance is analyzed using numerical simulations.

This chapter is an important step for optimal control of the most general form of the distributed parameter systems. The main contributions of this chapter can be summarized as

- Formulation and solution of an optimal boundary control problem for coupled parabolic PDE-ODE systems with in-domain coupling;
- Stability analysis of coupled parabolic PDE-ODE system with in-domain coupling.

5.1 Coupled PDE-ODE Systems: Mathematical Description

The problem of interest in this chapter is a system that consists of a set of parabolic PDEs coupled with a set of ODEs. Since most chemical processes are nonlinear in nature, we will start with nonlinear model of the system and will then linearize the model around the steady state profile of the system. Following a few transformations that will be introduced in this section, the linearized coupled PDE-ODE system will be formulated as a well-posed infinite dimensional system with bounded input and output operators, which is suitable for controller formulation.

For the rest of this chapter, it is assumed that the PDE part of the system is similar to what we have considered in Chapter 4. It is also assumed that the parameters of the kinetic terms in the parabolic equations are variable and modelled by a set of ODEs. The mathematical representation of such a system can be given as the following set

of quasi-linear parabolic PDEs and nonlinear ODEs:

$$\begin{aligned} \frac{\partial X}{\partial t} &= \mathbf{D}\frac{\partial^2 X}{\partial z^2} - \mathbf{V}\frac{\partial X}{\partial z} + \mathbf{R}(k, X) \\ \frac{dk}{dt} &= f(k) \end{aligned} \tag{5.1}$$

With the following initial and boundary conditions

$$\begin{aligned} &\mathbf{D}\frac{\partial X}{\partial z}|_{z=0} = \mathbf{V}(X_{z=0} - X_{in}) \\ &\frac{\partial X}{\partial z}|_{z=l} = 0 \\ &X(z,0) = X_0 \\ &k(0) = k_0 \end{aligned} \tag{5.2}$$

where $X(.,t) = \left[\begin{array}{ccc} X_1(.,t) & \cdots & X_n(.,t) \end{array} \right]^T \in \mathcal{H} := L^2(0,l)^n$ denotes the vector of state variables of the distributed parameter portion, $k = \left[\begin{array}{ccc} k_1(t) & \cdots & k_m(t) \end{array} \right]^T \in \mathcal{K} := \mathbb{R}^m$ denotes the vector of state variables for the lumped parameter portion of the model. $z \in [0,l] \in \mathbb{R}$ and $t \in [0,\infty)$ denote position and time, respectively. $\mathbf{D}$ and $\mathbf{V}$ are matrices of appropriate sizes. $\mathbf{R}$ is a Lipschitz continuous nonlinear operator from $\mathcal{H} \oplus \mathcal{K}$ into $\mathcal{H}$. f is a matrix of appropriate size whose entries are functions defined in $\mathbb{R}$. In a catalytic reactor, $\mathbf{R}$ represents the reaction term and f represents the deactivation kinetics.

The nonlinear system (5.1)-(5.2) can be linearized around the steady state profile and the resulting linear system is:

$$\frac{\partial X'}{\partial t} = \mathbf{D}\frac{\partial^2 X'}{\partial z^2} - \mathbf{V}\frac{\partial X'}{\partial z} + \mathbf{N}_1(z)X' + \mathbf{N}_2(z)k' \tag{5.3a}$$

$$\frac{dk'}{dt} = \frac{df(k)}{dk}|_{ss}k' \tag{5.3b}$$

the boundary and initial conditions are:

$$\begin{aligned}
&\mathbf{D}\frac{\partial X'}{\partial z}|_{z=0} = \mathbf{V}(X'_{z=0} - X'_{in}) \\
&\frac{\partial X'}{\partial z}|_{z=l} = 0 \\
&X'(z,0) = X'_0 \\
&k'(0) = k'_0
\end{aligned} \tag{5.4}$$

where $'$ indicates that the variables are in deviation form and $\mathbf{N}_1(z) = \frac{\partial \mathbf{R}(k,X)}{\partial X}|_{ss}$ and $\mathbf{N}_2(z) = \frac{\partial \mathbf{R}(k,X)}{\partial k}|_{ss}$.

The equation (5.3a) is a diffusion-convection-reaction system. To simplify the solution of the eigenvalue problem, it can be converted to a diffusion-reaction system by the following transformation

$$\theta = \mathbf{T}X' = \exp(-\frac{\mathbf{D}^{-1}\mathbf{V}}{2}z)X' \tag{5.5}$$

The resulting system is:

$$\frac{\partial \theta}{\partial t} = \mathbf{D}\frac{\partial^2 \theta}{\partial z^2} + \mathbf{M}_1(z)\theta + \mathbf{M}_2(z)k' \tag{5.6a}$$

$$\frac{dk'}{dt} = \mathbf{M}_3 k' \tag{5.6b}$$

where $\mathbf{M}_1(z) = (\mathbf{T}\mathbf{N}_1(z)\mathbf{T}^{-1} - \frac{\mathbf{V}\mathbf{D}^{-1}\mathbf{V}}{4})$, $\mathbf{M}_2(z) = \mathbf{T}\mathbf{N}_2(z)$ and $\mathbf{M}_3 = \frac{df(k)}{dk}|_{ss}$. The boundary and initial conditions are:

$$\begin{aligned}
&\mathbf{D}\frac{\partial \theta}{\partial z}|_{z=0} = \frac{\mathbf{V}}{2}\theta_{z=0} - \mathbf{V}X'_{in} \\
&\mathbf{D}\frac{\partial \theta}{\partial z}|_{z=l} = -\frac{\mathbf{V}}{2}\theta_{z=l} \\
&\theta(z,0) = \theta_0 = \mathbf{T}^{-1}X'_0 \\
&k'(0) = k'_0
\end{aligned} \tag{5.7}$$

Assuming that $u = \mathbf{V}X'_{in}$, and by defining a new state vector

$$x = \begin{bmatrix} x_d \\ x_l \end{bmatrix} = \begin{bmatrix} \theta \\ k' \end{bmatrix} \tag{5.8}$$

the system (5.6)-(5.7) can be formulated as an abstract boundary control problem on the space $H = \mathcal{H} \oplus \mathcal{K}$ given by

$$\begin{cases} \frac{dx(t)}{dt} = \mathfrak{A}x(t) \\ x(0) = x_0 \\ \mathfrak{B}x(t) = u(t) \\ y(t) = \mathfrak{C}x(t) \end{cases} \tag{5.9}$$

where $\mathfrak{A}$ is a linear operator defined on the domain

$$\mathcal{D}(\mathfrak{A}) = \{x \in H : x_d \text{ and } \frac{dx_d}{dz} \text{ are a.c., } \frac{dx_d^2}{dz^2} \in \mathcal{H}, \mathbf{D}\frac{dx_d}{dz}|_{z=l} = -\frac{\mathbf{V}}{2}x_d|_{x=l}\} \tag{5.10}$$

and is given by

$$\mathfrak{A} = \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \frac{d^2.}{dz^2} + \begin{bmatrix} \mathbf{M}_1 & \mathbf{M}_2 \\ \mathbf{0} & \mathbf{M}_3 \end{bmatrix} .I := \begin{bmatrix} \mathfrak{A}_{11} & \mathfrak{A}_{12} \\ 0 & \mathfrak{A}_{22} \end{bmatrix} \tag{5.11}$$

The boundary operator $\mathfrak{B} : H \to U := \mathbb{R}^n$ is given by

$$\mathfrak{B}x(.) = \left[\begin{array}{c|c} -\mathbf{D}\frac{\partial}{\partial z} + \frac{\mathbf{V}}{2} & 0 \end{array} \right] \begin{bmatrix} x_d \\ \hline x_l \end{bmatrix}_{z=0} \tag{5.12}$$

Since $\mathbf{M}_2$ in Equation (5.11) is generally non-zero, x_d and x_l are coupled. By introducing the following transformation, the system can be transformed to decoupled subsystems:

$$\Lambda = \left[\begin{array}{c|c} I & J \\ \hline 0 & I \end{array} \right] \in \mathcal{L}(H) \quad \& \quad \hat{x} = \Lambda x \tag{5.13}$$

The operator $\mathfrak{A}$ will be transformed to

$$\hat{\mathfrak{A}} = \Lambda\mathfrak{A}\Lambda^{-1} = \left[\begin{array}{c|c} \mathfrak{A}_{11} & -\mathfrak{A}_{11}J + \mathfrak{A}_{12} + J\mathfrak{A}_{22} \\ \hline 0 & \mathfrak{A}_{22} \end{array} \right] \tag{5.14}$$

with $\mathcal{D}(\hat{\mathfrak{A}}) = \mathcal{D}(\mathfrak{A})$. Therefore, if there exists a J that satisfies the following equation, operator $\hat{\mathfrak{A}}$ will be decoupled.

$$-\mathfrak{A}_{11}J + \mathfrak{A}_{12} + J\mathfrak{A}_{22} = 0 \tag{5.15}$$

Remark 5.1.1. The Equation (5.15) is a Sylvester equation and admits a unique solution if and only if $\sigma(-\mathfrak{A}_{11}) \cap \sigma(\mathfrak{A}_{22}) = \emptyset$. (Laub, 2005)

The solution is given by

$$J = \int_0^\infty T_{11}(t)\mathfrak{A}_{12}T_{12}(t)dt \tag{5.16}$$

where T_{11} and T_{22} are C_0-semigroups generated by $-\mathfrak{A}_{11}$ and $\mathfrak{A}_{22}$ respectively (Emirsajlow, 1999). ■

The resulting decoupled system is

$$\begin{cases} \frac{d\hat{x}(t)}{dt} = \hat{\mathfrak{A}}\hat{x}(t) \\ \hat{x}(0) = \hat{x}_0 \\ \hat{\mathfrak{B}}\hat{x}(t) = u(t) \\ y(t) = \hat{\mathfrak{C}}\hat{x}(t) \end{cases} \tag{5.17}$$

where $\hat{\mathfrak{B}} = \mathfrak{B}\Lambda^{-1}$ and $\hat{\mathfrak{C}} = \mathfrak{C}\Lambda^{-1}$

The boundary control problem (5.17) is in the form of a standard abstract boundary control problem and following a similar approach to §4.2, the abstract boundary control problem (5.17) can be converted to a well-posed infinite dimensional system with bounded input and output operators. The procedure is given below.

Define a new operator $\mathcal{A}$ by

$$\begin{aligned} \mathcal{A}x &= \hat{\mathfrak{A}}x \\ \mathcal{D}(\mathcal{A}) &= \mathcal{D}(\hat{\mathfrak{A}}) \cap \ker(\hat{\mathfrak{B}}) \\ &= \{\hat{x} \in H : \hat{x} \text{ and } \frac{d\hat{x}}{dz} \text{ are a.c., } \frac{d^2\hat{x}}{dz^2} \in H \\ &\qquad \text{and } \mathbf{D}\frac{d\hat{x}_d}{dz}|_{z=0} = \frac{\mathbf{V}}{2}\hat{x}_d|_{z=0}, \mathbf{D}\frac{d\hat{x}_d}{dz}|_{z=l} = -\frac{\mathbf{V}}{2}x_d|_{z=l}\} \end{aligned} \tag{5.18}$$

If $\mathcal{A}$ generates a C_0-semigroup on H and there exist a B such that the following conditions hold:

$$Bu \in \mathcal{D}(\hat{\mathfrak{A}}) \tag{5.19a}$$

$$\hat{\mathfrak{B}}Bu = u, \quad u \in U \tag{5.19b}$$

the system (5.17) can be transformed into the following infinite dimensional system with bounded input operator on the state space $H^e = H \oplus U$

$$\begin{aligned} \dot{x}^e(t) &= A^e x^e(t) + B^e \tilde{u}(t) \\ y^e(t) &= C^e x^e(t) \end{aligned} \tag{5.20}$$

where

$$A^e = \begin{bmatrix} 0 & 0 \\ \hat{\mathfrak{A}}B & \mathcal{A} \end{bmatrix}, \quad B^e = \begin{bmatrix} I \\ -B \end{bmatrix}, \quad C^e = \mathfrak{C} \begin{bmatrix} B & I \end{bmatrix} \tag{5.21}$$

and $\tilde{u}(t) = \dot{u}(t)$ and $x^e(t) = \begin{bmatrix} u(t) & \hat{x}(t) - Bu(t) \end{bmatrix}^T$ are the new input and state variables.

Remark 5.1.2. Consider $\tilde{B} = \Lambda^{-1}B$, then the conditions (5.19a)-(5.19b) become $\tilde{B}u \in \mathcal{D}(\hat{\mathfrak{A}})$ and $\mathfrak{B}\tilde{B}u = u$, respectively. One can assume that $\tilde{B} = \left[\begin{array}{c|c} B_d & B_l \end{array}\right]^T$, then the following conditions are equivalent to (5.19a)-(5.19b).

$$\begin{aligned} &\mathbf{D}\frac{dB_d(0)}{dz} - \frac{\mathbf{V}}{2}B_d(0) = I \\ &\mathbf{D}\frac{dB_d(l)}{dz} + \frac{\mathbf{V}}{2}B_d(l) = 0 \\ &B_l \in \mathcal{K} \end{aligned} \tag{5.22}$$

B_d can be any function that satisfies the above conditions. For simplicity one can assume that B_d is a matrix of polynomials. B_l is any arbitrary matrix in $\mathcal{K}$. Finally B can be calculated by

$$B = \Lambda\tilde{B} = \begin{bmatrix} B_d + JB_l \\ B_l \end{bmatrix} \tag{5.23}$$

■

The infinite dimensional system (5.20) is in the form of a standard infinite dimensional system and now we are in the position to proceed with stability analysis and controller formulation for this system. It should be mentioned that, since all of the transformations introduced in this chapter are exact transformations and there was no approximation involved, all of the dynamical properties of the original linearized

system are preserved. Hence, we can perform stability analysis and controller formulation on the transformed system (5.20), and then apply the designed controller to the original system. In order to perform the stability analysis, we need to solve the eignenvalue problem for the system (5.20).

5.2 Coupled PDE-ODE Operator: Eigenvalue Problem

In this section the solution of the eigenvalue problem that was introduced in Chapter 4 is extended to the case of coupled PDE-ODE systems. As discussed in Chapter 4, there is no general algorithm for analytical solution of eigenvalue problem for a general form of parabolic operator. Therefore, in this section we will consider the following assumptions:

1. $\mathbf{N}_1$ in (5.3a) is lower triangular, which leads to lower triangular form of $\mathfrak{A}_{11}$. For most of chemical engineering processes, one can use a transformation to triangularize the system.

2. The number of state variables in (5.3a) is two. Extension to more than two variables is straightforward.

3. Without loss of generality, N_3 is diagonal. Note that, N_3 is a matrix and is always diagonalizable, if its eigenvalues are simple.

Then the eigenvalue problem of interest will be:

$$A^e\phi = \lambda\phi \tag{5.24}$$

where A^e has the following form

$$A^e = \begin{bmatrix} 0 & 0 \\ \hat{\mathfrak{A}}B & \mathcal{A} \end{bmatrix} \tag{5.25}$$

and

$$\begin{aligned}
\mathcal{A} &= \begin{bmatrix} \mathcal{A}_{11} & 0 \\ 0 & \mathcal{A}_{22} \end{bmatrix} \\
\mathcal{A}_{11} &:= \begin{bmatrix} F_{11} & 0 \\ F_{21} & F_{22} \end{bmatrix} = \begin{bmatrix} D_{11}\frac{d^2}{dz^2} + M_{11}(z) & 0 \\ M_{21}(z) & D_{22}\frac{d^2}{dz^2} + M_{22}(z) \end{bmatrix} \\
\mathcal{A}_{22} &= \begin{bmatrix} \alpha_{11} & 0 \\ 0 & \alpha_{22} \end{bmatrix}
\end{aligned} \tag{5.26}$$

Eigenvalues and Eigenfunctions of $\mathcal{A}$

The operator $\mathcal{A}$ is a block diagonal operator, therefore $\sigma(\mathcal{A}) = \sigma(\mathcal{A}_{11}) \cup \sigma(\mathcal{A}_{22})$. Since $\mathcal{A}_{11}$ is a lower triangular operator $\sigma(\mathcal{A}_{11}) = \sigma(F_{11}) \cup \sigma(F_{22})$. Then, $\sigma(\mathcal{A}) = \sigma(F_{11}) \cup \sigma(F_{22}) \cup \sigma(\mathcal{A}_{22})$

The operator $\mathcal{A}_{11}$ is similar to operator $\mathcal{A}$ in Chapter 4 and its spectrum can be calculated by the same approach. Let λ_n and χ_n be eigenvalues and eigenfunctions of the operator F_{11} and μ_n and ψ_n be eigenvalues and eigenfunctions of the operator F_{22}. Then according to §4.2.1, the eigenvalues of the operator $\mathcal{A}_{11}$ are

$$\sigma(\mathcal{A}_{11}) = \sigma(F_{11}) \cup \sigma(F_2) = \{\lambda_n, \mu_n\} \quad n = 1, \cdots, \infty \tag{5.27}$$

and the associated eigenvectors are:

$$\left\{ \begin{bmatrix} \chi_n \\ (\lambda_n I - \mathcal{A}_{22})^{-1}\mathcal{A}_{21}\chi_n \end{bmatrix}, \begin{bmatrix} 0 \\ \psi_n \end{bmatrix} \right\} \quad n = 1, \cdots, \infty \tag{5.28}$$

The corresponding bi-orthonormal eigenfunctions can be computed by solving the eigenvalue problem for $\mathcal{A}_{11}^*$ and are given by:

$$\left\{ \begin{bmatrix} \chi_n \\ 0 \end{bmatrix}, \begin{bmatrix} (\mu_n I - \mathcal{A}_{11})^{-1}\mathcal{A}_{21}\psi_n \\ \psi_n \end{bmatrix} \right\} \quad n = 1, \cdots, \infty \tag{5.29}$$

$\mathcal{A}_{22}$ is a diagonal matrix and its eigenvalues are $\{\alpha_{11}, \alpha_{22}\}$ with the associated eigenvectors $\{[1,0]^T, [0,1]^T\}$. Finally:

$$\sigma(\mathcal{A}) = \{\lambda_n, \mu_n, \alpha_{11}, \alpha_{22}\} \quad n = 1, \cdots, \infty \tag{5.30}$$

and the associated eigenfunctions are

$$\left\{ \begin{bmatrix} \chi_n \\ (\lambda_n I - \mathcal{A}_{22})^{-1}\mathcal{A}_{21}\chi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \psi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\} \quad n = 1, \cdots, \infty \tag{5.31}$$

The corresponding bi-orthonormal eigenfunctions are

$$\left\{ \begin{bmatrix} \chi_n \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} (\mu_n I - \mathcal{A}_{11})^{-1}\mathcal{A}_{21}\psi_n \\ \psi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\} \quad n = 1, \cdots, \infty \tag{5.32}$$

Eigenvalues and Eigenfunctions of A^e

Assume that the operator $\mathcal{A}$ has eigenvalues $\{\sigma_k, k \geq 1\}$ and biorthonormal pair $\{(\phi_k, \psi_k), k \geq 1\}$. The operator A^e is similar to operator A^e in Chapter 4, and its spectrum is calculated by the same approach. $\sigma(A^e) = \sigma(\mathcal{A}) \cup \{0\}$ and $\lambda_0 = 0$ has a multiplicity of m, where m is the number of manipulated variables. The corresponding eigenfunctions for λ_0 are

$$\Phi_0^i = \begin{bmatrix} e_i \\ -\mathcal{A}^{-1}(\hat{\mathfrak{A}}B) \end{bmatrix} = \begin{bmatrix} e_i \\ \sum_{k=0}^{\infty} \frac{1}{\sigma_k} \langle \hat{\mathfrak{A}}B, \psi_k \rangle \phi_k \end{bmatrix}, \quad i = 1, \cdots, m \tag{5.33}$$

where $e_i, i = 1, \cdots, m$ is the orthonormal basis for $U = \mathbb{R}^n$.

The corresponding bi-orthonormal eigenfunction of A^e is

$$\Psi_0^i = \begin{bmatrix} e_i \\ 0 \end{bmatrix}, \quad i = 1, \cdots, m \tag{5.34}$$

For $\lambda \in \sigma(\mathcal{A})$, the associated bi-orthonormal pair are

$$\Phi_n = \begin{bmatrix} 0 \\ \phi_n \end{bmatrix} \quad \& \quad \Psi_n = \begin{bmatrix} \frac{1}{\sigma_n}(\hat{\mathfrak{A}}B)^* \psi_n \\ \psi_n \end{bmatrix} \tag{5.35}$$

The procedure for solution of eigenvalue problem for operator A^e can be summarized as:

- Compute the spectra of the operators F_{11} and F_{22} using the method proposed in Chapter 4
- Given the spectra of F_{11} and F_{22}, compute the spectrum of $\mathcal{A}_{11}$ using Equations (5.27)-(5.29)
- Compute spectrum of $\mathcal{A}_{22}$
- Given the spectra of $\mathcal{A}_{11}$ and $\mathcal{A}_{22}$, compute the spectrum of $\mathcal{A}$ using Equations (5.30)-(5.32)
- Compute the spectrum of A^e using Equations (5.33)-(5.35)

Now we have all the required information for stability analysis of the system, which is the topic of the following section.

5.3 Stability Analysis of PDE-ODE Systems

Theorem 5.3.1. *Consider operator $\mathcal{A}$ given by Equation* (5.26)*. Then $\mathcal{A}$ is an infinitesimal generator of C_0-semigroup on H.*

Proof. Operators $-F_{11}$ and $-F_{22}$, the diagonal entries of operator $-\mathcal{A}_{11}$, are Sturm-Liouville operators. Therefore, $-F_{11}$ and $-F_{22}$ are infinitesimal generators of C_0-semigroups T_{11} and T_{22}, respectively. They both have real, countable and distinct eigenvalues.

Operator $\mathcal{A}_{11}$ has a lower triangular form and its eigenvalues consist of eigenvalues of F_{11} and F_{22}. Therefore, the operator $\mathcal{A}_{11}$ also has real, countable and distinct eigenvalues. Furthermore, eigenfunctions of $\mathcal{A}_{11}$ and its adjoint are bi-orthonormal. Thus, the operator $\mathcal{A}_{11}$ is a Riesz spectral operator (Delattre *et al.*, 2003). By Curtain and Zwart (1995), Lemma 3.2.2, the operator $\mathcal{A}_{11}$ is the generator of the C_0-semigroup $\mathcal{T}_{11}$ given by

$$\mathcal{T}_{11}(t) = \begin{bmatrix} T_{11}(t) & 0 \\ T_{21}(t) & T_{22}(t) \end{bmatrix} \tag{5.36}$$

where

$$T_{21}(t)x_1 = \int_0^t T_{22}(t-s)F_{21}T_{11}(s)x_1 ds \tag{5.37}$$

Operator $\mathcal{A}_{22}$, is a diagonal finite dimensional operator and therefore is the generator of the semigroup $\mathcal{T}_{22} = \exp(-\mathcal{A}_{22}t)$. Thus, the operator $\mathcal{A}$ is the infinitesimal generator of the following C_0-semigroup

$$\mathcal{T}(t) = \begin{bmatrix} \mathcal{T}_{11}(t) & 0 \\ 0 & \mathcal{T}_{22}(t) \end{bmatrix} \tag{5.38}$$

■

Theorem 5.3.2. *Consider operator A^e given by Equation* (5.20)*. Then A^e is an infinitesimal generator of C_0-semigroup on H^e.*

Proof. Eigenvalues of operator A^e consist of eigenvalues of $\mathcal{A}$ and 0 with finite multiplicity m. It is shown in Theorem 5.3.1 that eigenvalues of $\mathcal{A}$ are real, countable and distinct. Therefore, A^e has real, countable eigenvalues with finite multiplicity. Moreover, generalized eigenfunctions of A^e and its adjoint are bi-orthonormal. Therefore, generalized egienfunctions of A^e form a Riesz basis for H^e. Furthermore, A^e is a Riesz spectral operator and is the generator of a C_0-semigroup given by

$$T^e(t) = \begin{bmatrix} I & 0 \\ \mathcal{S}(t) & \mathcal{T}(t) \end{bmatrix} \tag{5.39}$$

where $\mathcal{S}(t)x = \int_0^t \mathcal{T}(s)\tilde{\mathfrak{A}}Bxds$, and $\mathcal{T}(t)$ is the C_0-semigroup generated by $\mathcal{A}$.

■

Theorem 5.3.3. *Consider the state linear system $\sum(A^e, B^e, C^e)$ given by Equation* (5.20)

A necessary and sufficient condition for $\sum(A^e, B^e, -)$ to be β-exponentially stabilizable is

$$rank \begin{pmatrix} \langle b_1, \psi_{n_1} \rangle & \cdots & \langle b_m, \psi_{n_1} \rangle \\ \vdots & & \vdots \\ \langle b_1, \psi_{n_{rn}} \rangle & \cdots & \langle b_m, \psi_{n_{rn}} \rangle \end{pmatrix} = r_n \tag{5.40}$$

for all n such that $\lambda_n \in \sigma^+_\beta(A)$.

Proof. A^e is a Riesz-Spectral operator and its eigenvalues consist of eigenvalues of $\mathcal{A}$ and 0 with finite multiplicity m. Based on Theorem (4.3.2), the necessary and sufficient conditions for $\sum(A^e, B^e, -)$ to be $\beta-$exponentially stable are that there exist an $\epsilon > 0$ such that $\sigma^+_{\beta-\epsilon}(A^e)$ comprises, at most, finitely many eigenvalues and the rank condition (5.40) holds.

Diagonal entries of $\mathcal{A}$ are Sturm-Liouville operators, the spectrum of $\mathcal{A}$ is finitely bounded (i.e., there exists a ω such that all $\lambda \in \sigma(\mathcal{A}) < \omega$). Therefore, for any arbitrary β and ϵ, $\sigma^+_{\beta-\epsilon}(A^e)$ comprises finitely many eigenvalues and the first condition holds. Therefore, the necessary and sufficient condition for $\beta-$exponential stability of $\sigma(A^e, B^e, -)$ reduces to (5.40). Validity of this condition depends on the choice of B and should be verified for each case study. ■

5.4 LQ Control of PDE-ODE Systems

The extended state space system (5.20) is similar to the extended system (4.30), therefore formulation of the LQ controller is similar to §4.2. The Algebraic Riccati Equation (4.33) is independent of the type of operators, but its solution depends on the properties of the infinite dimensional system. In the previous section we discussed that the infinite dimensional system (5.20) is a Riesz Spectral system and therefore the solution of optimal control problem for this system can also be found by solving the set of algebraic equations given in (4.36).

In the following section, a case study involving a catalytic reactor with catalyst deactivation will be investigated and the performance of the optimal controller will be explored.

5.5 Case study: Catalytic Cracking Reactor with Catalyst Deactivation

In this section, the proposed approach is applied to the catalytic cracking reactor discussed in Chapter 4 with the assumption that the catalyst deactivates with time. The control objective is to regulate the trajectory of C_B, gasoline, at the steady state profile using the inlet concentration of A as the manipulated variable. The system will be represented as an infinite dimensional system using the procedures discussed in previous sections. The transformations required to decouple the PDE-ODE system and to convert the system to a well-posed infinite dimensional system will be computed in detail. Finally, numerical simulations will be performed to analyze the closed loop performance of the controller.

Model description

The model that is used is similar to the model of the catalytic cracking reactor in Chapter 4. The only difference is that the deactivation of the catalyst should also be considered. The reaction scheme is given by Equations

$$\begin{aligned} A &\xrightarrow{k_1} B \xrightarrow{k_2} C \\ A &\xrightarrow{k_3} C \end{aligned} \tag{5.41}$$

with the kinetic equations given by

$$\begin{aligned} r_A &= -(k_1 + k_3)y_A^2 = -k_0 y_A^2 \\ r_B &= k_1 y_A^2 - k_2 y_B \end{aligned} \tag{5.42}$$

It is assumed that the catalyst deactivation will only affect the pre-exponential factor of the main reaction, and k_1 will be modelled by

$$\frac{dk_1}{dt} = \alpha k_1 + \beta, \qquad k_1(0) = k_{1_0} \tag{5.43}$$

The above equation for the rate of deactivation of the catalyst, is equivalent to the exponential decay assumption, which is a common assumption for modelling catalyst

deactivation. It is in agreement with the observation that the catalyst deactivation consists of three phases: rapid initial deactivation, slow deactivation and stabilization (Kallinikos *et al.*, 2008).

The model of the reactor will consist of Equations (4.88)-(4.89) and (5.43). The linearization of the model can be performed similar to Chapter4. By defining the new state and input variables

$$\theta(t) = \begin{bmatrix} y_A - y_{A_{ss}} \\ y_B - y_{B_{ss}} \\ k_1 - k_{1_{ss}} \end{bmatrix}, \quad u(t) = v(y_{A_{in}} - y_{A_{in,ss}}) \tag{5.44}$$

the linearized model will have the form of

$$\frac{\partial}{\partial t}\begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} = \begin{bmatrix} D_a\frac{\partial^2}{\partial z^2} - v\frac{\partial}{\partial z} - 2(k_{1_{ss}} + k_3)y_{A_{ss}} & 0 & -y_{A_{ss}}^2 \\ 2k_{1_{ss}}y_{A_{ss}} & D_a\frac{\partial^2}{\partial z^2} - v\frac{\partial}{\partial z} - k_2 & y_{A_{ss}}^2 \\ 0 & 0 & \alpha \end{bmatrix}\begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} \tag{5.45}$$

with the initial and boundary conditions:

$$\begin{aligned} D_a\frac{\partial}{\partial z}\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{z=0} &= v\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{z=0} - \begin{bmatrix} u \\ 0 \end{bmatrix}, \\ D_a\frac{\partial}{\partial z}\begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}_{z=l} &= \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \\ \theta(z,0) = \theta_0 = \begin{bmatrix} \theta_{1_0}(z) \\ \theta_{2_0}(z) \\ \theta_{3_0} \end{bmatrix} &= \begin{bmatrix} y_{A_0} - y_{A_{ss}} \\ y_{A_0} - y_{A_{ss}} \\ k_{1_0} - k_{1_{ss}} \end{bmatrix} \end{aligned} \tag{5.46}$$

The set of equations (5.45) can be converted to a diffusion-reaction system by using the transformation given by Equation (5.5). The resulting system is

$$\frac{\partial}{\partial t}\left[\begin{array}{c} x_1 \\ x_2 \\ \hline x_3 \end{array}\right] = \left[\begin{array}{cc|c} D_a\frac{\partial^2}{\partial z^2} - \hat{k}_1(z) & 0 & -y_{A_{ss}}^2 \\ 2k_{1_{ss}}y_{A_{ss}}(z) & D_a\frac{\partial^2}{\partial z^2} - \hat{k}_2 & y_{A_{ss}}^2 \\ \hline 0 & 0 & \alpha \end{array}\right]\left[\begin{array}{c} x_1 \\ x_2 \\ \hline x_3 \end{array}\right] \tag{5.47}$$

with the following initial and boundary conditions

$$\begin{aligned} D_a\frac{\partial}{\partial z}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{z=0} &= \frac{v}{2}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{z=0} - \begin{bmatrix} u \\ 0 \end{bmatrix} \\ D_a\frac{\partial}{\partial z}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{z=l} &= -\frac{v}{2}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{z=l} \\ x(z,0) &= x_0 \end{aligned} \tag{5.48}$$

where

$$x = \begin{bmatrix} e^{-\frac{v}{2D}z}\theta_1 \\ e^{-\frac{v}{2D}z}\theta_2 \\ \theta_3 \end{bmatrix}^T \in H := L^2(0,l)^2 \oplus R, \quad x_0 = \begin{bmatrix} e^{-\frac{v}{2D}z}\theta_{1_0} \\ e^{-\frac{v}{2D}z}\theta_{2_0} \\ \theta_{3_0} \end{bmatrix}^T \in H$$

$$\hat{k}_1(z) = -\frac{v^2}{4D} - 2(k_{1_{ss}} + k_3)y_{A_{ss}}, \text{ and } \hat{k}_2 = -\frac{v^2}{4D} - k_2$$

The infinite dimensional representation of the system (5.47)-(5.48) on Hilbert space H has the form of (5.9) by defining the operator $\mathfrak{A}$ as:

$$\mathfrak{A} = \left[\begin{array}{cc|c} D_a\frac{\partial^2}{\partial z^2} - \hat{k}_1(z) & 0 & -y_{A_{ss}}^2 \\ 2k_{1_{ss}}y_{A_{ss}}(z) & D_a\frac{\partial^2}{\partial z^2} - \hat{k}_2 & y_{A_{ss}}^2 \\ \hline 0 & 0 & \alpha \end{array}\right] \tag{5.49}$$

$$\begin{aligned} \mathcal{D}(\mathfrak{A}) = \{x \in H : x \text{ and } \frac{dx}{dz} \text{ are a.c.}, \frac{dx^2}{dz^2} \in H, D_a\frac{dx_1}{dz}|_{z=l} = -\frac{v}{2}x_1|_{x=l} \\ D_a\frac{dx_2}{dz}|_{z=l} = -\frac{v}{2}x_2|_{x=l}, D_a\frac{dx_1}{dz}|_{z=0} = \frac{v}{2}x_1|_{x=0}\} \end{aligned} \tag{5.50}$$

and the boundary operator $\mathfrak{B}$ by

$$\mathfrak{B}x(.) = \left[\begin{array}{cc|c} -D_a\frac{\partial}{\partial z} + \frac{v}{2} & 0 & 0 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \\ \hline x_3 \end{array}\right]_{z=0} \tag{5.51}$$

Assuming that, the control variable is x_2, the output operator $\mathfrak{C}$ is:

$$\mathfrak{C} = \mathfrak{C}_0 I = \left[\begin{array}{cc|c} 0 & 1 & 0 \end{array}\right] \tag{5.52}$$

By performing the transformation (5.13), the operator $\mathfrak{A}$ can be converted to a block diagonal form and the decoupled infinite dimensional system (5.17) will be computed. Using Equation (5.16), the operator J in Equation (5.13) is

$$J = \int_0^\infty \mathfrak{T}_{11}(t)\mathfrak{A}_{12}\mathfrak{T}_{22} \tag{5.53}$$

$\mathfrak{T}_{11}$ and $\mathfrak{T}_{22}$ are the C_0-semigroups generated by $-\mathfrak{A}_{11}$ and $\mathfrak{A}_{22}$. $\mathfrak{A}_{11}, \mathfrak{A}_{22}$ and $\mathfrak{A}_{12}$ are given by

$$\mathfrak{A}_{11} = \begin{bmatrix} D_a\frac{\partial^2}{\partial z^2} - \hat{k}_1(z) & 0 \\ 2k_{1_{ss}}y_{A_{ss}}(z) & D_a\frac{\partial^2}{\partial z^2} - \hat{k}_2 \end{bmatrix}, \quad \mathfrak{A}_{12} = \begin{bmatrix} -y_{A_{ss}}^2 \\ y_{A_{ss}}^2 \end{bmatrix}, \quad \mathfrak{A}_{22} = \begin{bmatrix} \alpha \end{bmatrix} \tag{5.54}$$

- **Computation of $\mathfrak{T}_{11}$**

  $\mathfrak{A}_{11}$ is a lower triangular operator and as discussed in §5.3 generates the C_0-semigroup $\mathfrak{T}_{11}$ given by

  $$\mathfrak{T}_{11}(t) = \begin{bmatrix} T_{11}(t) & 0 \\ T_{21}(t) & T_{22}(t) \end{bmatrix} \tag{5.55}$$

  Where T_{11} and T_{22} are the semigroups generated by the diagonal elements of $-\mathfrak{A}_{11}$ and are given by

  $$T_{11}(t)x = \sum_{n=1}^{\infty} e^{-\lambda_n t}\langle x, \chi_n\rangle\chi_n \tag{5.56}$$

  $$T_{22}(t)x = \sum_{n=1}^{\infty} e^{-\mu_n t}\langle x, \psi_n\rangle\psi_n \tag{5.57}$$

  λ_n, μ_n, χ_n and ψ_n can be calculated using the approach discussed in §5.2. $T_{21}(t)$ can be calculated using $T_{11}(t)$ and $T_{22}(t)$ by

  $$T_{21}(t)x = \int_0^t T_{22}(t-s)FT_{11}(s)xds \tag{5.58}$$

  where F is the off-diagonal element of $\mathfrak{A}_{11}$ and is equal to $2k_{1_{ss}}y_{A_{ss}}(z)$. By performing simple calculations, $T_{21}(t)$ becomes

  $$T_{21}(t)x = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} -\frac{e^{-\lambda_m t} - e^{-\mu_n t}}{\lambda_m - \mu_m}\langle x, \chi_m\rangle\langle F\chi_m, \psi_n\rangle\psi_n \tag{5.59}$$

- **Computation of $\mathfrak{T}_{22}$**

  $\mathfrak{A}_{22}$ is just an scalar and the semigroup generated by it is

$$\mathfrak{T}_{22} = e^{\alpha t} \tag{5.60}$$

- **Computation of J**

  Using Equation (5.53) and Equations (5.55)-(5.60), and assuming that $\mathfrak{A}_{12} = \begin{bmatrix} N_1 \\ N_2 \end{bmatrix}$, J can be computed as:

$$J = \begin{bmatrix} J_1 \\ J_2 \end{bmatrix} \tag{5.61}$$

$$J_1 x = \sum_{n=1}^{\infty} \frac{1}{\lambda_n + \alpha} \langle N_1 x, \chi_n \rangle \chi_n \tag{5.62}$$

$$J_2 x = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{(\lambda_n + \alpha)(\mu_m + \alpha)} \langle N_1 x, \chi_n \rangle \langle F\chi_n, \psi_m \rangle \psi_m \tag{5.63}$$

$$+ \sum_{m=1}^{\infty} \frac{1}{\mu_m + \alpha} \langle N_2 x, \psi_m \rangle \psi_m \tag{5.64}$$

Finally, by defining $\hat{\mathfrak{A}} = \Lambda \mathfrak{A} \Lambda^{-1}$, $\hat{\mathfrak{B}} = \mathfrak{B}\Lambda^{-1}$ and $\hat{\mathfrak{C}} = \mathfrak{C}\Lambda^{-1}$, the decoupled abstract boundary control problem becomes:

$$\begin{cases} \frac{d\hat{x}(t)}{dt} = \hat{\mathfrak{A}}\hat{x}(t) \\ \hat{x}(0) = \hat{x}_0 \\ \hat{\mathfrak{B}}\hat{x}(t) = u(t) \\ y(t) = \hat{\mathfrak{C}}\hat{x}(t) \end{cases} \tag{5.65}$$

The abstract boundary control problem (5.65), can be converted to a well-posed infinite dimensional system with bounded input and output operators using Equations (5.18)-(5.21). In the Equation (5.21), B can be calculated using the discussion in Remark 5.1.2. Since $\tilde{B}$ is any arbitrary function that satisfies conditions (5.22), we assume that $B_d = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}$ and B_1 and B_2 are both second order polynomials. Using

the conditions (5.22), B_1 and B_2 are:

$$B_1 = \frac{-2}{4D_a l + v l^2} z^2 + \frac{2}{v} \tag{5.66}$$

$$B_2 = -\frac{1}{4D_a l + v l^2} z^2 + \frac{1}{4D_a + v l} z + \frac{2D_a}{4D_a v + v^2 l} \tag{5.67}$$

B_l is any arbitrary number in $\mathbb{R}$ and we assume that $B_l = 1$. Finally B becomes:

$$B = \begin{bmatrix} B_1 + J_1 B_l \\ B_2 + J_2 B_l \\ B_l \end{bmatrix} \tag{5.68}$$

Now we are in a position to use the formulated LQ controller in §4.2 to control the resulting well-posed infinite dimensional system of form (5.20) and analyze its performance by numerical simulation.

5.6 Numerical Simulations

In this section the performance of the proposed approach is demonstrated. The LQ controller discussed in the previous section was studied via a simulation that used a nonlinear model of the reactor given in Equations (4.87)-(4.89) and (5.43). Values of the model parameters are given in Table 5.1 (Weekman, 1969).

Table 5.1: Model Parameters

Parameter	Value	Unit
k_1	18.1	(hr×weight fraction)$^{-1}$
k_2	1.7	hr^{-1}
k_3	4.8	(hr×weight fraction)$^{-1}$
D_a	0.5	m^{2}hr^{-1}
v	2	m×hr^{-1}
$y_{A_{in}}$	0.7	weight fraction
$y_{B_{in}}$	0	weight fraction
α	-0.001	hr^{-1}
β	9.05×10^{-3}	

The control objective is to regulate the trajectory of y_B at the desired steady state

profile. Deactivation of catalyst has a negative impact on y_B and our objective is to calculate the optimal values of inlet y_A to keep trajectory of y_B at the desired profile and eliminate the effect of deactivation. Using the nominal operating conditions, and the model given in Equations (4.87)-(4.89) and (5.43), the steady-state profiles of y_A and y_B were computed. Then, the nonlinear model was linearized around the stationary states and transformed to the self-adjoint form of Equations (5.47)-(5.48). Spectra of operators A_{11} and A_{22} were calculated using the algorithm discussed in §5.2. In order to compute the spectrum of A_{11}, it was assumed that the length of the reactor is divided into 50 equally-spaced sections and the coefficient of the reaction term is constant in each section. First five eigenvalues of the operator A_{11} are:

$$\lambda = \{-2.39 \times 10^{-5}, -1.34 \times 10^{-4}, -4.46 \times 10^{-4}, -1.12 \times 10^{-3}, -2.35 \times 10^{-3}\}$$

The spectrum of A_{22} can be computed using Equations (4.41)-(4.43). First five eigenvalues of A_{22} are:

$$\lambda = \{-2.04 \times 10^{-6}, -1.096 \times 10^{-5}, -5.68 \times 10^{-5}, -2.08 \times 10^{-4}, -5.78 \times 10^{-4}\}$$

Finally, the spectrum of A^e was computed using Equations (5.33)-(5.35). The first six eigenvalues of A^e is:

$$\sigma(A^e) = \{0, -0.001, -2.39\times10^{-5}, -2.04\times10^{-6}, -1.34\times10^{-4}, -1.096\times10^{-5}\} \quad (5.69)$$

and the associated eigenfunctions are shown in Figures 5.1-5.2. Once the eigenvalues and eigenfunctions of the operator A^e are calculated, the LQ-feedback controller can be computed using Equation (4.36). Note that since Π is a self-adjoint operator, $\langle \phi_n, \Pi\phi_m \rangle = \langle \phi_m, \Pi\phi_n \rangle$, therefore $\Pi_{nm} = \Pi_{mn}$. As a result, Equation (4.36) gives $\frac{n(n+1)}{2}$ coupled algebraic equations that should be solved simultaneously where n is the number of modes that are used to formulate the controller. Since there are two orders of magnitude difference between the first and sixth eigenvalues of the operator A^e, the effect of higher order eigenvalues on the dynamic of the system is considered to be negligible; therefore, in this work the first five modes were used for numerical

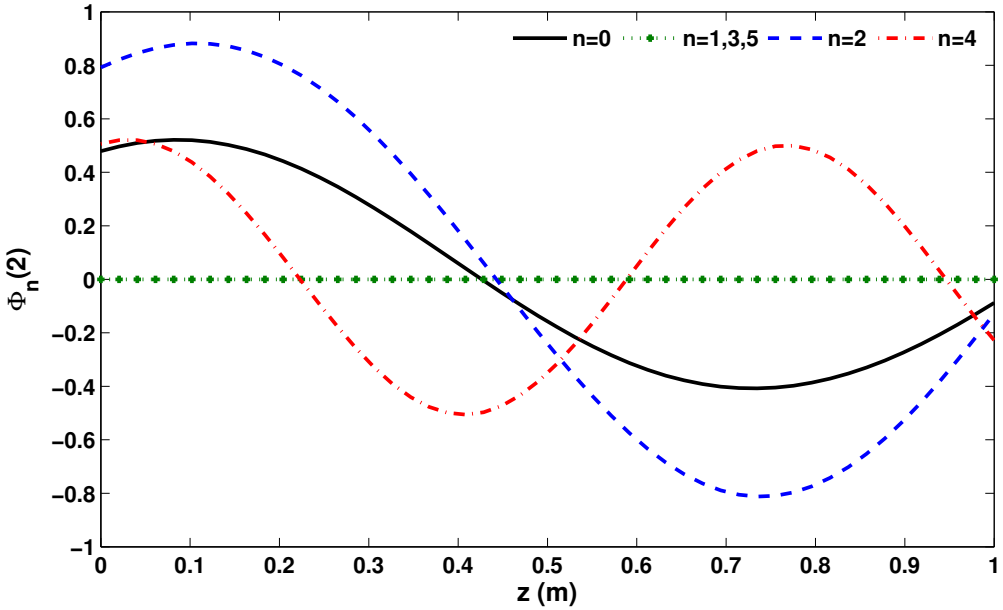


Figure 5.1: Second element of $\hat{\phi}_n$ given by Equation (4.67) and Equations (4.62)-(4.63)

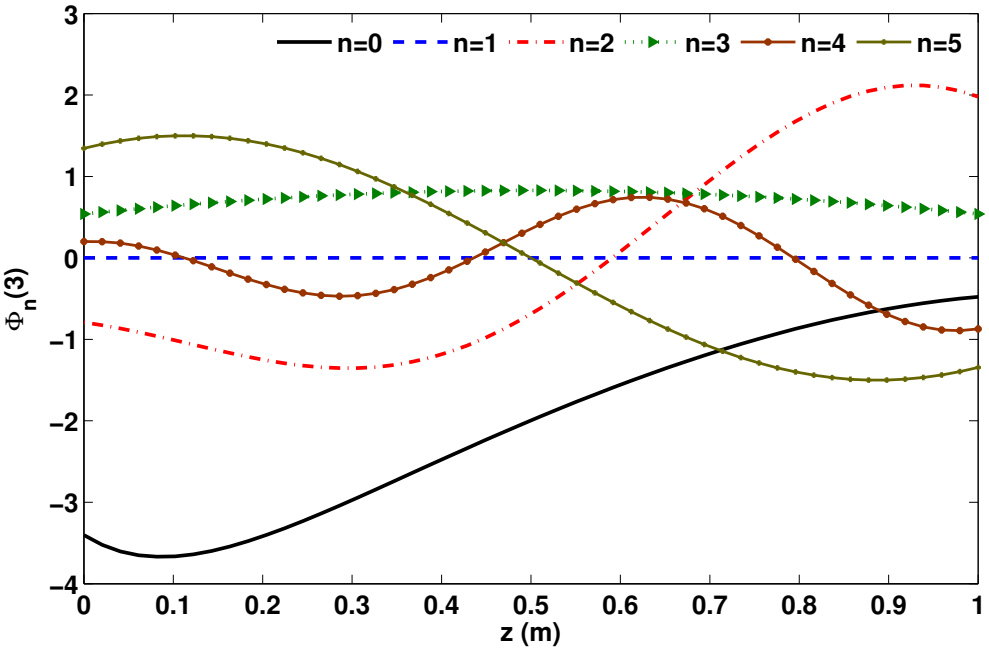


Figure 5.2: Third element of $\hat{\phi}_n$ given by Equation (4.67) and Equations (4.62)-(4.63)

simulation. The computed LQ controller was applied to the nonlinear model of the reactor. Simulation of the nonlinear system was performed using COMSOL®. The closed loop trajectory of error is shown in Figure 5.3 and the optimal input trajectory is shown in Figure 5.4. Figure 5.3 illustrates that, as catalyst deactivates, the controller is able to regulate the trajectory of y_B at the desired steady state trajectory.

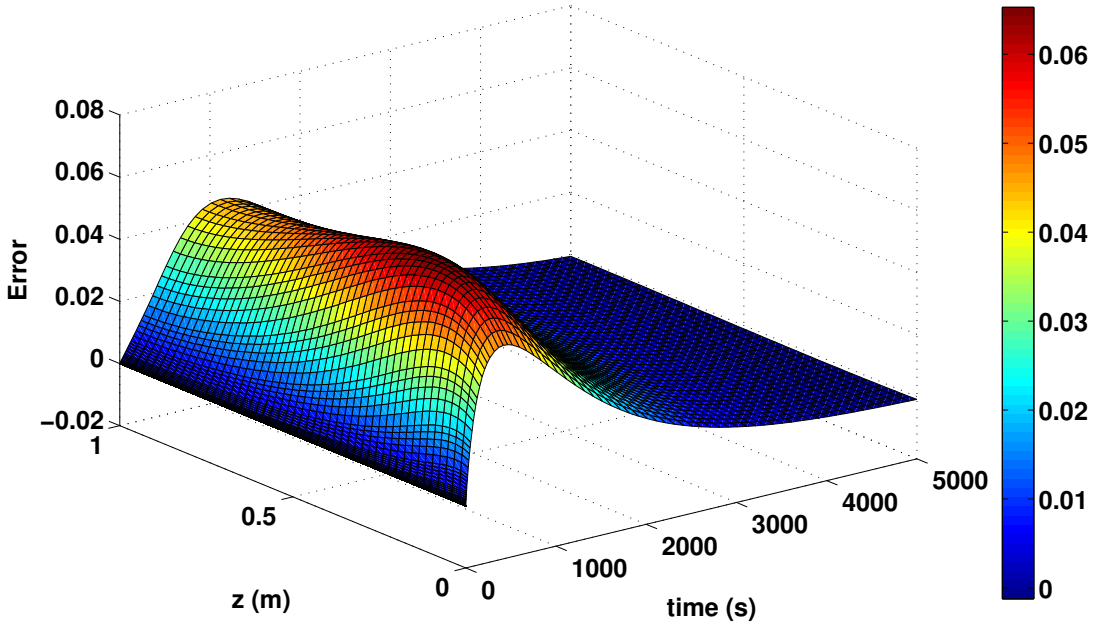


Figure 5.3: Closed loop trajectory of error $y_B - y_{B_{ss}}$

5.7 Summary

The infinite dimensional LQ controller for boundary control of an infinite dimensional system modelled by coupled Parabolic PDE-ODE equations was studied. This chapter was a very important step in formulation of an optimal controller for the most general form of distributed parameter systems consisting of coupled parabolic and hyperbolic PDEs, as well as ODEs. The coupled PDE-ODEs were converted to a decoupled form using an exact transformation. Conditions on existence of

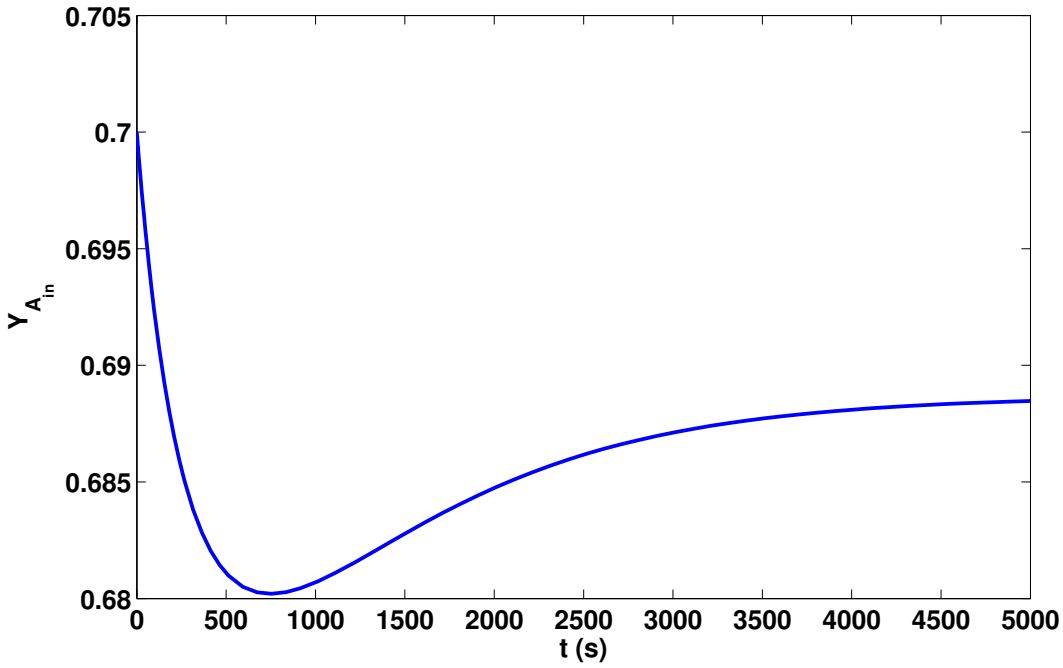


Figure 5.4: Optimal input trajectory

this transformation were studied. The decoupled system was then formulated as a well-posed infinite dimensional system by extension of the approach introduced in Chapter 4. It was shown that the resulting system is a Reisz Spectral system and using the properties of Riesz spectral systems, the stabilizability of the system was proven. Since the transformed well-posed system was a Riesz Spectral system, the LQ controller formulated in Chapter 4 was applicable to this system as well. The LQ controller was applied to a catalytic fixed bed reactor, where the rate of catalyst deactivation was modelled by an ODE. The closed loop performance of the controller was studied via numerical simulations. It was illustrated that the formulated controller is able to eliminate the effect of the catalyst deactivation.

6

Conclusions and Recommendations

This thesis was concerned with the problem of the infinite dimensional optimal controller design for distributed parameter systems with special emphasis on transport-reaction processes (i.e., fixed-bed reactors) that are normally modelled by partial differential equations. Since the governing transport phenomenon in a transport-reaction system determines the type of the PDEs involved in the modelling (e.g., hyperbolic or parabolic), this thesis was divided to two parts to address each type of PDE system independently. The goal was to develop the required mathematical tools for solution of the optimal control problem for a general class of distributed parameter systems representing a fixed-bed reactor with minimum number of simplifying assumptions in the modelling of the reactor.

The first part of the thesis concentrated on catalytic reactors with negligible diffusion that are modelled by a set of hyperbolic systems. In Chapter 2, a LQ controller for a set of time-varying coupled hyperbolic equations was formulated. Exponential stability of these systems was analyzed using the Lyapunov approach. It

was shown that the solution of the optimal control problem could be found by solving an equivalent matrix Riccati partial differential equation. Numerical simulations were performed to evaluate the closed loop performance of the designed controller on a hydrotreating fixed-bed reactor. The performance of the proposed controller was compared to the performance of an infinite dimensional controller formulated by ignoring the catalyst deactivation. Simulation results showed that the performance of the proposed controller is better than the controller that ignores catalyst deactivation, when the deactivation time is comparable to the residence time of the reactor. In case of very slow deactivation the two controllers had comparable performance.

Input and output constraints, as well as parameter uncertainty, are issues that shall be considered in designing a controller. Chapter 3 addressed the problem of constrained model predictive control of hyperbolic systems under parameter uncertainty. A characteristic based robust model predictive control algorithm was developed for a set of two time-scale hyperbolic PDEs. This class of hyperbolic systems have two characteristic curves along which the set of PDEs can be represented as a set of ODEs. Using this feature, the set of partial differential equations was transformed to a set of ODEs. In order to construct the state space model of the system, the spatial domain was discretized by a finite number of discretization points. The structure of the resulting state space model was explored. It was shown that the resulting state space system has certain periodic features depending on the ratio of the slopes of two characteristic curves. A very nice feature of the proposed algorithm is preservation of finite impulse response property of the co-current hyperbolic systems. This means the proposed method can tolerate discontinuities in the boundary conditions as opposed to other discretization methods. In order to specify the uncertainty of the plant, it was assumed that the real model of the system lies inside a polytopic set Ω generated by uncertain models of the system. The MPC problem was defined by nominal performance index but constraint satisfaction for all polytopic models was ensured. A case study involving a hydrotreating reactor was used to evaluate the closed loop response of the controller. In this case study two uncertain

parameters leading to four polytopic models existed. Simulation results indicated that this algorithm is able to satisfy input and output constraints under parameter uncertainty.

The second part of the thesis dealt with systems modelled by a set of parabolic PDES. In chapter 4, optimal boundary control of infinite dimensional systems described by a set of parabolic PDEs with spatially varying coefficients was studied. Such systems are results of linearization of nonlinear PDE model of the process around its steady state profile. Using an exact transformation, the boundary control problem was transformed to a well-posed infinite dimensional system. It was proven that the resulting system is a Riesz Spectral system. Stabilizability of the system was investigated using the spectral properties of the system. The most challenging part of this chapter was to solve the eigenvalue problem for the set of coupled PDEs with spatially varying coefficients. The spectrum of the system is required to solve the optimal control problem for Riesz-Spectral systems and unfortunately there is no method available for analytical solution of a general form of the parabolic operator. Therefore, some simplifying assumptions were made and then an innovative approach for solution of eigenvalue problem was proposed. The basic idea for solution of the problem was the solution method for the heat equation in composite media. Moreover, by using the spectral properties of the system, the operator Riccati equation was converted to a set of algebraic equations that could be solved numerically.

A tubular reactor with axial dispersion was considered as the case study. The reactor can be modelled by a set of nonlinear parabolic partial differential equations. Linearization around the steady state profile of the system results in a set of linear PDEs with spatially varying coefficients. The performance of the formulated controller was compared to a LQ controller based on finite difference algorithm. Simulation results showed that the infinite dimensional controller leads to better performance in terms of l^2-norm of the error.

In Chapter 5, the tools developed for optimal control of parabolic systems in Chapter 4 were extended to the boundary control of an infinite dimensional system

modelled by coupled Parabolic PDE-ODE equations. An exact transformation was introduced to convert the system to a decoupled form. Conditions on existence of such a transformation were studied. Using another transformation, the boundary control problem was formulated as a well-posed infinite dimensional system. It was shown that the resulting system is a Reisz Spectral system and using the properties of the Riesz spectral systems, the stabilizability of the system was proven. Since the transformed well-posed system was a Riesz Spectral system, the LQ controller formulated in Chapter 4 could be applied to it. This chapter took a very important step in controller formulation for more general forms of distributed parameter systems consisting of coupled parabolic and hyperbolic PDEs and ODES.

6.1 Future Work

This thesis took a significant step towards building required tools for solution of optimal control problem for a general class of distributed parameter systems with special focus on catalytic reactors. A number of challenges remain in the development of the infinite dimensional controller for processes modelled by a general form of infinite dimensional systems.

The Robust MPC studied in Chapter 3 used the method of characteristics as a tool to convert the set of hyperbolic equations to state space system. This method performs very well for systems with up to two characteristic equations, but for systems with more than two characteristic equations the computation of the state space model becomes very complicated. The method of characteristics is a special case of invariant transformations in mathematics. For general case of hyperbolic system, an invariant transformation approach might be useful in conversion of PDEs to ODEs. This approach has not been used in engineering and could lead to significant contributions in the area of infinite dimensional controllers.

The method proposed in Chapters 4 and 5 had a limitation on the structure of the operator A. In order to solve the eigenvalue problem it was assumed that the infinite dimensional operator had a triangular form, which means the coupling of the state

variables is one way. Solution of the eigenvalue problem for general form of infinite dimensional operators cannot be performed analytically. For special cases the infinite dimensional operator can be triangularized using a transformation. Exploration of the conditions for existence of such a transformation is the topic that needs to be addressed in future work.

A final important area for future work is to formulate infinite dimensional controllers for systems modelled by a set of hyperbolic-parabolic PDEs. Many chemical processes heat transfer can be represented by a hyperbolic PDE, but mass transfer is modelled by a set of parabolic PDEs. Since the approaches for solution of these two types of PDEs are different, it would be worthwhile to investigate how to exploit two different approaches within one problem.

Bibliography

Aksikas, I. (2005). Analysis and LQ-Optimal Control of Infinite-Dimensional Semilinear Systems: Application to a Plug Flow Reactor. PhD thesis. Université catholique de Louvain.

Aksikas, I., A. Fuxman, J. F. Forbes and J. J. Winkin (2009). LQ-Control Design of a Class of Hyperbolic PDE Systems: Application to Fixed-Bed Reactor. *Automatica* **45**, 1542–1548.

Aksikas, I., A. M. Fuxman and J. F. Forbes (2008*a*). Control of Time Varying Distributed Parameter Plug Flow Reactor by LQR. In: *Proceedings of the IFAC World Congress, Seoul Korea*.

Aksikas, I. and J. F. Forbes (2007). State LQ-Feedback Control of Hyperbolic PDE's Systems : Application to a Fixed-bed Reactor. In: *Proceedings of the European Control Conference, ECC 07, kos, Greece*. pp. 5595–5601.

Aksikas, I., J. J. Winkin and D. Dochain (2008*b*). Optimal LQ-feedback control for a class of first-order hyperbolic distributed parameter systems. *ESAIM: Control, Optimisation and Calculus of Variations*.

Banks, H. T. and K. Kunisch (1984). The linear regulator problem for parabolic systems. *Siam Journal on Control and Optimization* **20**, 684–698.

Bensoussan, A., G. Da Prato, M. C. Delfour and S. K. Mitter (2007). *Representation and Control of Infinite Dimensional Systems*. 2nd ed.. Birkhäuser, Boston.

Byrnes, C.I., D.S. Gilliam, A. Isidori and V.I. Shubov (2006). Zero dynamics modeling and boundary feedback design for parabolic systems. *Mathematical and Computer Modelling* **44**, 857 – 869.

Callier, F.M. and J. Winkin (1992). LQ-Optimal Control of Infinite-Dimensional Systems by Spectral Factorization. *Automatica* **28:4**, 757–770.

Callier, F.M. and J.Winkin (1990). Spectral Factorization and LQ-Optimal Regulation for Multivariable Distributed Parameter Systems. *International Journal of Control* **52**, 55–75.

Camacho, E. F. (1999). *Model Predictive Control*. Springer.

Chen, J., Z. Ring and T. Dabros (2001). Modeling and simulation of a fixed-bed pilot-plant hydrotreater. *Industrial & Engineering Chemistry Research* **40**, 3294–3300.

Choi, J. and K. S. Lee (2005). Model Predictive Control of Cocurrent First-Order Hyperbolic PDE Systems. *Industrial & Engineering Chemistry Research* (44), 1812–1822.

Christofides, P. D. (2001). *Nonlinear and Robust Control of PDE Systems: Methods and Applications to Tarnsport-Reaction Processes*. Birkhäuser.

Curtain, R.F. and H.J. Zwart (1995). *Introduction to Infinite-Dimensional Linear Systems Theory*. Springer-Verlag.

de. Monte, F. (2002). An analytic approach to the unsteady heat conduction processes in one-dimensional composite media. *International Journal of Heat and Mass Transfer* **45**, 1333–1343.

Delattre, C., D. Dochain and J. Winkin (2003). Sturm-liouville systems are riesz-spectral systems. *Applied mathematics and computer science* **13**, 481–484.

Dubljevic, S. and P. D. Christofides (2006). Predictive control of parabolic PDEs with boundary control actuation. *Chemical Engineering Science* **61**(18), 6239 – 6248.

Dubljevic, S., P. Mhaskar, N. H. El-Farra and P. Christofides (2005). Predictive control of transport-reaction processes. *Computers and Chemical Engineering* **29**, 2335–2345.

Emirsajlow, Z. (1999). A Composite Semigroup for the Infinite-Dimensional Differential Sylvester Equation. In: *Proceedings of the 7th Mediterranean Conference on Control and Automation (MEHD99)*.

Emirsjlow, Z. and S. Townley (2000). From pdes with boundary control to the abstract state equation with an unbounded input operator: A tutorial. *European Journal of Control* **6**(1), 27–49.

Friedman, A. (1976). *Partial differential equations*. R. E. Krieger Publishing Company.

Froment, G. F. (1990). *Chemical Reactor Analysis and Design*. Wiley.

Guo, B. Z. and H. J. Zwart (2001). Riesz spectral systems. Memorandum No. 1594. Faculty of Mathematical Science, University of Twente.

Jaree, A., B. Boonsomlanijit and J. Limtrakul (2008). On the dynamic instability of packed-bed reactors in the presence of catalyst deactivation. *Computers & Chemical Engineering* **32**, 2897–2902.

Jaree, A., H. Budman, R. R. Hudgins, P. L. Silveston, V. Yakhnin and M. Menzinger (2001). Temperature excursions in packed bed reactors with an axial variation of catalyst activity. *Catalysis Today* **69**, 137–146.

Kallinikos, L.E., G.D. Bellos and N.G. Papayannakos (2008). Study of the catalyst deactivation in an industrial gasoil HDS reactor using a mini-scale laboratory reactor. *Fuel* **87**(12), 2444 – 2449.

Kappel, F. and D. Salamon (1990). An approximation theorem for algebraic Riccati equation. *Siam Journal on Control and Optimization* **28**, 1136–1147.

Kothare, M. V., V. Balakrishnan and M. Morari (1996). Robust constrained model predictive control using linear matrix inequalities. *Automatica* **32**(10), 1361 – 1379.

Krstic, M. (2009). Compensating a String PDE in the Actuation or Sensing Path of an Unstable ODE. *Automatic Control, IEEE Transactions on* **54**(6), 1362 –1368.

Laub, A. J. (2005). *Matrix analysis for scientists and engineers*. Siam.

Lions, J. L. (1971). *Optimal Control of Systems Governed by Partial Differential Equations*. Springel-Verlag.

Maciejowski, J. M. (2002). *Predictive control with constraints*. Prentice Hall.

Mohammadi, L., I. Aksikas and J. F. Forbes (2009). Optimal Control of a Catalytic Fixed-Bed Reactor with Catalyst Deactivation. In: *Proceedings of the American Control Conference*.

Mohammadi, L., I. Aksikas, S. Dubljevic and J. F. Forbes (2011). Linear Quadratic Optimal Boundary Control of a Diffusion-Convection-Reaction System. In: *Proceedings of the 18th IFAC World Conference*.

Mohammadi, L., I. Aksikas, S. Dubljevic and J. F. Forbes (2012*a*). LQ-boundary control of a diffusion-convection-reaction system. *International Journal of Control* **85**, 171–181.

Mohammadi, L., I. Aksikas, S. Dubljevic, J. F. Forbes and Y. Belhamadia (Submitted 2012*b*). Optimal Control of a Catalytic Fixed-Bed Reactor With Catalyst Deactivation. *Journal of Process Control*.

Mohammadi, L., S. Dubljevic and J. F. Forbes (2010). Robust Characteristic-Based MPC of a Fixed-Bed Reactor. In: *Proceedings of the American Control Conference*.

Muske, K. R. and J. B. Rawlings (1993). Model Predictive Control with Linear Models. *Process Systems Engineering*.

Pandolfi, L. (1992). Existence of Solutions to the Riccati Equation for Time-Varying Distributed Systems. *IMA Journal of Mathematical Control & Information* **9**, 265–273.

Pazy, A. (1983). *Semigroups of Linear Operators and Applications to Partial Differential Equations*. Springer-Verlag.

Rawlings, J. B. (2000). Tutorial overview of model predictive control. *IEEE Control Systems Magazine* **20**(3), 38:52.

Ray, W. H. (1981). *Advanced process control*. McGraw-Hill, New York :.

Rossiter, J. A (2003). *Model-based predictive control:a practical approach*. CRC Press.

Schnaubelt, R. and G. Weiss (2010). Two classes of passive time-varying well-posed linear systems. *Mathematics of Control, Signals, and Systems (MCSS)* **21**, 265–301.

Shang, H., J. F. Forbes and M. Guay (2004). Model predictive control for quasilinear hyperbolic distributed parameter systems. *Industrial & Engineering Chemistry Research* **43**, 2140–2149.

Shang, H., J. F. Forbes and M. Guay (2007). Computationally efficient model predictive control for convection dominated parabolic systems. *Journal of Process Control* **17**, 379–386.

Susto, G.A. and M. Krstic (2010). Control of PDE-ODE cascades with Neumann interconnections. *Journal of the Franklin Institute* **347**(1), 284 – 314.

Weekman, V. W. (1969). Kinetics and dynamics of catalytic cracking selectivity in fixed-bed reactors. *Industrial & Engineering Chemistry: Process Design and Development*.

Winkin, J. J., D. Dochain and P. Ligarius (2000). Dynamical analysis of distributed parameter tubular reactors. *Automatica* **36**(3), 349 – 361.