OPTIMAL BOUNDARY LQ-CONTROL OF SELECTIVE CATALYTIC REDUCTION

by

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Abstract

The objective of this thesis is to design an optimal LQ-boundary controller for SCR, which is a model of coupled parabolic-hyperbolic PDEs with an ODE. The problem is a boundary control one because the manipulated variable **u** is the ammonia gas at the inlet ($z = 0$).Our purpose is to find an optimal $\mathbf{u}^{opt}$ to reduce the amount of NO_x and ammonia slip as much as possible.

The augmented infinite-dimensional state space representation is used to solve the optimal state-feedback control problem. By using the perturbation theorem, the thesis shows that the system generates a C0-semigroup on the augmented state space. Furthermore, the dynamical properties of both the original and the augmented systems are examined. Under some technical conditions, we show that the augmented system generates an exponentially stabilizable and detectable C0-semigroups. The linear-quadratic control problem has been solved for the augmented system. A decoupling technique is implemented to decouple and solve the corresponding Riccati equation. Monolithic catalyst reactor and Selective Catalyst Reduction (SCR) models are used to test the performances of the developed controller through numerical simulations.

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Chapter 1

Introduction

Diesel engine is one of the most extensively used categories of engines in industrial equipment and commercial vehicles, especially in heavy duty ones such as trains, buses, trucks, and ships. This is due to its durability, low cost and also because of the safety of the diesel fuel, since it is less volatile and its vapor less explosive than gasoline [43]. A diesel engine is a compression ignition engine. Air is introduced into the piston during the cylinder downstroke. The piston then moves upwards, compressing the air which increases its temperature and pressure. Near the top of the stroke, fuel is injected, which ignites. The chemical reaction releases heat, which forces the piston down, changing chemical energy into mechanical work. However, diesel engines have many disadvantages, especially environmental ones. The pollution is one of the major drawbacks of diesel engines, especially for NO_x and ammonia slip NH_3 which are dirty and hazardous to health [40]. To deal with this challenging problem many approaches have been developed in various aspects such as improvement of the fuel quality, diesel oxidation catalysts (DOC), diesel particulate filters (DPF) and also exhaust gas recirculation (EGR) to control the oxides nitrogen (NO_x) and the engine efficiency. All of these desirable techniques are called after-treatment techniques. Reduction of NO_x emissions using the selective catalytic reduction (SCR) technology is one of the most cost-effective technologies for this task. SCR can convert NO_x into N_2 with the aid of a catalyst .This is done by injecting urea solution, which is stored in a special tank, into the hot stream at the inlet of SCR, where urea decomposes into gaseous NH_3 and can be stored in the catalyst. After that we use the stored NH_3 to convert NO_x into N_2, H_2O and a small amount of carbon dioxide (CO_2). Nevertheless, the SCR is not a perfect device since there are some technological drawbacks such as its high cost, high back pressure of pipes and space requirement. In addition, there is a risk to produce the ammonia slip during the process. Ammonia slip refers to the emission of ammonia, which is the result of excessive ammonia injection. However, when comparing to its advantages we can say that the SCR technique is one of the most promising technologies which guarantees the reduction of toxic emissions and saves a large amount of fuel [48]. It is obvious that the injection of urea would be the most important factor to get good results in reducing NO_x, however, inappropriate urea injection can lead to bad results. For instance, if we inject an amount of urea that is less than the optimal amount it would result in the insufficient input of NH_3 needed to optimize the reduction of NO_x. On the other side, injecting a higher amount than the optimal one of the urea results in the ammonia slip which is undesirable ([37,38]) and here appears the main challenge. Therefore, we need to build an optimal control system that can reduce the emissions of NO_x and at the same time make sure that the ammonia slip is below the allowed limit. Unfortunately, few studies have been done to perform this task especially because the entire model of SCR is a huge system with a complex Partial differential equations (PDEs).

Partial differential equations (PDEs) are used to describe a wide variety of phenomena in science and engineering. Dynamic systems that are described by PDEs are usually called distributed parameter systems. Control problems for those systems can be studied by using infinite-dimensional state space description. This representation has a main advantage of keeping the distributed nature of the system ([22, 23, 34]). PDEs are classified into hyperbolic, parabolic and elliptic, and each one has its applications in real life. Moreover, the dynamics of some systems can be described by coupled PDEs of different types. In our case, SCR that carries out gas-solid phases, such that the transport phenomena in the gas phase are dominated by convective mechanism and are modeled by first-order hyperbolic PDEs concerning the concentrations and temperature, whereas the dominant transport mechanism of the temperature in the solid phase is diffusion and the transport phenomena are modeled by second-order parabolic PDE. Moreover, in the same solid phase the concentrations are modeled by ODEs.

Linear quadratic (LQ) optimal control plays an important role in the control literature. The linear quadratic regulator design involves the determination of an input signal to drive a linear system from initial state to a desired state while minimizing certain quadratic cost criteria. The main advantage is that the optimal input is expressed as a state feedback that guarantees the exponential stability of the closed-loop system ([20, 23]). The infinite-dimensional state space approach, which is based on the well-known operator Riccati equation, has been used for both hyperbolic PDEs ([5–8, 10, 12, 13, 16, 19]) and parabolic PDEs ([11, 14, 28, 31]). In the hyperbolic case, the operator Riccati equation has been converted into a matrix differential equation, while in the parabolic case, the eigenvalues and eigenfunctions of the system generator have been used to convert the ORE into a set of finite number of algebraic Riccati equations. In [17], optimal control of coupled parabolic and hyperbolic PDEs has been solved by using state-space approach combined with a decoupling base technique to solve the corresponding Riccati equation. The present paper extends the state-space approach to a system of interacting parabolic-hyperbolic PDEs with an ODE. Moreover, the focus here is on a boundary control system in which the input variable appears in the boundary conditions. Hence, an extended state space approach is used to solve the control problem ([23]).

This thesis is organized in the following manner. In Chapter 2, an introduction of Distributed Parameters is presented, then the notion of Semi Group Theory is introduced, and some properties of Reisz spectral operators are shown. Then we highlight the Cauchy problem in a Hilbert space and introduce the method of dealing with the boundary control systems. We also introduce important concepts in the control problems, such as stability, stabilizability and detectability. Finally, we gave a brief idea about the Linear quadratic problems. In chapter 3, we describe of the Linear quadratic (LQ) optimal control in the general case of coupled parabolic-hyperbolic PDEs and an ODE with a description of the scalar coefficients of the non-linear PDEs model of interest and its linearization. Moreover, the augmented infinite-dimensional state-space representation of the linearized system is demonstrated on a Hilbert space. The has been solved for the parabolic subsystem .Also we focuse on the analysis of the dynamical proper ties (generation property, exponential stabilizability and exponential detectability) of the system, which are needed to guarantee the existence and uniqueness of solution of the control problem .Then we show the main work, where the linear-quadratic optimal control problem is solved and develop an algorithm to solve the corresponding operator Riccati equation. We then give an expression of the state feedback regulator. Finally, the case study of monolithic catalytic reactor is studied and our developed algorithm is applied to the reactor model where numerical simulations are performed to show the performances of the LQ-feedback controller. chapter 4 focuses on the entire model of SCR as a case study of the general case the only difference is that the coefficients of the system are not anymore scalars but matrices, so we applied the same algorithm where numerical simulations were performed to show the performances of the LQ-feedback controller in the case of the entire model of SCR.

Chapter 2

Introduction of Distributed Parameters systems

A wide variety of phenomena can be described by partial differential equations (PDEs) and this kind of system is called distributed parameter system. Concerning control problems, distributed parameter systems can be formulated in the same way as lumped parameter systems (those described by ordinary differential equations) just instead of working with finite-dimensional space and matrices we work in appropriate infinite-dimensional space and appropriate operators. The power of the control of infinite-dimensional systems is that you will be able to catch all phenomena, because neglecting the distributed nature of the original system may lead to false conclusion. In the next section we introduce an important notion in the infinite-dimensional systems, which is the semigroup theory.

2.1 Semigroup Theory

In finite-dimensional spaces we always study matrix exponential functions as a solution of any type of our control problem $\dot{x} = Ax + Bu$, so it is natural to ask whether similar properties of those exponential functions can be found in infinite-dimensional spaces. Semigroup can be considered as the exponential function of an operator, which, however, is no longer bounded [24]

Definition 2.1.1. *:*
Let $\mathbb{X}$ be Hilbert space and $(T(t))_{t\geq 0} \subset \mathfrak{L}(\mathbb{X})$ linear bounded operators
$\forall\ t \geq 0$ *T(t):$\mathbb{X} \to \mathbb{X}$ is called C_0-semigroup on $\mathbb{X}$ if it satisfies:*

$$T(0) = I$$

$$T(t+s) = T(t)T(s) \ t, s \geq 0$$

$$T(t)x \to x, t \to 0^{+} \forall x \in \mathbb{X}$$

Example 2.1.1. *If we consider A as a real matrix such that $A \in \mathbb{R}^{m\times m}$, the family $(e^{At})_{t\geq 0}$ is C_0-semigroup on the Hilbert space $\mathbb{R}^n$*

Definition 2.1.2. *Let $(T(t))_{t\geq 0}$ be a C_0-semigroup on Hilbert space H . The operator A is called the infinitesimal generator of the $C_0 -$ semigroup $(T(t))_{t\geq 0}$ if*

$$Ax = \lim_{t\to o^{+}} \frac{T(t)x - x}{t}, \ \forall x \in D(A)$$

D(A) is the set of elements in H such that the limit exists.

Theorem 2.1.1. *Let $(T(t))_{t\geq 0}$ be a $C_0 -$ semigroup on Hilbert space H with the infinitesimal generator A . $\forall x \in D(A)$ and $\forall t \geq 0$ the following properties hold:*
(i) $T(t)x \in D(A)$ *and* $\frac{d}{dt}(T(t)x) = AT(t)x = T(t)Ax$.
(ii) $T(t)x - x = \int_0^t T(z)Axdz$.

As the infinitesimal generator of any C0-semigroup is very important we always need necessary and sufficient conditions for a linear operator on Hilbert space H to be the infinitesimal generator and those conditions are described in the following Hille-Yosida theorem .

Theorem 2.1.2 (Hille-Yosida Theorem)**.** *: Let H be a Hilbert space and A is a linear operator on H. A is the infinitesimal generator of a $C_0 -$ semigroup $(T(t))_{t\geq 0}$ if and only if*
(i) *A is closed and D(A) is dense in H.*
(ii) *there exist positive constants M ,ω and $\beta \in \mathbb{R}$*
$\forall \ \beta > \omega$, *such that $\beta \in \rho(A)$ the resolvent set of A,The following hold*
$\|R(\beta, A)^p\| \leq \frac{M}{(\beta-\omega)^p} \quad \forall p \geq 1$
where $R(\beta, A) = (\beta I - A)^{-1}$ is the resolvent operator
in this case $\|T(t)\| \leq Me^{\omega t}$.

After introducing some notions of a linear operator, we introduce adjoint of this linear operator which is always needed in control problems.

2.1.1 Adjoint of a linear operator

Calculus of Adjoint of linear operator is very important in the domain of control because it is very useful to solve Lyapunov or Reccati equations.
The inner product on Hilbert space H is given by :

$$< x, y >= \overline{< y, x >} = \int_0^1 x(z)\overline{y(z)}dz \quad \forall x, y \in H$$

Definition 2.1.3. *Let $A \in \mathfrak{L}(H_1, H_2)$, where H_1 and H_2 are Hilbert spaces.the adjoint operator is the unique operator $A^* \in \mathfrak{L}(H_2, H_1)$ that satisfies :*

$$< Ax, y >_{H_2} = < x, A^*y >_{H_1}$$

Definition 2.1.4. *Let A be a linear operator on Hilbert space H. D(A) Domaine of definition of A which is supposed to be dense in H. The adjoint operator $A^* : D(A^*) \subset Z \to Z$ of A is defined as follows. $D(A^*) = [y \in H such\ that\ there\ exists\ a\ y^* \in H\ satisfying < Ax, y >=< x, y^* > \forall x \in D(A)]$*
$\forall y \in D(A^*)$ the adjoint operator A^* is defined in terms of y^* by $A^*y = y^*$

Example 2.1.2. *Let $H = \mathbf{L}_2(0, 1)$ and A the operator which is given by :*
$(Ax)(\xi) = -\frac{dx}{d\xi}(\xi)$, where $D(A) = \{x \in \mathbf{L}_2(0, 1)|x$ is absolutely continuous with $\frac{dx}{d\xi} \in \mathbf{L}_2(0, 1), x(0) = 0\}$ A is a closed linear operator .
We caclulate its adjoint as follows:
$< Ax, y >= -\int_0^1 \frac{dx}{d\xi}(\xi)\overline{y(\xi)}d\xi = -[x(\xi)\overline{y(\xi)}]_0^1 + \int_0^1 x(\xi)\frac{\overline{dy}}{d\xi}(\xi)d\xi$
this can be written in the form $< x, y^* >$ if and only if $y(1) = 0$ and $\frac{dy}{d\xi} \in H$ .So $A^*y = \frac{dy}{dx}$ with $D(A^*) = \{y \in \mathbf{L}_2(0, 1)|y$ is absolutely continuous with $\frac{dy}{d\xi} \in \mathbf{L}_2(0, 1), y(1) = 0\}$

Example 2.1.3. *Let $H = \mathbf{L}_2(0, 1)$ and A the operator which is given by :*
$(Ax)(\xi) = -\frac{d^2x}{d\xi^2}(\xi)$, where $D(A) = \{x \in \mathbf{L}_2(0, 1)|x, \frac{dx}{d\xi}$ is absolutely continuous with $\frac{d^2x}{d\xi^2} \in \mathbf{L}_2(0, 1), \frac{dx}{d\xi}(0) = \frac{dx}{d\xi}(1) = 0\}$
A is a closed linear operator .
We caclulate its adjoint as follows:

$$< Ax, y >= \int_0^1 \frac{d^2x}{d\xi^2}(\xi)\overline{y(\xi)}d\xi = [\frac{dx}{d\xi}(\xi)\overline{y(\xi)}]_0^1 - \int_0^1 \frac{dx}{d\xi}(\xi)\frac{d\overline{y}}{d\xi}(\xi)d\xi$$

$$= [x(\xi)\frac{d\overline{y}}{d\xi}(\xi)]_0^1 - \int_0^1 x(\xi)\frac{d^2\overline{y}}{d^2\xi}(\xi)d\xi$$

This can be written in the form $< x, y^* >$ *if and only if* $\frac{dy}{d\xi}(0) = \frac{dy}{d\xi}(1) = 0$ *and* $\frac{d^2y}{d\xi^2} \in H$
So $A^*y = \frac{d^2y}{d\xi^2}$ *with* $D(A^*) = \{y, \frac{dy}{d\xi} \in \mathbf{L}_2(0,1) | y$ *are absolutely continuous with* $\frac{d^2y}{d\xi^2} \in \mathbf{L}_2(0,1), \frac{dy}{d\xi}(0) = \frac{dy}{d\xi}(1) = 0\}$.
In the most of cases concerning linear partial differential systems it is hard to find the exact solution .So we always need to find the best approach to deal with this situation that's it is very important to introduce the following section of Riesz-spectral operators.

2.2 Riesz-spectral operators

This section gives a representation of a large classes of linear partial differential systems of both parabolic and hyperbolic types.

Definition 2.2.1. *A sequence of vectors* $\{\phi_n, n \geq 1\}$ *in Hilbert space* H *can be a Reisz basis for* H *if the following two conditions hold:*

$$(i) \quad \overline{span}\{(\phi_n)_{n\geq 1}\} = H$$

(ii) there exist positive constants r *and* R *such that :* $\forall N \in \mathbb{N}$ *and* $(\alpha_n)_{1<n\leq N} \in \mathbb{R}$

$$r\sum_{n=1}^{N} |\alpha_n|^2 \leq \| \sum_{n=1}^{N} \alpha_n\phi_n\|^2 \leq R\sum_{n=1}^{N} |\alpha_n|^2$$

Theorem 2.2.1. *Let* A *closed linear operator on Hilbert space* H *has simple eigenvalues* $\{\lambda_n, n \geq 1\}$ *and its corresponding eigenvectors* $\{\phi_n, n \geq 1\}$ *form a Riesz basis in* H.
(i) If $\{\psi_n, n \geq 1\}$ *are the eigenvectors of the adjoint of* A *corresponding to the eigenvalues* $\{\lambda_n, n \geq 1\}$*.Then the* $\{\psi_n\}$ *can be suitably scaled so that* $\{\phi_n\}, \{\psi_n\}$ *are biorthogonal*
(ii) $\forall z \in H$ *has a unique representation*

$$z = \sum_{n=1}^{\infty} < z, \psi_n > \phi_n$$

Definition 2.2.2. *Let A be a linear closed operator on a Hilbert space H, with eigenvalues $\{\lambda_n, n \geq 1\}$ and corresponding eigenvectors $\{\phi_n, n \geq 1\}$ form a Riesz basis in H*

A is a Riesz-spectral operator If there is no two points $a, b \in \overline{\{\lambda_n, n \geq 1\}}$ can be joined by segment entirely $\in \overline{\{\lambda_n, n \geq 1\}}$.

The next theorem gives us the representation of operators based on its eigenfunctions and eigenvalues.

Theorem 2.2.2. *Suppose that A is a Riesz-spectral operator with eigenvalues $\{\lambda_n, n \geq 1\}$ and corresponding eigenvectors $\{\phi_n, n \geq 1\}$.$\{\psi_n, n \geq 1\}$ are eigenvectors of A^* such that $< \phi_n, \psi_m >= \delta_{nm}$ .Then A has the following representation :*

$$Az = \sum_{n=1}^{\infty} \lambda_n < z, \psi_n > \phi_n \quad \forall z \in D(A)$$

With

$$D(A) = \{z \in H | \sum_{n=1}^{\infty} |\lambda_n|^2 | < z, \psi_n > |^2 < \infty\}$$

Example 2.2.1. *Let $H = \mathbf{L}_2(0,1)$ and A the operator which is given by :*
$(Ax)(\xi) = -\frac{d^2x}{d\xi^2}(\xi)$, where $D(A) = \{x \in \mathbf{L}_2(0,1) | x, \frac{dx}{d\xi}$ is absolutely continuous with $\frac{d^2x}{d\xi^2} \in \mathbf{L}_2(0,1), \frac{dx}{d\xi}(0) = \frac{dx}{d\xi}(1) = 0\}$
A has the eigenvalues $\lambda_n = -n^2\pi^2, n \geq 0$ and the corresponding eigenvectors $\phi_n(\xi) = \sqrt{2}cos(n\pi\xi)$ for $n \geq 1$, $\phi_0 = 1$ form an orthonormal basis for $\mathbf{L}_2(0,1)$ A is the Riesz-spectral operator given by

$$Az = \sum_{n=1}^{\infty} -2n^2\pi^2 < z, cos(n\pi\xi) > cos(n\pi\xi) \quad \forall z \in D(A)$$

Where

$$D(A) = \{z \in \mathbf{L}_2(0,1) | \sum_{n=1}^{\infty} n^4\pi^4 | < z, \sqrt{2}cos(n\pi\xi) > |^2 < \infty\}.$$

2.3 Cauchy Problem in a Hilbert space

Let A be the infinitesimal generator of a $C_0 - semigroup$ $(T(t))_{t\geq 0}$ on H homogenous Cauchy problem is given by:

$$\begin{cases} \dot{x}(t) = Ax(t) \quad t \geq 0 \\ x(0) = x_0 \in D(A) \end{cases} \tag{2.1}$$

Based on Theorem 3.1.1 the solution of this Cauchy problem is that :

$$x(t) = T(t)x_0$$

On the other hand the non-homogeneous Cauchy problem is that:

$$\begin{cases} \dot{x}(t) = Ax(t) + f(t) & t \geq 0 \\ x(0) = x_0 \in D(A) \end{cases} \tag{2.2}$$

Definition 2.3.1. *x(t) is a classical solution of* (2.2) *on* $[0, t_f]$ *if the following properties hold:*
(i) the function x *and its derivative are continuous on* $[0, t_f]$
(ii) $x(t) \in D(A)$ *and satisfies* (2.2) $\forall t \in [0, t_f]$

Remark 1. *x(t) is the solution of* (2.2) *on* $[0, \infty)$ *if x(t) is the classical solution on* $[0, t_f]$ $\forall t \in [0, t_f]$

if f is a continuous function on $[0, t_f]$ and x is a classical solution of (2.2) on $[0, t_f]$.So $Ax(.)$ is a continuous function on $[0, t_f]$ and x is given by:

$$x(t) = T(t)x_0 + \int_0^t T(t-\theta)f(\theta)d\theta \tag{2.3}$$

2.3.1 Perturbations and Triangular systems

In control f of the non-homogeneous Cauchy problem is determined by the following state feedback:

$$f(t) = Dx(t) \quad D \in \mathfrak{L}(H)$$

The new Cauchy problem :

$$\begin{cases} \dot{x}(t) = (A + D)x(t), & t \geq 0 \\ x(0) = x_0 \end{cases} \tag{2.4}$$

With the corresponding mild solution:

$$x(t) = T(t)x_0 + \int_0^t T(t-\theta)Dx(\theta)d\theta$$

Theorem 2.3.1. *The operator* $A+D$ *is the infinitesimal generator of a* C_0-*semigroup* $(T_D(t))_{t\geq 0}$ *which is the unique solution of the following equation*

$$T_D(t)x_0 = T(t)x_0 + \int_0^t T(t-\theta)DT_D(\theta)x_0 d\theta, \quad x_0 \in H$$

In a large scale of control applications , we often deal with multivariable and coupled systems . It may be easier to make those systems on the triangular form to use the next theorem, which gives us a good way to deal with $C_0 - semigroup$ generated by multivariable triangular operator from the one which is generated by the diagonal entries of such operator

Theorem 2.3.2. *A_1 and A_2 are the infinitesimal generators of respective $C_0 -$ semigroups $T_1(t)$ and $T_2(t)$ on respective Hilbert spaces H_1 and H_2 Assume that :*
$\|T_i(t)\| \leq M_i e^{r_i t}$, $\quad i = 1, 2.$ *and* $D \in \mathfrak{L}(H_1, H_2)$ *Then the operator* $A = \begin{pmatrix} A_1 & 0 \\ D & A_2 \end{pmatrix}$
is the infinitesimal generator of the $C_0 - semigroup$ $T(t)$ on $H = H_1 \oplus H_2$
with $D(A) = D(A_1) \oplus D(A_2)$, $T(t) = \begin{pmatrix} T_1(t) & 0 \\ S(t) & T_2(t) \end{pmatrix}$ *and ,*
$S(t)x = \int_0^t T_2(t - \theta) D T_1(\theta) d\theta$

2.3.2 Boundary control systems

In many applications the model does not fit into the standard formulation (2.2). Therefore we need to reformulate this problem to get the standard form and that is possible for sufficiently inputs. However to do that we need to extend the state space. Let a class of abstract boundary control problems to be on this form:

$$\begin{cases} \dot{x}(t) = \mathfrak{A}x(t), \quad x(0) = x_0 \\ \mathfrak{B}x(t) = u(t), \\ y(t) = Cx(t), \end{cases} \tag{2.5}$$

where $\mathfrak{A} : D(\mathfrak{A}) \subset H \to H$, $u(t) \in U$ a separable Hilbert space
$\mathfrak{B} : D(\mathfrak{B}) \subset H \to U$ such that $D(\mathfrak{A}) \subset D(\mathfrak{B})$

Definition 2.3.2. *The control system* (2.5) *is considered a boundary control system if the following hold:*
(i) The operator $A : D(A) \to H$ which is defined by:
$Ax = \mathfrak{A}x \quad \forall x \in D(A)$ *with* $D(A) = D(\mathfrak{A}) \cap D(\mathfrak{B})$ *is the infinitesimal generator of a $C_0 - semigroup$ on H*
(ii) There exists a $B \in \mathfrak{L}(U, H)$ such that $\forall u \in U, Bu \in D(\mathfrak{A})$. the operator $\mathfrak{A}\mathfrak{B}$ is an element of $\mathfrak{L}(U, H)$ and $\mathfrak{B}Bu = u, u \in U$

Let suppose that (2.5) is a boundary control system .The following abstract differential equation on H is well posted

$$\begin{cases} \dot{z}(t) = Az(t) - B\dot{u}(t) + \mathfrak{A}Bu(t), \\ z(0) = z_0 \end{cases} \tag{2.6}$$

Theorem 2.3.3. *Lets take the boundary control system* (2.5) *and the abstract Cauchy problem* (2.6)*.by considering that* $u \in \mathbf{C}^2([0,\tau];U)$ $\forall \tau > 0$.
if $z_0 = x_0 - Bu(0) \in D(A)$*, then the relation between the solutions of* (2.5) *and* (2.6) *is :*

$$z(t) = x(t) - Bu(t)$$

and the classical solution of (2.5) *is unique*

However, and after reformulating (2.5) to (2.6) the derivative of the control term is included, and to avoid this undesirable term we have to extend the state space to $H^e = U \oplus H$ and we put the new augmented state as follows: $x^e(t) = \begin{pmatrix} u(t) \\ z(t) \end{pmatrix}$, and the new input is $\tilde{u} = \dot{u}$.Then we get the new augmented system :

$$\dot{x}^e(t) = \begin{pmatrix} 0 & 0 \\ \mathfrak{A}B & A \end{pmatrix} x^e(t) + \begin{pmatrix} I \\ -B \end{pmatrix} \tilde{u}(t) \tag{2.7}$$

$$x^e(0) = \begin{pmatrix} (x_0^e)_1 \\ (x_0^e)_2 \end{pmatrix}$$

2.4 Stability, Stabilizability,and Detectability

In the design of feedback controls the stability is one of the most important phenomena.It is always desirable to guarantee this aspect of stability.

2.4.1 exponential stability

Definition 2.4.1. *A* C_0*-semigroup* $(T(t))_{t\geq 0}$ *on a Hilbert space* H *is exponentially stable if there exist positive constants* M *and* r *such that:* $\|T(t)\| \leq Me^{-rt} \quad t \geq 0$
r *is called the decay rate*

An important criterion to prove the exponential stability is Lyapunov criterion

Theorem 2.4.1. *Let $(T(t))_{t\geq 0}$ be C_0- semigroup on Hilbert space H, and A be its infinitesimal generator.*

$(T(t))_{t\geq 0}$ is exponentially stable if and only if there exists a positive operator $P \in \mathfrak{L}(H)$ which is the solution of the following Lyapunov algebraic equation

$$PAx + A^*Px + x = 0 \quad \forall x \in D(A) \text{ such that } P(D(A)) \subset D(A^*)$$

2.4.2 Exponential stabilizability and detectability

Definition 2.4.2. *Let A be the infinitesimal generator of the C_0- semigroup T(t) on Hilbert space H and $B \in \mathfrak{L}(U,H)$, where U is a Hilbert space .*
(i) We say that $\sum(A,B,-)$ is exponentially stabilizable if there exists a feedback operator $K \in \mathfrak{L}(H,U)$ such that $A+BK$ generates an exponentially stable C_0-semigroup $T_{BK}(t)$
Let $C \in \mathfrak{L}(H,Y)$ which Y is a Hilbert space
(ii) We say that $\sum(A,-,C)$ is exponentially detectable if there exists an operator $L \in \mathfrak{L}(Y,H)$ such that $A+LC$ generates an exponentially stable C_0- semigroup $T_{LC}(t)$

To relate between the stability and detectability properties of the boundary control systems to the extended systems we introduce the following theorem:

Theorem 2.4.2. *Considering that the boundary control system (2.5) is exponentially stabilizable $\sum(A,B,C)$ and its extended system is that $\sum(A^e,B^e,C^e)$,*
(i) Assuming that $0 \in \rho(A)$ and $\mathfrak{A}B \neq 0$ the $\sum(A^e,B^e,C^e)$ is exponentially stabilizable if and only if

$$ker(sI \quad (\mathfrak{A}B)^*) \cap ker(0 \quad (sI-A)^*) \cap ker(I \quad -B^*) = 0 \quad \forall s \in \overline{\mathbb{C}_0^+}$$

(ii) Assuming that $0 \in \rho(A)$, the $\sum(A^e,B^e,C^e)$ is exponentially detectable if and only if

$$ker(sI - A^e) \cap kerC^e = \{0\}$$

2.5 Linear Quadratic problem

LQ-optimal control is widely used in control problems for infinite-dimensional state space systems which can be obtained from the Operator Riccati Algebraic Equation. Let, $\sum(A, B, C)$ denote the following linear time-invariant infinite-dimensional state-space systems:

$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t), \quad x(0) = x_0 \\ y(t) = Cx(t) \end{cases} \tag{2.8}$$

Such that the state $x(t) \in H$ a real separable Hilbert space with inner product $< ., . >$, the input $u(t) \in U$ and the output $y(t) \in Y$, where U and Y are real separable Hilbert spaces also $B \in \mathfrak{L}(U, H)$,$C \in \mathfrak{L}(U, H)$

Let put the cost functional as follow:

$$I(x_0; u) = \int_0^{\infty} (< y(p), y(p) > + < u(p), u(p) >)dp \tag{2.9}$$

Our main goal is to minimize this cost functional. According to Zwart and Curtain([23]) if the system $\sum(A, B, C)$ is exponentially stabilizable then $\forall x_0 \in H$ and there exists an input $u \in \mathbf{L}^2([0, \infty); U)$ such that the cost functional I is finite. That's why the exponential stabilizability guarantees the well posedness of the minimization problem. We can get this optimal feedback by solving the following Operator Riccati Algebraic Equation .:

$$[A^*Q + QA + C^*C - QBB^*Q]x = 0 \forall x \in D(A); \tag{2.10}$$

where $Q \in \mathfrak{L}(H)$ is a positive $self-adjoint$ operator and $Q(D(A)) \subset D(A^*)$.

Theorem 2.5.1. *Consider the infinit-dimenstional system* $\sum(A, B, C)$. *Assume that* (A, B) *is exponentially stabilizable and* (C, A) *is exponentially detectable. The Operator Riccati Algebraic Equation* (2.10) *has a unique positive self-adjoint solution* $Q \in \mathfrak{L}(H)$ *and* $\forall x_0 \in H$. *The functional cost I is minimized by the unique control* u_{opt} *which is :*

$$u_{opt}(t) = Kx(t) \ t \geq 0, \quad x(t) = e^{(A+BK)t}x_o;$$

where $K = -B^*Q \in \mathfrak{L}(H, U)$

The feedback semigroup $(e^{(A+BK)t})_{t \geq 0}$ is exponentially stable .

Chapter 3

Control of parabolic-hyperbolic PDEs-ODE

3.1 Mathematical Model

In this chapter, we are interested in the following coupled 3 by 3 parabolic-hyperbolic PDEs and ODE in one spatial dimension.

$$\begin{cases} \dfrac{\partial z_p}{\partial t} = d\dfrac{\partial^2 z_p}{\partial \xi^2} + f_1(z_p, z_h, k) \\ \dfrac{\partial z_h}{\partial t} = -v\dfrac{\partial z_h}{\partial \xi} + f_2(z_p, z_h, k) \\ \dfrac{dk}{dt} = f_3(z_p, z_h, k) \end{cases} \tag{3.1}$$

with the following initial and boundary conditions

$$\begin{gathered} \frac{\partial z_p}{\partial \xi}|_{\xi=0} = \frac{\partial z_p}{\partial \xi}|_{\xi=1} = 0 \quad \text{and} \quad z_h(\xi = 0) = z_{h,in} \\ z_p(\xi, 0) = z_{p,0}(\xi) \text{ and } z_h(\xi, 0) = z_{h,0}(\xi) \text{ and } k(0) = k_0 \end{gathered} \tag{3.2}$$

where $(z_p, z_h, k) \in H = L^2(0,1) \times L^2(0,1) \times \mathbb{R}$ denotes the state variables of the system, $\xi \in [0,1]$ and $t \in [0,\infty)$ represent the space variable and time, respectively. The functions f_1, f_2 and f_3 are non-linear continuous functions. The function $z_{h,in} \in L^2(0,1)$ is the input variable. The parameter d and v are positive constants.

To solve the corresponding linear-quadratic control problem, the linearization of the above system around a steady-state profile is needed. For this purpose, let us denote by $z_{p,ss}$ and $z_{h,ss}$ and k_{ss} the components of the system steady state.

$$\left\{\begin{array}{rcl}\dfrac{\partial \tilde{z}_p}{\partial t} &=& d\dfrac{\partial^2 \tilde{z}_p}{\partial \xi^2}+m_{11}(\xi)\tilde{z}_p+m_{12}(\xi)\tilde{z}_h+m_{13}(\xi)\tilde{k}\\ \dfrac{\partial \tilde{z}_h}{\partial t} &=& -v\dfrac{\partial \tilde{z}_h}{\partial \xi}+m_{21}(\xi)\tilde{z}_p+m_{22}(\xi)\tilde{z}_h+m_{23}(\xi)\tilde{k}\\ \dfrac{d\tilde{k}}{dt} &=& m_{31}(\xi)\tilde{z}_p+m_{32}(\xi)\tilde{z}_h+m_{33}(\xi)\tilde{k}\end{array}\right. \tag{3.3}$$

with the following new initial and boundary conditions

$$\begin{array}{l}\dfrac{\partial \tilde{z}_p}{\partial \xi}|_{\xi=0}=0 \qquad \dfrac{\partial \tilde{z}_p}{\partial \xi}|_{\xi=l}=0 \quad \text{and} \qquad \tilde{z}_h(\xi=0)=z_h(\xi=0)-z_{h,ss}(\xi=0)\\ \tilde{z}_p(\xi,0)=z_{p,0}(\xi)-z_{p,ss}(\xi),\ \tilde{z}_h(\xi,0)=z_{h,0}(\xi)-z_{h,ss}(\xi) \text{ and } \tilde{k}(0)=k_0-k_{ss}\end{array} \tag{3.4}$$

where $\tilde{z}_p = z_p - z_{p,ss}$, $\tilde{z}_h = z_h - z_{h,ss}$, and $\tilde{k} = k - k_{ss}$ are the state variables in deviation form and the functions $m_{ij}, 0 \le i, j \le 3$ are the Jacobians of the nonlinear terms evaluated at the system steady state.

$$m_{11}(\xi)=\frac{\partial f_1(z_p,z_h,k)}{\partial z_p}|_{ss}, \qquad m_{12}(\xi)=\frac{\partial f_1(z_p,z_h,k)}{\partial z_h}|_{ss}, \qquad m_{13}(\xi)=\frac{\partial f_1(z_p,z_h,k)}{\partial k}|_{ss}$$

$$m_{21}(\xi)=\frac{\partial f_2(z_p,z_h,k)}{\partial z_p}|_{ss}, \qquad m_{22}(\xi)=\frac{\partial f_2(z_p,z_h,k)}{\partial z_h}|_{ss}, \qquad m_{23}(\xi)=\frac{\partial f_1(z_p,z_h,k)}{\partial k}|_{ss}$$

$$m_{31}(\xi)=\frac{\partial f_3(z_p,z_h,k)}{\partial z_p}|_{ss}, \qquad m_{32}(\xi)=\frac{\partial f_3(z_p,z_h,k)}{\partial z_h}|_{ss}, \qquad m_{33}(\xi)=\frac{\partial f_3(z_p,z_h,k)}{\partial k}|_{ss}.$$

Let us denote by $z = \begin{bmatrix} \tilde{z}_p & \tilde{z}_h & \tilde{k} \end{bmatrix}^T$ the new state and by $w = \tilde{z}_h(\xi = 0)$ the new input. Then, the above linear system can be formulated as an abstract boundary control problem on the Hilbert space H [23],

$$\left\{\begin{array}{l}\dfrac{dz(t)}{dt}=\mathfrak{A}z(t) \qquad z(0)=z_0\\ \mathcal{B}z(t)=w(t)\end{array}\right. \tag{3.5}$$

where $\mathfrak{A}$ is the linear operator defined by

$$\mathfrak{A}=\begin{bmatrix} d\dfrac{\partial^2}{\partial \xi^2}+m_{11}(\xi) & m_{12}(\xi) & m_{13}(\xi)\\ m_{21}(\xi) & -v\dfrac{\partial}{\partial \xi}+m_{22}(\xi) & m_{23}(\xi)\\ m_{31}(\xi) & m_{32}(\xi) & m_{33}(\xi)\end{bmatrix} \tag{3.6}$$

on its domain of definition

$$D(\mathfrak{A})=\left\{z\in H: \tilde{z}_p,\tilde{z}_h,\frac{d\tilde{z}_p}{d\xi} \text{ are absolutely continous}, \frac{d\tilde{z}_h}{d\xi}\times\frac{d\tilde{z}_p}{d\xi}\times\frac{d^2\tilde{z}_p}{d\xi^2}\in(L^2(0,1))^3\right.$$

and $\frac{\partial \tilde{z}_p}{\partial \xi}|_{\xi=0} = 0)$, and $\frac{\partial \tilde{z}_p}{\partial \xi}|_{\xi=l} = 0\Big\}$.
The input operator $\mathcal{B} : H \to \mathbb{R}$ is given by

$$\mathcal{B} = \left[\begin{array}{ccc} 0 & I_{\xi=0} & 0 \end{array}\right]$$

The objective is to find an operator $B \in \mathcal{L}(\mathbb{R}, H)$ such that for all $w \in \mathbb{R}$, $Bw \in D(\mathfrak{A})$, the operator $\mathfrak{A}B$ is an element of $\mathcal{L}(\mathbb{R}, H)$ and $\mathcal{B}Bw = w$. If B is chosen under the following form

$$B = \left[\begin{array}{c} b_p(\xi) \\ b_h(\xi) \\ b_k(\xi) \end{array}\right] \cdot I \tag{3.7}$$

then the condition $Bu \in D(\mathfrak{A})$ is satisfied if:

$$\frac{d(b_p(\xi)w)}{d\xi}(\xi = 0) = w\frac{db_p}{d\xi}(\xi = 0) = 0 \Leftrightarrow \frac{db_p}{d\xi}(\xi = 0) = 0 \tag{3.8}$$

and

$$\frac{d(b_p(\xi)w)}{d\xi}(\xi = l) = w\frac{db_p}{d\xi}(\xi = l) = 0 \Leftrightarrow \frac{db_p}{d\xi}(\xi = l) = 0 \tag{3.9}$$

Also, the condition $\mathcal{B}Bw = w$ is satisfied if:

$$(b_h(\xi)w)_{|\xi=0} = b_{h_{|\xi=0}}w = w \Leftrightarrow b_h(\xi = 0) = 1 \tag{3.10}$$

Now we are in a position to define the operator $A : D(A) \to H$ by $Az = \mathfrak{A}z$ on its domain $D(A) = D(\mathfrak{A}) \bigcap ker(\mathcal{B})$. Let us consider the new state $v(t) = z(t) - Bw(t)$ and the new input $u(t) = \dot{w}(t)$. Then

$$\dot{v}(t) = \dot{z}(t) - B\dot{w}(t) = \mathfrak{A}z(t) - B\dot{w}(t)$$

$$= \mathfrak{A}(v(t) + Bw(t)) - B\dot{w}(t) = Av(t) - Bu(t) + \mathfrak{A}Bw(t)$$

By using the augmented state $x = \left[\begin{array}{c} w \\ v \end{array}\right] \in \mathcal{H} := \mathbb{R} \oplus H$, the system can be written as follows

$$\begin{cases} \dot{x}(t) = \hat{A}x(t) + \hat{B}u(t) \qquad x(0) = x_0 \\ y(t) = \hat{C}x(t) \end{cases} \tag{3.11}$$

where the operators $\hat{A}, \hat{B}$ and $\hat{C}$ are given by

$$\hat{A} = \left[\begin{array}{cc} 0 & 0 \\ \mathfrak{A}B & A \end{array}\right]; \quad \hat{B} = \left[\begin{array}{c} I \\ -B \end{array}\right], \quad \hat{C} = C[B \quad I] \tag{3.12}$$

The operator $\mathfrak{A}B$ is given by

$$\mathfrak{A}B = \begin{bmatrix} (\mathfrak{A}B)_1 \\ (\mathfrak{A}B)_2 \\ (\mathfrak{A}B)_3 \end{bmatrix} = \begin{bmatrix} d\frac{\partial^2}{\partial\xi^2} + m_{11} & m_{12} & m_{13} \\ m_{21} & -v\frac{\partial}{\partial\xi} + m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{bmatrix} \begin{bmatrix} b_p \\ b_h \\ b_k \end{bmatrix}$$

Due to the fact that the operator $\mathfrak{A}B$ acts on elements on R (space independent elements), then if we assume that the functions b_p and b_h are constants (In this case and according to Equation (4.31) b_h should equal to 1), the operator $\mathfrak{A}B$ can be simplified and becomes

$$\mathfrak{A}B = \begin{bmatrix} m_{11}b_p + m_{12} + m_{13}b_k \\ m_{12}b_p + m_{22} + m_{23}b_k \\ m_{31}b_p + m_{32} + m_{33}b_k \end{bmatrix} \cdot I := \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{bmatrix} \cdot I$$

In this case, the operator $\hat{B}$ becomes

$$\hat{B} = \begin{bmatrix} 1 \\ -b_p \\ -1 \\ -b_k \end{bmatrix} \cdot I \tag{3.13}$$

3.2 Eigenvalues Problem

In functional analysis the eigenvectors of a compact self-adjoint operator form an orthogonal basis for the Hilbert space, but for large classes of linear partial differential systems of parabolic and hyperbolic types the operators are non-self-adjoint, whose eigenvectors may not be orthogonal but that do form a Riesz basis, which is a very important concept. Indeed, any element in the state space can be uniquely represented as a linear combination of the Riesz basis (even if the basis is not orthogonal) by using the corresponding bi-orthogonal sequence (i.e. the eigenfunctions of the adjoint operator). This concept plays an important role in view of solving the Riccati equation associated with the parabolic subsystem. In this section, the eigenvalues and eigenfunctions of parabolic operator A_{11} are found, which are used in Section 4.3 to solve the optimal control problem.

$$A_{11} = d\frac{d^2\cdot}{d\xi^2} + m_{11}(\xi) \cdot I$$

The domain of definition of A_{11} is:

$$D(A_{11}) = \{z \in L^2(0,1) : z \text{ and } \frac{dz}{d\xi} \text{ are absolutely continuous} \frac{dz}{d\xi}_{|\xi=0} = \frac{dz}{d\xi}_{|\xi=1} = 0\}$$

If λ is an eigenvalue of the operator A_{11} and ϕ is the eigenfunction associated with λ. The eigenvalue problem associated with the operator A_{11} is given by

$$A_{11}\phi(\xi) = \lambda\phi(\xi)$$

which can be written as:

$$\begin{aligned} &d\frac{d^2\phi(\xi)}{d\xi^2} + (m_{11}(\xi) - \lambda)\phi(\xi) = 0, \qquad \xi \in [0,1] \\ &\phi'(0) = \phi'(1) = 0 \end{aligned} \tag{3.14}$$

The above problem is challenging due to the fact that $\alpha = m_{11}(\xi) - \lambda$ is space-dependent. To address this issue, we divide the interval $[0, 1]$ into a finite number of segments (h), such that the value of α is constant at each segment and equal to the average value of the function $\alpha(\xi)$, which is defined by

$$\overline{\alpha}_i = h\int_{(i-1)/h}^{i/h} \alpha(\xi)d\xi, \quad i = 1, 2, \cdots, h$$

Under this assumption, the boundary value problem (3.14) can be approximated by:

$$\frac{d^2\phi_i(\xi)}{d\xi^2} + \frac{m_{11}(\xi_i) - \lambda_i}{d}\phi_i(\xi) = 0, \qquad \xi \in [\xi_i, \xi_{i+1}], \quad i = 1, 2, \cdots, s \tag{3.15}$$

subject to boundary conditions:

$$\phi_1'(0) = 0 \tag{3.16}$$

$$\phi_{i-1}(\xi_i) = \phi_i(\xi_i), \quad \phi_{i-1}'(\xi_i) = \phi_i'(\xi_i), \quad i = 2, 3, \cdots, s \tag{3.17}$$

$$\phi_s'(1) = 0 \tag{3.18}$$

Condition (3.17) is a consequence of the fact that ϕ and ϕ' are absolutely continuous. Each boundary value problem has a non-trivial solution if

$$\omega_i^2 = \frac{m_{11}(\xi_i) - \lambda_i}{d} > 0, \quad i = 1, 2, \cdots, s \tag{3.19}$$

Under this condition, the solution of (3.15) is given by :

$$\phi_i(\xi) = a_i \sin(\omega_i\xi) + b_i \cos(\omega_i\xi), \quad \xi \in [\xi_i, \xi_{i+1}], \quad i = 1, 2, \cdots, s \tag{3.20}$$

where a_i and b_i are integration constants. Observe that conditions (3.16)-(3.18) consists of 2s equations, however, 3s unknowns (a_i, b_i and ω_i) should be found. Then to simplify the calculations, it is assumed that for all $1 \leq i \leq s$, $a_i = b_i - b_1$ (this assumption is compatible with condition (3.16) which gives us that $a_1 = 0$). In this case, the eigenfunctions are given by

$$\phi_i(\xi) = b_i\left[\cos\left(\omega_i \xi\right) + \sin\left(\omega_i \xi\right)\right] - b_1 \sin\left(\omega_i \xi\right), \quad \xi \in [\xi_i, \xi_{i+1}],\ i = 1, 2, \cdots, s \quad (3.21)$$

Conditions (3.17) can be rewritten explicitly for all $1 \leq i \leq s$ as follows

$$b_i\left[\sin(\omega_i\xi_i) + \cos(\omega_i\xi_i)\right] - b_{i-1}\left[\sin(\omega_{i-1}\xi_i) + \cos(\omega_{i-1}\xi_i)\right] = b_1\left[\sin(\omega_i\xi_i) - \sin(\omega_{i-1}\xi_i)\right] \quad (3.22)$$

and

$$b_1\left[\omega_i \cos(\omega_i\xi_i) - \omega_{i-1}\cos(\omega_{i-1}\xi_i)\right] = b_i\omega_i\left[\cos(\omega_i\xi_i) - \sin(\omega_i\xi_i)\right] + b_{i-1}\omega_{i-1}\left[\sin(\omega_{i-1}\xi_i) - \cos(\omega_{i-1}\xi_i)\right] \quad (3.23)$$

The above equations can be written in the following compact form

$$\begin{bmatrix} A_i & B_i \\ A_i' & B_i' \end{bmatrix}\begin{bmatrix} b_i \\ b_{i-1} \end{bmatrix} = \begin{bmatrix} C_i \\ C_i' \end{bmatrix} \quad (3.24)$$

where $A_i, B_i, C_i, A_i', B_i'$ and C_i' are given by

$$\begin{cases} A_i = \sin(\omega_i\xi_i) + \cos(\omega_i\xi_i) \\ B_i = -\sin(\omega_{i-1}\xi_i) - \cos(\omega_{i-1}\xi_i) \\ C_i = b_1\left[\sin(\omega_i\xi_i) - \sin(\omega_{i-1}\xi_i)\right] \\ A_i' = \omega_i\left[\cos(\omega_i\xi_i) - \sin(\omega_i\xi_i)\right] \\ B_i' = \omega_{i-1}\left[\sin(\omega_{i-1}\xi_i) - \cos(\omega_{i-1}\xi_i)\right] \\ C_i' = b_1\left[\omega_i\cos(\omega_i\xi_i) - \omega_{i-1}\cos(\omega_{i-1}\xi_i)\right] \end{cases} \quad (3.25)$$

The solution of Equation (3.24) is given by (provided $\Delta_i = A_iB_i' - A_i'B_i \neq 0$)

$$b_i = \frac{B_i'C_i - B_iC_i'}{\Delta_i} \quad \text{and} \quad b_{i-1} = \frac{A_iC_i' - A_i'C_i}{\Delta_i} \quad (3.26)$$

which leads to the following relation between $\omega_i, \omega_{i-1}, and\ \omega_{i-2}$

$$\frac{B_{i-1}'C_{i-1} - B_{i-1}C_{i-1}'}{\Delta_{i-1}} = \frac{A_iC_i' - A_i'C_i}{\Delta_i} \quad (3.27)$$

On the other hand, Equation (3.18) implies

$$b_s\omega_s\cos(\omega_s) - b_s\omega_s\sin(\omega_s) - b_1\omega_s\cos(\omega_s) = 0 \quad (3.28)$$

and then

$$b_s = \frac{b_1}{1 - \tan(\omega_s)} \tag{3.29}$$

Also, by using the expression of ω_s in Equation (3.26), one gets

$$\frac{b_1}{1 - \tan(\omega_s)} = \frac{B_s' C_s - B_s C_s'}{\Delta_s} := h(\omega_s, \omega_{s-1}) \tag{3.30}$$

To get all ω_i, it is assumed that ω_s is known. Here it is chosen to be an infinite sequence of the form $\omega_s = (\omega_s^n)_{n\geq 1} = (n\pi)_{n\geq 1}$. In this case, Equation (3.29) implies that $b_s = b_1$ and consequently $\phi_s^n = b_s \cos(\omega_s^n \xi)$. If we choose $b_s = b_1 = \sqrt{2}$, then the orthonormality of the base ϕ_i^n is guaranteed. Therefore, $\omega_{s-1} = (\omega_{s-1}^n)_{n\geq 1}$ can be found by solving Equation (3.30). Finally, we can get all ω_i^n by solving Equation (3.27). The corresponding eigenvalues are given by the following equation:

$$\lambda_i^n = m_{11}(\xi_i) - d(\omega_i^n)2 \tag{3.31}$$

3.3 Dynamical System Properties

This section is devoted to the dynamical properties of system such as generation property, exponential stabilizability and exponential detectability. These properties are needed to guarantee the existence and the uniqueness of the solution of LQ-control problem. The following result holds.

Lemma 1. Let us consider the operator $\hat{A}$ defined by Equation (4.33), then $\hat{A}$ is the infinitesimal generator of a C_0 semigroup on $\mathcal{H}$.

Proof. According to [23, Lemma 3.2.2], it is enough to show that A is infinitesimal generator of a C_0-semigroup on H since $\mathfrak{A}B \in \mathcal{L}(\mathbb{R}, H)$. Note that the operator A given by (4.38a) can be written as

$$A = \begin{bmatrix} d\dfrac{\partial^2}{\partial \xi^2} & 0 & 0 \\ 0 & -v\dfrac{\partial}{\partial \xi} & 0 \\ 0 & 0 & m_{33} \end{bmatrix} + \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & 0 \end{bmatrix} := A_0 + D$$

The operator $d\dfrac{\partial^2}{\partial \xi^2}$ is the infinitesimal generator of C_0-semigroup on $L^2(0,1)$ (see Example 2.3.7 in [23]). Also, the operator $-v\dfrac{\partial}{\partial \xi}$ is the infinitesimal generator of

C_0-semigroup on $L^2(0,1)$ (see Example 2.2.4 in [23]). Hence, the operator $\mathbf{A}_0$ is the generator of a C_0-semigroup on H since all diagonal entries of A_0 are the generators of C_0-semigroups (see [23, Lemma 3.2.2].

On the other hand, D is a bounded operator (since all the functions $m_{ij}, 1 \leq i,j \leq 3$ are bounded), therefore we can conclude by the perturbation theorem that the operator A generates a C_0-semigroup on H, see [23, Theorem 3.2.1]. $\square$

The following result states that, under some technical conditions, the functions b_p and b_k can be chosen to guarantee the exponential stabilizability of the pair $(\hat{A}, \hat{B})$.

Proposition 1. Let us consider the operator pair (A, B), where A and B are given by Equations (4.38a) and (4.38b), respectively. Then, b_p and b_k can always be chosen to guarantee that there exists an operator $K \in \mathcal{L}(H, \mathbb{R})$ such that $A + BK$ generates an exponentially stable C_0-semigroup on H. Moreover, if $0 \in \rho(A)$ and $\forall s \in \overline{\mathbb{C}_0^+}$, $ker(sI \quad (\mathfrak{A}B)^*) \cap ker(0 \quad (sI - A^*)) \cap ker(I \quad - B^*) = \{0\}$, then the operator pair $(\hat{A}, \hat{B})$ generates an exponentially stabilizable C_0-semigroup on $\mathcal{H}$.

Proof. First, let us prove the exponential stabilizability of (A, B). If $K = [k_1, k_2, k_3] \in \mathcal{L}(H, \mathbb{R})$, then the operator $A + BK$ can be expressed as follows

$$A + BK = \begin{bmatrix} d\frac{\partial^2}{\partial \xi^2} + m_{11} + b_p k_1 & m_{12} + b_p k_2 & m_{13} + b_p k_3 \\ m_{21} + k_1 & -v\frac{\partial}{\partial \xi} + m_{22} + k_2 & m_{23} + k_3 \\ m_{31} + b_k k_1 & m_{32} + b_k k_2 & m_{33} + b_k k_3 \end{bmatrix}$$

Now let us choose $k_1 = -(\beta + m_{11}) b_p^{-1} (\beta > 0)$, $k_2 = -m_{12} b_p^{-1}$ and $k_3 = -m_{13} b_p^{-1}$ and substitute in the operator $A + BK$. This results the following form

$$A + BK = \begin{bmatrix} d\frac{\partial^2}{\partial \xi^2} - \beta & 0 & 0 \\ m_{21} + k_1 & -v\frac{\partial}{\partial \xi} + \alpha_{11} & \alpha_{12} \\ m_{31} + b_k k_1 & \alpha_{21} & \alpha_{22} \end{bmatrix}$$

where the functions $\alpha_{ij}, 1 \leq i, j \leq 2$ are given by

$$\alpha_{11} = m_{22} - m_{12} b_p^{-1}, \quad \alpha_{12} = m_{23} - m_{13} b_p^{-1}$$

$$\alpha_{21} = m_{32} - b_k m_{11} b_p^{-1}, \quad \alpha_{22} = m_{33} - b_k m_{13} b_p^{-1}$$

According to [35, Lemma 5.1], the operator $d\frac{\partial^2}{\partial\xi^2}-\beta$ generates an exponentially stable C_0-semigroup on $L^2(0,1)$. Therefore, it is enough to show that the operator

$$\mathcal{A}=\begin{bmatrix} -v\frac{\partial}{\partial\xi}+\alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{bmatrix}$$

generates an exponentially stable C_0-semigroup. To do so, the operator $\mathcal{A}$ can be written as follows

$$\mathcal{A}=\begin{bmatrix} -v\frac{\partial}{\partial\xi}+\alpha_{11} & 0 \\ \alpha_{21} & \alpha_{22} \end{bmatrix}+\begin{bmatrix} 0 & \alpha_{12} \\ 0 & 0 \end{bmatrix}:=\mathcal{A}_0+\mathcal{D}_0$$

Since the operator $-v\frac{\partial}{\partial\xi}+\alpha_{11}$ generates an exponentially stable C_0-semigroup (see [6]), then the operator $\mathcal{A}_0$ generates an exponentially stable C_0-semigroup $T_0(t)$ if the function α_{22} is negative. In this case, there exist positive constants M and α such that

$$\|T_0(t)\|\leq Me^{-\alpha t},\qquad \text{for}\qquad t\geq 0.$$

Therefore by using the perturbation theorem [23, Theorem 3.2.1], the operator $\mathcal{A}$ generates a C_0-semigroup $T_D(t)$ such that

$$\|T_D(t)\|\leq Me^{(-\alpha+M|\alpha_{12}|)t}$$

Hence b_p and b_k can be chosen in such a way to guarantee both (1) $\alpha_{22}<0$ and (2) $-\alpha+M|\alpha_{12}|<0$. Consequently, the operator $\mathcal{A}$ generates an exponentially stable C_0-semigroup and so is the opeartor $A+BK$. The exponential stabilizability of $(\hat{A},\hat{B})$ is an immediate consequence of [23, Exercise 5.25]. $\square$

Similarly, the exponential detectability of the operator pair $(\hat{C},\hat{A})$ is stated in the following proposition.

Proposition 2. Let us consider the operator A given by Equation (4.38a) and $C=C_0\cdot I$, where C_0 is any matrix of bounded functions and $rank(C_0)=2$. Then there exists an operator $L\in\mathcal{L}(H)$ such that $A+LC$ generates an exponentially stable C_0-semigroup on H. Moreover, if $0\in\rho(A)$, then the operator pair $(\hat{A},\hat{C})$ generates an exponentially stabilizable C_0-semigroup on $\mathcal{H}$.

Proof. Let $C_0=(c_{ij})_{1\leq i,j\leq 3}$ and let us consider L under the following form

$$L=\begin{bmatrix} l_1 & 0 & 0 \\ 0 & l_2 & 0 \\ l_3 & l_4 & l_5 \end{bmatrix}$$

The operator $A + LC$ is

$$\begin{bmatrix} d\frac{\partial^2}{\partial\xi^2} + m_{11} + l_1c_{31} & m_{12} + l_1c_{32} & m_{13} + l_1c_{33} \\ m_{21} + l_2c_{31} & -v\frac{\partial}{\partial\xi} + m_{22} + l_2c_{32} & m_{23} + l_2c_{33} \\ m_{31} + l_3c_{11} + l_4c_{21} + l_5c_{31} & m_{32} + l_3c_{12} + l_4c_{22} + l_5c_{32} & m_{33} + l_3c_{13} + l_4c_{23} + l_5c_{33} \end{bmatrix}$$

Let us choose $l_1 = -m_{11}c_{31}^{-1}, l_2 = m_{21}c_{31}^{-1}(c_{31} \neq 0)$ and l_3, l_4, l_5 are the solutions of the following system of equations

$$\begin{array}{rcl} l_3c_{11} + l_4c_{21} + l_5c_{31} & = & -m_{31} \\ l_3c_{12} + l_4c_{22} + l_5c_{32} & = & -m_{32} \\ l_3c_{13} + l_4c_{23} + l_5c_{33} & = & -m_{33} - \eta \quad \text{for some} \quad \eta > 0 \end{array}$$

provided that $rank(C_0) = 2$. In this case, the operator $A + LC$ becomes

$$A + LC = \begin{bmatrix} d\frac{\partial^2}{\partial\xi^2} & m_{12} + l_1c_{32} & m_{13} + l_1c_{33} \\ 0 & -v\frac{\partial}{\partial\xi} + m_{22} + l_2c_{32} & m_{23} + l_2c_{33} \\ 0 & 0 & -\eta \end{bmatrix}$$

The resulting operator is triangular and all its diagonal entries generates an exponentially stable C_0-semigroup and so is the operator $A + LC$. The exponential detectability of $(\hat{C}, \hat{A})$ is an immediate consequence of [23, Exercise 5.25]. □

Remark 2. *Note that the choice of L assumes that $c_{31} \neq 0$ however, if $c_{31} = 0$ it is possible to change the form of L to triangularize $A + LC$. More general, if we choose a full matrix L, it may be possible to generate a weaker condition of detectability. Indeed, it is enough to have L as solution of the equation $LC_0 = D_0$ where D_0 is a diagonal matrix with negative entries.*

3.4 Optimal Control Design

In this section, the aim is to design an optimal linear-quadratic (LQ) state feedback controller for the linearized system $\Sigma(\hat{A}, \hat{B}, \hat{C})$ given by Equations (4.32)-(4.33). Our objective is to find a control law to minimize the following cost functional:

$$J(x_0, u) = \int_0^\infty (\langle y(s), \mathbf{P}y(s)\rangle + \langle u(s), \mathbf{R}u(s)\rangle)ds \qquad (3.32)$$

where the operator $\mathbf{P} = P \cdot I = (p_{ij} \cdot I)_{1\leq i,j\leq 4}$ such that the matrix P is symmetric and positive semi-definite and $\mathbf{R} = \mathbf{r} \cdot I$ such that $\mathbf{r} > 0$. It has been shown in the previous section that the pair $(\hat{A}, \hat{B})$ is exponentially stabilizable and the pair $(\mathbf{P}^{1/2}\hat{C}, \hat{A})$ is exponentially detectable. It is well-known that, under those conditions, the solution of the LQ-control problem can be obtained via the corresponding Operator Riccati Equation (ORE) ([23]).

$$[\hat{A}^*\mathbf{Q} + \mathbf{Q}\hat{A} + \hat{C}^*\mathbf{P}\hat{C} - \mathbf{Q}\hat{B}\mathbf{R}\hat{B}^*\mathbf{Q}]x = 0 \quad \forall x \in D(\hat{A}) \text{ and } \mathbf{Q}(D(\hat{A})) \subset D(\hat{A}^*) \tag{3.33}$$

which admits a unique non-negative self adjoint solution and for any $x_0 \in H$, the quadratic cost (4.34) is minimized by the unique control u given for any $t \geq 0$ by

$$u(t) = \mathbf{K}x(t) := -\mathbf{R}^{-1}\hat{B}^*\mathbf{Q}x(t), \quad x(t) = e^{(\hat{A}+\hat{B}\mathbf{K})t}x_0 \tag{3.34}$$

Moreover, the C_0-semigroup $e^{(\hat{A}+\hat{B}\mathbf{K})t}$ generated by the closed-loop system is exponentially stable on H. Let us assume the operator Riccati equation (4.35) admits a diagonal solution of the following form:

$$\mathbf{Q} = \begin{bmatrix} q_1 & 0 & 0 & 0 \\ 0 & q_2 & 0 & 0 \\ 0 & 0 & q_3 & 0 \\ 0 & 0 & 0 & q_4 \end{bmatrix} \tag{3.35}$$

where $q_i \in \mathcal{L}(L^2(0,1))$, $1 \leq i \leq 4$ are non-negative and self-adjoint operators. Equation (4.35) gives the following system of equations:

$$0 = p_{11}c_1^2 - \mathbf{r}q_1^2 \tag{3.36a}$$

$$0 = \gamma_1 q_2 + p_{12}c_1c_2 + \mathbf{r}b_p q_1 q_2 \tag{3.36b}$$

$$0 = \gamma_2 q_3 + p_{13}c_1c_3 + \mathbf{r}q_1 q_3 \tag{3.36c}$$

$$0 = \gamma_3 q_4 + p_{14}c_1c_4 + \mathbf{r}b_k q_1 q_4 \tag{3.36d}$$

$$0 = A_{11}^* q_2 + q_2 A_{11} + p_{22}c_2^2 - \mathbf{r}b_p^2 q_2^2 \tag{3.36e}$$

$$0 = m_{21}q_3 + q_2 m_{12} + p_{23}c_2c_3 - \mathbf{r}b_p q_2 q_3 \tag{3.36f}$$

$$0 = m_{31}q_4 + q_2 m_{13} + p_{24}c_2c_4 - \mathbf{r}b_p b_k q_2 q_4 \tag{3.36g}$$

$$0 = A_{22}^* q_3 + q_3 A_{22} + p_{33}c_3^2 - \mathbf{r}q_3^2 \tag{3.36h}$$

$$0 = m_{32}q_4 + q_3 m_{23} + p_{34}c_3c_4 - \mathbf{r}b_k q_3 q_4 \tag{3.36i}$$

$$0 = m_{33}q_4 + q_4 m_{33} + p_{44}c_4^2 - \mathbf{r}b_k^2 q_4^2 \tag{3.36j}$$

Note that the operators b_p, b_h , andb_k are operators defined from $\mathbb{R}$ to $L^2(0,1)$ under the form $Bu = b(z)u$. The adjoint operator of B is defined from $L^2(0,1) \rightarrow \mathbb{R}$

and is given by

$$B^*x = \int_0^1 b(z)x(z)dz$$

which represents the average value of the function bx on the interval $[0, 1]$. With this fact, the Riccati equation is to become a set of integro-differential equations that are not easy to solve. To avoid this problem, the output of the adjoint operators b_p^*, b_h^* and b_k^* are to be substituted by the distributed functions instead of the average values. However, the average values will be used to calculate the optimal input which is defined in Equation (3.34) and can be found by the following expression:

$$u(t) = -r^{-1}\left[q_1x_1(t) - b_p\int_0^1 q_2(z)x_2(t,z)dz \right.$$
$$\left. -\sum_{i=1}^{5} b_{h_i}\int_0^1 \left[q_3(z)x_3(t,z)\right]_i dz - b_k\int_0^1 q_4(z)x_4(t,z)dz\right] \tag{3.37}$$

where q_1, q_2, q_3, q_4 are the unique solutions of Equations (3.36a), (3.36e), (3.36h) and (3.36j), respectively. Now, we can solve these four equations separately and use the matrix $\mathbf{P}$ to force the other equations to be satisfied.

- **Equation (3.36a):** This equation is very easy to solve

  $$p_{11}c_1^2 - rq_1^2 = 0$$

  which gives

  $$q_1 = |c_1|\sqrt{\frac{p_{11}}{r}} \tag{3.38}$$

- **Equation (3.36e):** The equation can be written as follows

  $$\left[A_{11}^*q_2 + q_2A_{11} + p_{22}c_2^2 - rb_p^2q_2^2\right]x = 0 \quad \forall x \in D(A_{11})$$

  Let us put $\alpha = p_{22}c_2^2$ and $\beta = b_prb_p$. To solve the above equation, the inner product form of the equation is to be used. For all $x, y \in D(A_{11})$, one has

  $$< q_2x, A_{11}y > + < A_{11}x, q_2y > + < \beta x, y > - < q_2x, \alpha q_2y >= 0$$

  If we take $x = \phi_m$ and $y = \phi_n$, we have the following equation

  $$< q_2\phi_m, A_{11}\phi_n > + < A_{11}\phi_m, q_2\phi_n > + < \beta\phi_m, \phi_n > - < q_2\phi_m, \alpha q_2\phi_n >= 0$$

To use the eigenvalues and eigenvectors found in Section 3, the above equation is solved on each subdivision of the interval $[0,1]$. Indeed, the equation can be written on $[\xi_i, \xi_{i+1}]$ as follows

$$\lambda_n^i < q_2^i\phi_m^i, \phi_n^i > +\lambda_m^i < \phi_m^i, q_2^i\phi_n^i > + < \beta\phi_m^i, \phi_n^i > - < q_2^i\phi_m^i, \alpha q_2^i\phi_n^i >= 0$$

By setting $\beta_{mn}^i =< \beta\phi_m^i, \phi_n^i >$ and $q_{2,mn}^i =< q_2^i\phi_m^i, \phi_n^i >$ for $i = 1, 2 \cdots s$, we obtain the following equation:

$$(\lambda_n^i + \lambda_m^i)q_{2,mn}^i + \beta_{mn}^i - < q_2^i\phi_m^i, \alpha q_2^i\phi_n^i >= 0 \tag{3.39}$$

On the other hand, any element $x \in L^2(0,1)$ can be written as follows:
$x = \sum_{k=0}^{\infty} < x, \phi_k > \phi_k$ and then the following holds:

$$< q_2^i\phi_m^i, \alpha q_2^i\phi_n^i >=< q_2^i\phi_m^i, \sum_{k=0}^{\infty} < \alpha q_2^i\phi_n^i, \phi_k^i > \phi_k^i >= \sum_{k=0}^{\infty} < \alpha q_2^i\phi_n^i, \phi_k^i >< q_2^i\phi_m^i, \phi_k^i >$$

$$= \sum_{k=0}^{\infty} < q_2^i\phi_n^i, \alpha\phi_k^i > q_{2,mk}^i = \sum_{k=0}^{\infty} < q_2^i\phi_n^i, \sum_{k=0}^{\infty} < \alpha\phi_k^i, \phi_l^i > \phi_l^i > q_{2,mk}^i$$

$$= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} < \alpha\phi_k^i, \phi_l^i >< q_2^i\phi_n^i, \phi_l^i > q_{2,mk}^i = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \alpha_{kl} q_{2,nl}^i q_{2,mk}^i$$

where $\alpha_{kl}^i =< \alpha\phi_k^i, \phi_l^i >$. Then Equation (3.39) becomes

$$(\lambda_n^i + \lambda_m^i)q_{2,mn}^i + \beta_{mn}^i - \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \alpha_{kl}^i q_{2,nl}^i q_{2,mk}^i = 0 \tag{3.40}$$

If it is assumed that $\forall$ n $\neq$ m $q_{2,mn}^i = 0$ is a solution of equation (3.40), one gets the following quadratic equation:

$$2\lambda_n^i q_{2,nn}^i + \beta_{nn}^i - \alpha_{nn}^i (q_{2,nn}^i)^2 = 0 \tag{3.41}$$

which admits two solutions and only the positive one is to be used.

$$q_{2,nn}^i = \frac{\lambda_n^i + \sqrt{(\lambda_n^i)^2 + \beta_{nn}^i \alpha_{nn}^i}}{\alpha_{nn}^i} \tag{3.42}$$

Finally, the expression of the function q_2 is given by

$$q_2^i x = \sum_{n=0}^{\infty} \frac{\lambda_n^i + \sqrt{(\lambda_n^i)^2 + \beta_{nn}^i \alpha_{nn}^i}}{\alpha_{nn}^i} < x, \phi_n^i > \phi_n^i \tag{3.43}$$

- **Equation (3.36h):** The equation can be written as

$$\left[A_{22}^{*}q_3 + q_3 A_{22} + p_{33}c_3^2 - rq_3^2\right] x = 0$$

Remember that $A_{22} = -v\frac{d}{d\xi} + m_{22}$ defined on $D(A_{22}) = \{h \in \mathcal{L}(0,1) : h \text{ is absolutely continuous } h(0) = 0\}$ and its adjoint $A_{22}^{*} = v\frac{d}{d\xi} + m_{22}$ defined $D(A_{22}^{*}) = \{h \in \mathcal{L}(0,1) : h \text{ is absolutely continuous } h(1) = 0\}$. Then Equation (3.36h) can be written as follows

$$v\frac{d(q_3 x)}{d\xi} + m_{22}q_3 x + q_3\left(-v\frac{dx}{d\xi} + m_{22}x\right) - rq_3^2 x + p_{33}c_3^2 x = 0$$

Then the function q_3 should satisfy the following differential equation

$$v\frac{dq_3}{d\xi} + 2m_{22}q_3 - rq_3^2 + p_{33}c_3^2 = 0, \quad q_3(1) = 0 \tag{3.44}$$

The condition $q_3(1) = 0$ is equivalent to $q_3 x \in D(A_{22}^{*})$ for all $x \in D(A_{22})$ then $(q_3 x)(1) = 0$.

Equation (3.44) can be solved numerically. However, if we assume that the function m_{22} is space independent, an explicit solution can be found. Indeed, let us introduce the following notations.

$$a_1 = \frac{r}{v}, \ a_2 = \frac{m_{22}}{v}, \ a_3 = \frac{p_{33}c_3^2}{v}$$

$$\mu_1 = \frac{-a_2 - \sqrt{a_2^2 + a_1 a_3}}{a_1}, \quad \mu_2 = \frac{-a_2 + \sqrt{a_2^2 + a_1 a_3}}{a_1}$$

$$\mu_3 = 2\sqrt{a_2^2 + a_1 a_3}, \qquad \overline{q}_3 = \frac{1}{q_3 + \mu_1}$$

Using the above notations, Equation (3.44) can be written as follows

$$\frac{dq_3}{d\xi} = a_1 q_3^2 - 2a_2 q_3 - a_3 = a_1(q_3 + \mu_1)(q_3 + \mu_2)$$

On the other hand, the derivative of $\overline{q}_3$ with respect to ξ is

$$\frac{d\overline{q}_3}{d\xi} = -\frac{dq_3}{d\xi}\frac{1}{(q_3 + \mu_1)^2} = -\frac{a_1(q_3 + \mu_1)(q_3 + \mu_2)}{(q_3 + \mu_1)^2} = -\frac{a_1(q_3 + \mu_2)}{q_3 + \mu_1}$$

$$= -\frac{a_1(q_3 + \mu_1 - \mu_1 + \mu_2)}{q_3 + \mu_1} = -a_1 - \mu_3\overline{q}_3$$

Consequently, Equation (3.44) is converted to the linear initial value differential equation

$$\frac{d\overline{q}_3}{d\xi} + \mu_3\overline{q}_3 = -a_1, \qquad \overline{q}_3(1) = \frac{1}{\mu_1}$$

which has the following explicit solution

$$\overline{q}_3(\xi) = \left(\frac{1}{\mu_1} + \frac{a_1}{\mu_3}\right) e^{\mu_3(1-\xi)} - \frac{a_1}{\mu_3}$$

and then the function q_3 is given by the following expression

$$q_3(\xi) = \left[\left(\frac{1}{\mu_1} + \frac{a_1}{\mu_3}\right) e^{\mu_3(1-\xi)} - \frac{a_1}{\mu_3}\right]^{-1} - \mu_1 \tag{3.45}$$

- **Equation (3.36j):** It is a quadratic equation that can be solved easily. It can be written as follows

$$rb_k^2 q_4^2 - 2m_{33}q_4 - p_{44}c_4^2 = 0 \tag{3.46}$$

which has two solutions and the positive one is given by

$$q_4 = \frac{m_{33} + \sqrt{m_{33}^2 + rb_k^2 p_{44} c_4^4}}{rb_k^2} \tag{3.47}$$

Remark 3. *It can be easily observed that in order to solve the equation (3.36a), (3.36e), (3.36h) and (3.36j), the values of the constants $p_{11}, p_{22}, p_{33}, p_{44}$ and r are needed. The remaining off-diagonal elements of P can be found by solving the remaining equations. In what follows, an algorithm to solve the general Riccati equation (4.35).*

- **Algorithm to solve ORE (4.35):**

  - Choose positive p_{11}, p_{22}, p_{33}, p_{44} and r to find q_1, q_2, q_3, q_4.
  - Solve the off diagonal equations (3.36b), (3.36c), (3.36d), (3.36f), (3.36g), (3.36i) to get explicitly $p_{ij},\ i \neq j$.
  - Check if the resulting P is positive. If P is not positive then,
  - Choose a new p_{11}, p_{22}, p_{33}, p_{44} and r to find new q_1, q_2, q_3, q_4 and solve again the off-diagonal equations until we get a positive P.

- **State feedback control:** To implement the state-feedback control given by Equation (4.39), we need to rewrite it in terms of the original variables. For this purpose, let us substitute $u = \dot{w}$ and $x_1 = w$, $x_2 = \tilde{z}_p - b_p w$ $x_3 = \tilde{z}_h - b_h w$ and $x_4 = \tilde{k} - b_k w$ in Equation (4.39)

$$-\mathbf{r}\dot{w}(t) = q_1 w(t) - b_p \int_0^1 q_2(z)(\tilde{z}_p - b_p w)dz$$
$$- \sum_{i=1}^{5} b_{h_i} \int_0^1 \left[q_3(z)(\tilde{z}_h - b_h w)\right]_i dz - b_k \int_0^1 q_4(z)(\tilde{k} - b_k w)dz$$
$$-\mathbf{r}\dot{w}(t) = \left[q_1 + \int_0^1 \left(b_p^2 q_2(z) + \sum_{i=1}^{5} b_{h_i} \left[q_3(z) b_h\right]_i + b_k^2 q_4(z)\right) dz\right] w(t)$$
$$- \int_0^1 \left(b_p q_2(z)\tilde{z}_p(z) + \sum_{i=1}^{5} b_{h_i} \left[q_3(z)\tilde{z}_h\right]_i + b_k q_4(z)\tilde{k}\right) dz$$

Then the function w satisfies the following linear differential equation

$$\dot{w}(t) + \tau w(t) = \gamma(t), \quad w(0) = 0 \tag{3.48}$$

where τ is a constant given by the following expression

$$\tau = \mathbf{r}^{-1} \left[q_1 + \int_0^1 \left(b_p^2 q_2(z) + \sum_{i=1}^{5} b_{h_i} \left[q_3(z) b_h\right]_i + b_k^2 q_4(z)\right) dz\right]$$

and γ is a function of the SCR states and given by

$$\gamma(\tilde{z}_p, \tilde{z}_h, \tilde{k}) = \mathbf{r}^{-1} \left[\int_0^1 \left(b_p q_2(z)\tilde{z}_p(z) + \sum_{i=1}^{5} b_{h_i} \left[q_3(z)\tilde{z}_h\right]_i + b_k q_4(z)\tilde{k}\right) dz\right]$$

Consequently, the optimal (to be injected ammonia) state feedback control is given by

$$C^g_{NH3}(0) = w(t) + z_{h,0}(0) = e^{-\tau t} \left[\int e^{\tau t} \gamma(\tilde{z}_p(t), \tilde{z}_h(t), \tilde{k}(t))dt - G(0)\right] + z_{h,0}(0) \tag{3.49}$$

where G is the anti-deriavtive function of $e^{\tau t}\gamma(t)$.

3.5 Case Study: Monolithic catalyst Reactor

Monolithic catalyst reactor (see Figure 1) is used to demonstrate all the above theoretical development. In this reactor, an endothermic reaction $A \rightarrow B$ takes place and

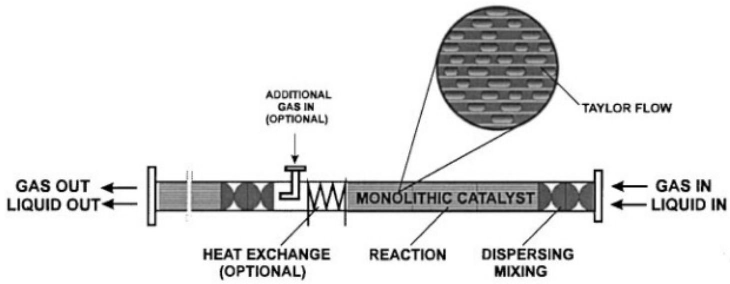

Figure 3.1: Monolithic catalyst

the objective is to keep the temperature at the surface as high as possible.

The energy balance law is used to describe the dynamics of the gas temperature, surface temperature and housing temperature. The gas temperature (T_g) is the temperature of the gas that enters to the monolithic reactor. Since the monolith represents the solid-phase in the catalytic, its temperature determines how fast or slow the surface reactions will take place, it is called the surface temperature (T_s). The housing temperature (T_h) represents the heat transfer from the monolith to the catalyst housing and subsequently to the ambient environment. It is assumed that diffusion transport phenomenon is negligible in the gas phase and the only controllable input is gas temperature inlet $T_g(0,t) = u$. Under these assumptions, the process dynamics can described by the following dimensionless PDEs (see [62]):

$$\frac{\partial T_s(z,t)}{\partial t} = \frac{\partial^2 T_c}{\partial \xi^2} + a_s e^{\frac{\gamma T_s}{1+T_s}} - b_s(T_s - T_g) - c_s(T_s - T_h) \tag{3.50}$$

$$\epsilon \frac{\partial T_g(z,t)}{\partial t} = -\frac{\partial T_g}{\partial \xi} + a_g(T_c - T_g) - b_g(T_g - T_h) \tag{3.51}$$

$$\frac{dT_h}{dt} = a_h(T_h^4 - T_a^4) + b_h(T_s - T_h) \tag{3.52}$$

with the following boundary and initial conditions:

$$\frac{\partial T_c(0,t)}{\partial \xi} = \frac{\partial T_c(1,t)}{\partial \xi} = 0, \quad T_g(0,t) = T_{g_{in}} = u, \quad T_c(\xi,0) = T_g(\xi,0) = T_h(\xi,0) = 0 \tag{3.53}$$

where T_a is the dimensionless ambient temperature; b_s, c_s, a_g, b_g, a_h and b_h are the dimensionless heat transfer coefficients; γ is the dimensionless activation energy and a_s is the dimensionless heat of the reaction (see [21]). The control objective is to regulate the catalyst temperature around its desired value along the reactor by manipulating the gas temperature at the inlet of the reactor.

To simulate the model equations (3.50)-(3.53) at steady-state, the values of the system parameters are given in Table 3.1. Also, we choose the manipulated variable at steady-state equal to 2. By using MATLAB, the steady-state profiles for the gas, surface and housing temperatures are given in Figure (3.2).

Table 3.1: Model parameters for Monolithic catalyst Reactor

Parameter	ϵ	a_s	γ	b_s	c_s	a_g	b_g	a_h
Value	0.01	-0.03	-1.4	1.0	15.62	0.5	0.5	0.001

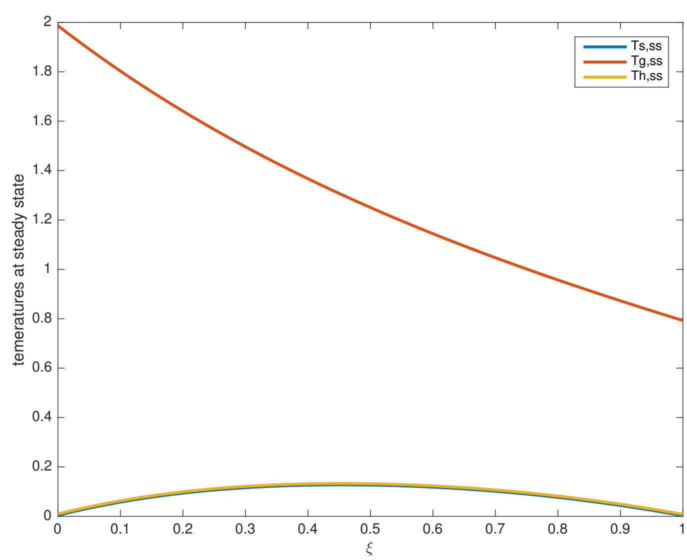

Figure 3.2: Surface,gas and housing temperatures at steady state

Except m_{11} and m_{33}, all the functions $m_{ij}, 1 \leq i, j \leq 3$ are constants and given by

$$m_{12} = 1,\ m_{13} = 15.62,\ m_{21} = 50,\ m_{22} = -100,\ m_{23} = 50,\ m_{31} = 0.02,\ m_{32} = 0.$$

On the other hand, it has been observed that the variation of m_{33} is very small and it can be estimated by $m_{33} = -0.02$. For m_{11}, the interval has been divided into 5 subin-

Table 3.2: Values of m_{11} over space

ξ	[0, 0.2]	[0.2, 0.4]	[0.4, 0.6]	[0.6, 0.8]	[0.8, 1]
$m_{11}(\xi)$	-18.2	-20.3	-21.4	-20.3	-18.3

tervals, where the function m_{11} is estimated by its average in each subinterval.Table (3.2)

To calculate the eigenvalues, it is assumed that the length of the reactor is divided into 5 equally spaces. The first five eigenvalues of the parabolic operator are given by:

$$\lambda_n^1 = \{-18.22, -18.62, -18.21, -20.22, -20.22, \dots\}$$

$$\lambda_n^2 = \{-20.38, -20.72, -20.31, -22.36, -22.36, \dots\}$$

$$\lambda_n^3 = \{-23.46, -23.42, -23.34, -23.46, -23.39, \dots\}$$

$$\lambda_n^4 = \{-20.30, -22.56, -20.64, -21.75, -23.95, \dots\}$$

$$\lambda_n^5 = \{-18.20, -28.07, -57.68, -107.03, -176.43, \dots\}$$

The corresponding eigenfunctions are given by:

$$\phi_n^1 = \left\{\sqrt{2}\cos(1.4\xi), \sqrt{2}\cos(0.65\xi), \sqrt{2}\cos(-0.12\xi), \sqrt{2}\cos(1.43\xi), \sqrt{2}\cos(1.42\xi), \dots\right\}$$

$$\begin{aligned}
\phi_n^2 &= \{1.5\cos(0.28\xi) + 0.13\sin(0.28\xi), 1.96\cos(0.65\xi) + 0.54\sin(0.65\xi), \\
&\quad 1.4\cos(1.4\xi) - 0.0025\sin(1.4\xi), 4.73\cos(1.43\xi) + 3.3\sin(1.43\xi), \\
&\quad 4.7\cos(1.42\xi) + 3.31\sin(1.42\xi), \dots\} \\
\phi_n^3 &= \{10\cos(1.4\xi) + 8.59\sin(1.4\xi), -7.72\cos(1.42\xi) - 9.14\sin(1.42\xi), \\
&\quad 3.1\cos(1.39\xi) + 1.67\sin(1.39\xi), -1.2\cos(1.4\xi) - 2.62\sin(1.4\xi), \\
&\quad -1.17\cos(1.41\xi) - 2.6\sin(1.41\xi), \dots\} \\
\phi_n^4 &= \{-13.37, -0.0037\cos(1.5\xi) - 1.418\sin(1.5\xi), -1.35\cos(0.58\xi) - 2.77\sin(0.58\xi), \\
&\quad 1.67\cos(-1.2\xi) + 0.25\sin(-1.2\xi), 0.22\cos(1.9\xi) - 1.2\sin(1.9\xi), \dots\}
\end{aligned}$$

$$\phi_n^5 = \left\{\sqrt{2}, \sqrt{2}\cos(\pi\xi), \sqrt{2}\cos(2\pi\xi), \sqrt{2}\cos(3\pi\xi), \sqrt{2}\cos(4\pi\xi), \dots\right\}$$

To solve the corresponding Riccati equation (3.44) in the case study, the algorithm developed in the previous section is implemented. The output operator is chosen to be $C = I$ and $p_{11} = 0.3, p_{22} = 0.2, p_{33} = 10, p_{44} = 10$ and $r = 10$. In this case, the functions $q_i, 1 \le i \le 4$ are given by the following expressions

$$q_1 = 3.1623 \quad \text{and} \quad q_4 = 1.2$$

The expression of the function q_2 at each subdivision is expressed by using (4.43) :

$$q_2^1 z = 4.29(z^T\phi_1^1)\phi_1^1 + 4.2(z^T\phi_1^2)\phi_1^2 + 4.3(z^T\phi_1^3)\phi_1^3 + 3.88(z^T\phi_1^4)\phi_1^4 + 3.87(z^T\phi_1^5)\phi_1^5$$

$$q_2^2 z = 3.85(z^T\phi_2^1)\phi_2^1 + 3.8(z^T\phi_2^2)\phi_2^2 + 3.864(z^T\phi_2^3)\phi_2^3 + 3.5(z^T\phi_2^4)\phi_2^4 + 3.52(z^T\phi_2^5)\phi_2^5$$

$$q_2^3 z = 3.3652(z^T\phi_3^1)\phi_3^1 + 3.36(z^T\phi_3^2)\phi_3^2 + 3.38(z^T\phi_3^3)\phi_3^3 + 3.3625(z^T\phi_3^4)\phi_3^4 + 3.372(z^T\phi_3^5)\phi_3^5$$

$$q_2^4 z = 3.87(z^T\phi_4^1)\phi_4^1 + 3.5(z^T\phi_4^2)\phi_4^2 + 3.8(z^T\phi_4^3)\phi_4^3 + 3.36(z^T\phi_4^4)\phi_4^4 + 3.3(z^T\phi_4^5)\phi_4^5$$

$$q_2^5 z = 4.3(z^T\phi_5^1)\phi_5^1 + 2.82(z^T\phi_5^2)\phi_5^2 + 1.32(z^T\phi_5^3)\phi_5^3 + 0.74(z^T\phi_5^4)\phi_5^4 + 0.45(z^T\phi_5^5)\phi_5^5$$

The exact expression of q_3 is given by the following expression:

$$q_3(\xi) = \left[200.05e^{201(1-\xi)} - 0.05\right]^{-1} - 0.05$$

By solving the off-diagonal equations, the matrix P is given by

$$P = \begin{bmatrix} 0.3 & 0.0054 & 0 & -1.7286 \\ 0.0054 & 0.2 & -0.0063 & -0.1004 \\ 0 & -0.0063 & 10 & -0.0009 \\ -1.7286 & -0.1004 & -0.0009 & 10 \end{bmatrix} \tag{3.54}$$

which has the eigenvalues $[0.0005,\ 0.1997,\ 10,\ 10.3]$ and then the positivity of P is guaranteed.

The state feedback is given by Equation (3.49). This controller is applied on the nonlinear system . The closed-loop responses are shown in Figures 3.3-3.5. It can be observed that, the designed optimal controller is able to reject the effect of the initial condition in 5 seconds and surface, gas, and housing temperatures converge to their desired steady-state profiles .

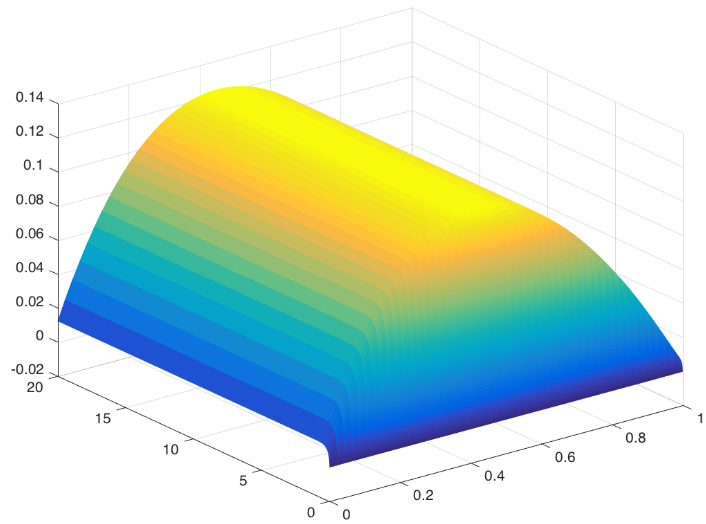

Figure 3.3: Closed-loop surface temperature.

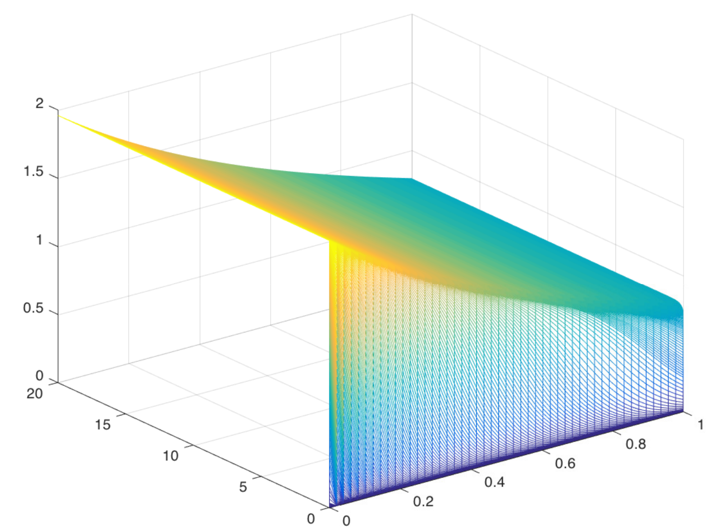

Figure 3.4: Closed-loop gas temperature.

The closed-loop errors are shown in Figures 3.6-3.7 confirms our results and it is observable that the errors converge to zero in 5 seconds which means that our controller drive the closed-loop to the steady states for any initial condition.

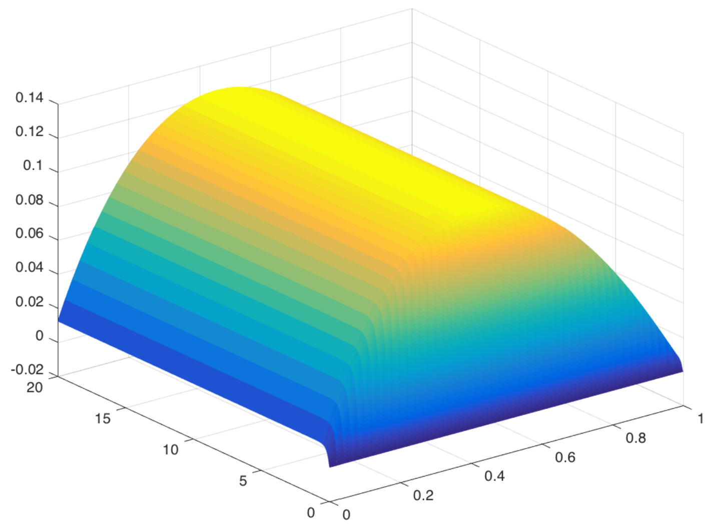

Figure 3.5: Closed-loop housing temperature.

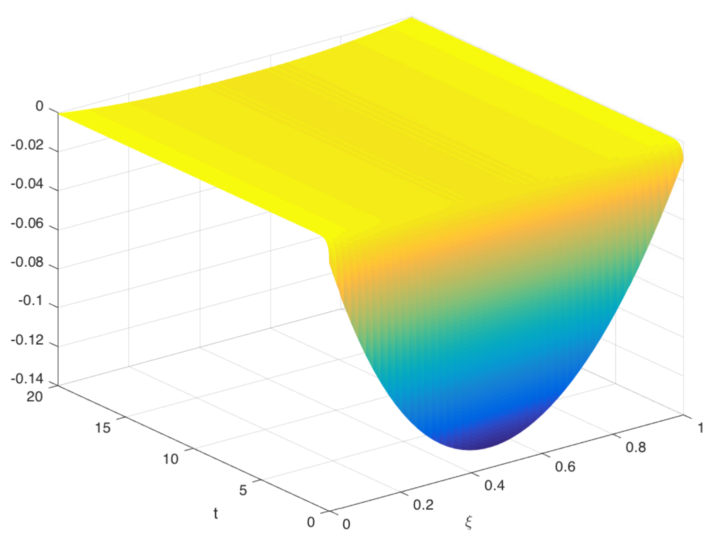

Figure 3.6: Closed-loop trajectory of $T_s - T_{s,ss}$.

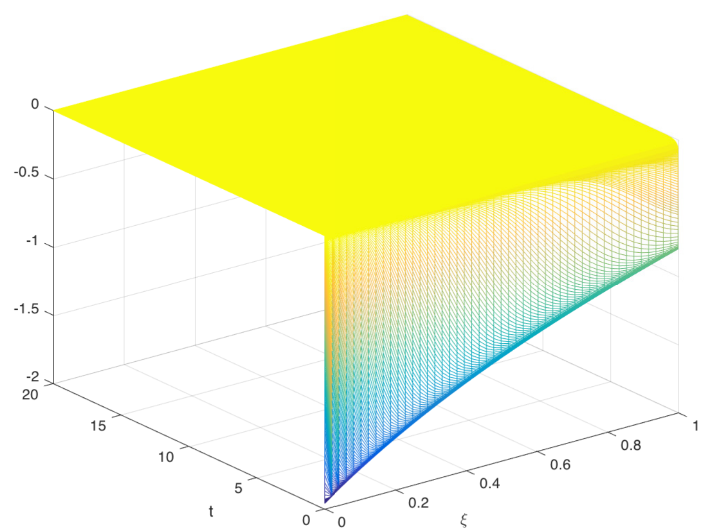

Figure 3.7: Closed-loop trajectory of $T_g - T_{g,ss}$.

Chapter 4

Optimal Control of Selective Catalytic Reduction

4.1 Process Description and Modelling

4.1.1 Reaction Mechanism

The reaction Mechanism describes how the chemical reactions occur. We consider that the only species adsorbed on surface is the NH_3. In this case many studies have been reported [39, 41, 42], where we can find the details of this mechanism

An aqueous urea solution is required to reduce NO_x. Urea plays the main role concerning the formation of gaseous ammonia. Urea decomposition is described in the following reactions [29]:

$$\mathrm{H_4N_2CO} \longrightarrow \mathrm{NH_3} + \mathrm{HNCO} \tag{4.1}$$

$$\mathrm{HNCO} + \mathrm{H_2O} \longrightarrow \mathrm{NH_3} + \mathrm{CO_2} \tag{4.2}$$

The thermal decomposition reaction (4.1) takes place upstream of the SCR catalyst. The $\mathrm{NH_3}$ formed is further adsorbed on the surface of the SRC catalyst.It has been observed that the hydrolysis reaction (4.2) has significant effect concerning the formation of NH_3.Then it is much better to take this reaction into account.
After the step of NH_3 formation we now describe the process how this NH_3 can reduced the nitrogen oxides by converting it to nitrogen and water which are less harmful than NO_x The reactions are [29]:

$$4\mathrm{NH_3} + 2\mathrm{NO} + 2\mathrm{NO_2} \longrightarrow 4\mathrm{N_2} + 6\mathrm{H_2O} \tag{4.3}$$

$$4\mathrm{NH_3} + 4\mathrm{NO} + \mathrm{O_2} \longrightarrow \mathrm{N_2} + 6\mathrm{H_2O} \tag{4.4}$$

$$8\mathrm{NH_3} + 6\mathrm{NO_2} \longrightarrow 7\mathrm{N_2} + 12\mathrm{H_2O} \tag{4.5}$$

The reaction (4.3) is the best pathway because it can convert NO_x to nitrogen and water very fast and it is preferable to reaction (4.4) and reaction (4.5).The oxidation of ammonia can be an obstacle for maximum conversion of NO_x The reaction mechanisms are [29]:

$$4\mathrm{NH_3} + 3\mathrm{O_2} \longrightarrow 2\mathrm{N_2} + 6\mathrm{H_2O} \tag{4.6}$$

$$\mathrm{NH_3} + 5\mathrm{O_2} \longrightarrow 4\mathrm{NO} + 6\mathrm{H_2O} \tag{4.7}$$

4.1.2 The Complete SCR Model

The SCR catalytic converter typically consists of a ceramic substrate in the form of a honeycomb monolith with thousands of parallel channels of about 1 mm hydraulic radius. The surface of the channels is covered with a washcoat containing a catalyst. We consider a single channel as being representative of the converter as a whole. We model the channel as a right circular cylinder and this case can use a 2D axisymetrical model. Further, by using a lumped capacitance model in the radial direction we can further reduce the model to a single spatial dimension [45]. We have to consider the bulk gas phase and the surface, with the two being coupled via heat and mass transfer coefficients. The complete model [46,47] of bulk gas contains four species (NO, NO_2, NH_3, and O_2). The mass balance equations are PDEs as follows:

The Mass balance

$$\frac{\partial c_j^g(z,t)}{\partial t} = -v\frac{\partial c_j^g}{\partial z} + \frac{k_m^j a}{\epsilon}(c_j^s - c_j^g), \quad j = NO, NO_2, NH_3, O_2 \tag{4.8}$$

Equation(4.8) describes the masse balances of each components, and it is considered as a hyperbolic class of PDEs.

There are three terms in Equation(4.8) which are: accumulation of species ,convective term, and diffusion of mass from bulk gas to washcoat

c_j,v,k_m,a, and ϵ are the concentration of component 'j',the linear gas velocity which is assumed constant along catalyst channel, the mass transfer coefficient; the mass and heat transfer area per unit of catalyst volume; the porosity in the catalytic washcoat layer or the void fraction .

The mass balances of each component in the washcoat pores are shown in the following equations

$$(1-\epsilon)\frac{\partial c_j^s(z,t)}{\partial t} = k_m^j a(c_j^g - c_j^s) \pm G\sum \sigma_k r_k, \quad j = NO, NO_2, NH_3, O_2 \tag{4.9}$$

Equation (4.9) is the same as the pervious one, just in this case the accumulation takes place only in $1-\epsilon$, and instead of a convective term we have a heat source which is generated by the chemical reactions. The accumulation of species in the surface is very small compared to other terms , that is the reason behind neglecting this accumulation term. So the final form of the mass balance at surface is, where G is active catalytic surface area and σ_k is the stoichiometric coefficient of each reaction, r_k are reaction rates of each reaction

$$k_m^j a(c_j^g - c_j^s) = \pm G\sum \sigma_k r_k, \quad j = NO, NO_2, NH_3, O_2 \tag{4.10}$$

The mass balances of intermediate species :

Intermediate species are the adsorption/desorption of gases on the reaction sites on the surface. They have have a significant role in modelling SCR. Thus the ammonia intermediate species surface coverage equation can be written as follows:

$$\frac{d\Omega_{NH_3}(z,t)}{dt} = \frac{a}{\Omega_{NH_3}^{cap}}(r_{ad} - r_{des} - r_4) \tag{4.11}$$

Ω_{NH3} is the coverage of stored ammonia on the surface of catalyst; Ω^{cap} is the storage capacity.

The Energy balance

The total enthalpy balance in the bulk gas gives us the gas temperature as follows:

$$\frac{\partial T^g(z,t)}{\partial t} = -v\frac{\partial T^g}{\partial z} + \frac{h_m a}{\rho^g cp^g \epsilon}(T^s - T^g) \tag{4.12}$$

Equation (4.12) is a hyperbolic PDE which consists of three terms :the accumulation of heat, the heat convection, and inter-phase heat transfer from gas to monolith.]h_m,ρ^g ,cp^g,T^g,and T^s e are the conductive heat transfer coefficient between bulk gas and monolith ,the exhaust gas density, an exhaust gas specific heat capacity, temperature of exhaust gas, and the surface temperature.

The total enthalpy balance in surface gives us the surface temperature as follows:

$$\begin{aligned}\frac{\partial T^s(z,t)}{\partial t} = \frac{\lambda^s}{\rho^s cp^s}\frac{\partial^2 T^s}{\partial z^2} - \frac{h_m a}{\rho^s cp^s(1-\epsilon)}(T^s - T^g) - \frac{h_{ext}a_{ext}}{\rho^s cp^s(1-\epsilon)}(T^s - T^{ext}) \\ - \frac{a}{\rho^s cp^s(1-\epsilon)}\sum_{j=1}^{5}\Delta H_j r_j \end{aligned} \tag{4.13}$$

The Equation (4.13) is a parabolic PDE λ is the thermal conductivity; T^{ext} is the temperature of surroundings; and ΔH is the standard reaction enthalpy. respectively.

We conclude that the model of SCR includes hyperbolic and parabolic partial differential equations (PDEs), and ordinary differential equation (ODE) that are coupled.

Reaction rates

The reaction rate defines how fast the chemical reaction consumes reactants and produces products. In our case reaction rates are introduced as the following:

$$r_1 = 2.53 * 10^6 e^{\dfrac{-3007}{T^s}} \frac{c^s_{NO} c^s_{NO_2} c^s_{NH_3}}{1 + 1.2042 * 10^{-3} c^s_{NH_3}} \tag{4.14}$$

$$r_2 = 2.36 * 10^8 e^{\dfrac{-7151}{T^s}} \frac{c^s_{NO} c^s_{NH_3}}{1 + 1.2042 * 10^{-3} c^s_{NH_3}} \tag{4.15}$$

$$r_3 = 7.56 * 10^8 e^{\dfrac{-8507}{T^s}} \frac{c^s_{NO_2} c^s_{NH_3}}{1 + 1.2042 * 10^{-3} c^s_{NH_3}} \tag{4.16}$$

$$r_4 = 1.32 * 10^7 e^{\dfrac{-15034}{T^s}} \Omega_{NH_3} \tag{4.17}$$

$$r_5 = 9.11 * 10^{10} e^{\dfrac{-14503}{T^s}} \frac{c^s_{O_2} c^s_{NH_3}}{(1 + 1.2042 * 10^{-3} c^s_{NH_3})(1 + 1.5053 * 10^{-3} c^s_{O_2})} \tag{4.18}$$

$$r_{ad} = 0.82 c^s_{NH_3} (1 - \Omega_{NH_3}) \tag{4.19}$$

$$r_{des} = 3.67 * 10^6 e^{\dfrac{-12992(1 - 0.310\Omega_{NH_3})}{T^s}} \Omega_{NH_3} \tag{4.20}$$

Note that the unit of the reaction rates $r_i, 1 \leq i \leq 5$ is $mol/s.m^2$ and the unit for r_{ad} and r_{des} is $mol/s.m^3$.

The parameters, mass and heat transfer coefficients, and functions used to express the reaction kinetics that are used in Equations (4.8)-(4.13) are shown in Tables 4.1 and 4.2, respectively.

Table 4.1: Model parameters for SCR [29]

Parameter	Value	Unit
a	2666	$[m^2m^{-3}]$
a_{ext}	1	$[m^2m^{-3}]$
h_{ext}	35	$[Wm^{-2}K^{-1}]$
ϵ	0.68	[%]
ρ^s	1770	$[kgm^{-3}]$
cp^s	900	$[Jkg^{-1}K^{-1}]$
λ_s	1	$[Wm^{-1}K^{-1}]$
$\Omega^{cap}_{NH_3}$	209	$[mol/m^3]$
ΔH_1	-378.534	$[kJmol^{-1}]$
ΔH_2	-407.129	$[kJmol^{-1}]$
ΔH_3	-341.664	$[kJmol^{-1}]$
ΔH_4	-316.839	$[kJmol^{-1}]$
ΔH_5	-226.549	$[kJmol^{-1}]$

Table 4.2: Mass and heat transfer coefficients for SCR [29]

Parameter	Equation	Unit
h_m	$= 19 + 0.1748T^g - 18.318 * 10^{-6}(T^g)^2$	$[Wm^{-2}K^{-1}]$
k_m^{NO}	$= 2.745 * 10^{-6}(T^g)^{1.75}$	$[ms^{-1}]$
$k_m^{NO_2}$	$= 2.212 * 10^{-6}(T^g)^{1.75}$	$[ms^{-1}]$
$k_m^{NH_3}$	$= 2.959 * 10^{-6}(T^g)^{1.75}$	$[ms^{-1}]$
$k_m^{O_2}$	$= 2.399 * 10^{-6}(T^g)^{1.75}$	$[ms^{-1}]$

4.1.3 Control Objectives

The SCR catalyst technology theoretically can reduce up to 90% percent of NO_x, but this is not the case for many reasons. For example, there are some disturbances that may affect the control performance of a SCR, and one of them is the continues fluctuations of NO_x concentrations because the speed of diesel engine is not constant, also the urea solution has a direct effect on the ammonia, so the under/overdosage of urea can lead to disturbance in the control of SCR, Finally the disturbance of the gas temperature at the inlet it may affect the SCR performances. Our control objective is to keep the performances of SCR as high as possible and to drive this system to achieve the optimal performances regardless, of the previous disturbances. The ammonia dosage at the inlet is the only manipulated variable, so finding the optimal dosage of ammonia is our challenging objective. Good control performance is achieved if the tailpipe concentration of NO_x is less than 50 ppm, and the ammonia slip is less than 20 ppm, so we need to perform some simulations by changing values of concentrations and temperature of gas at the inlet to determine which is the perfect steady states that we can linearize around.

4.1.4 Abstract Cauchy problem on the Hilbert space Z

In this section we reformulate our boundary control problem to an abstract Cauchy problem which fits our standard formulation (2.2) . It is possible to reformulate such problems on an extended state space so that they do lead to an associated system in the standard form [23].

The Final models of SCR with the Boundary Conditions are given as follows:

$$\begin{cases} \dfrac{\partial T^s(z,t)}{\partial t} = \dfrac{\lambda^s}{\rho^s cp^s}\dfrac{\partial^2 T^s}{\partial z^2} - \dfrac{h_m a}{\rho^s cp^s(1-\epsilon)}(T^s - T^g) - \dfrac{h_{ext}a_{ext}}{\rho^s cp^s(1-\epsilon)}(T^s - T^{ext}) \\ -\dfrac{a}{\rho^s cp^s(1-\epsilon)}\sum_{j=1}^{5}\Delta H_j r_j \\ \\ \dfrac{\partial T^g(z,t)}{\partial t} = -v\dfrac{\partial T^g}{\partial z} + \dfrac{h_m a}{\rho^g cp^g \epsilon}(T^s - T^g) \\ \dfrac{\partial c^g_{NO}(z,t)}{\partial t} = -v\dfrac{\partial c^g_{NO}}{\partial z} + \dfrac{k_m^{NO} a}{\epsilon}(c^s_{NO} - c^g_{NO}), \\ \dfrac{\partial c^g_{NO2}(z,t)}{\partial t} = -v\dfrac{\partial c^g_{NO2}}{\partial z} + \dfrac{k_m^{NO2} a}{\epsilon}(c^s_{NO2} - c^g_{NO2}) \\ \dfrac{\partial c^g_{NH3}(z,t)}{\partial t} = -v\dfrac{\partial c^g_{NH3}}{\partial z} + \dfrac{k_m^{NH3} a}{\epsilon}(c^s_{NH3} - c^g_{NH3}) \\ \dfrac{\partial c^g_{O2}(z,t)}{\partial t} = -v\dfrac{\partial c^g_{O2}}{\partial z} + \dfrac{k_m^{O2} a}{\epsilon}(c^s_{O2} - c^g_{O2}) \\ \dfrac{d\Omega_{NH_3}(z,t)}{dt} = \dfrac{a}{\Omega^{cap}_{NH_3}}(r_{ad} - r_{des} - r_4) \end{cases} \tag{4.21}$$

With the following Boundary Conditions:

$$\begin{cases} T^g(0,t) = T^g_{in} \\ c^g_j(0,t) = c^g_{j,in}, \quad j = NO, NO_2, NH_3, O_2 \\ \dfrac{\partial T^s(0,t)}{\partial z} = \dfrac{\partial T^s(L,t)}{\partial z} = 0, \end{cases} \tag{4.22}$$

We reformulate the problem to match the general case. The system can be written as follows:

$$\begin{cases} \frac{\partial z_p}{\partial t} = \mathbf{d}\frac{\partial^2 z_p}{\partial \xi^2} + \mathbf{f}(z_p, z_h, k) \\ \frac{\partial z_h}{\partial t} = -\mathbf{V}\frac{\partial z_h}{\partial \xi} + \mathbf{g}(z_p, z_h, k) \\ \frac{dk}{dt} = \mathbf{h}(z_p, z_h, k) \end{cases} \tag{4.23}$$

Such that the states are:

$$z_p = T^s, \quad z_h = \begin{bmatrix} T^g & c^g_{NO} & c^g_{NO2} & c^g_{NH3} & c^g_{O2} \end{bmatrix}^T = \begin{bmatrix} z_{h1} & z_{h2} & z_{h3} & z_{h4} & z_{h5} \end{bmatrix}^T, \quad k = \Omega_{NH3}$$

The coefficients are: $\mathbf{d} = \dfrac{\lambda^s}{\rho^s cp^s}, \qquad \mathbf{V} = diag(v.I_4)$

Finally the non-linear functions are:

$$\mathbf{f}(z_p, z_h, k) = -\frac{h_m a}{\rho^s cp^s(1-\epsilon)}(T^s - T^g) - \frac{h_{ext} a_{ext}}{\rho^s cp^s(1-\epsilon)}(T^s - T^{ext}) - \frac{a}{\rho^s cp^s(1-\epsilon)} \textstyle\sum_{j=1}^5 \Delta H_j r_j$$

$$\mathbf{h}(z_p, z_h, k) = \frac{1}{\Omega^{cap}_{NH_3}}(r_{ad} - r_{des} - a r_4)$$

$$\mathbf{g}(z_p, z_h, k) = \begin{bmatrix} \dfrac{h_m a}{\rho^g cp^g \epsilon}(T^s - T^g) \\ \dfrac{k_m^{NO} a}{\epsilon}(c^s_{NO} - c^g_{NO}) \\ \dfrac{k_m^{NO2} a}{\epsilon}(c^s_{NO2} - c^g_{NO2}) \\ \dfrac{k_m^{NH3} a}{\epsilon}(c^s_{NH3} - c^g_{NH3}) \\ \dfrac{k_m^{O2} a}{\epsilon}(c^s_{O2} - c^g_{O2}) \end{bmatrix} = \begin{bmatrix} \mathbf{g_1}(z_p, z_h, k) \\ \mathbf{g_2}(z_p, z_h, k) \\ \mathbf{g_3}(z_p, z_h, k) \\ \mathbf{g_4}(z_p, z_h, k) \\ \mathbf{g_5}(z_p, z_h, k) \end{bmatrix}$$

The final models with the boundary conditions are stated as follows:

$$\begin{cases} \dfrac{\partial z_p}{\partial t} = \mathbf{d}\dfrac{\partial^2 z_p}{\partial \xi^2} + \mathbf{f}(z_p, z_h, k) \\ \dfrac{\partial z_h}{\partial t} = -\mathbf{V}\dfrac{\partial z_h}{\partial \xi} + \mathbf{g}(z_p, z_h, k) \\ \dfrac{dk}{dt} = \mathbf{h}(z_p, z_h, k) \end{cases} \tag{4.24}$$

Where the boundary conditions are:

$$\begin{aligned} \frac{\partial z_p}{\partial \xi}|_{\xi=0} = \frac{\partial z_p}{\partial \xi}|_{\xi=1} = 0 \quad \text{and} \quad z_h(\xi=0) = z_{h,in} \\ z_p(\xi,0) = z_{p,0}(\xi) \text{ and } z_h(\xi,0) = z_{h,0}(\xi) \text{ and } k(0) = k_0 \end{aligned} \tag{4.25}$$

where $(z_p, z_h, k) \in H = L^2(0,1) \times (L^2(0,1))^5 \times \mathbb{R}$ denote the state variables of the system, $\xi \in [0,1]$ and $t \in [0,\infty)$ represent the space variable and time, respectively. The functions $\mathbf{f}$ and $\mathbf{g}$ and $\mathbf{h}$ are non-linear continuous functions. $c^g_{NH3}(\xi=0)$ the component number 4 of the function $z_{h,in} \in L^2(0,1)$ is the input variable. The only difference between the previous case and this case is that $\mathbf{V}$ is diagonal matrix rather than scalar .

To solve the corresponding linear-quadratic control problem, the linearization of the above system around a steady-state profile is needed. For this purpose, let us denote by $z_{p,ss}$ and $z_{h,ss}$ and k_{ss} the components of the system steady state.

$$\begin{cases} \dfrac{\partial \tilde{z}_p}{\partial t} = \mathbf{d}\dfrac{\partial^2 \tilde{z}_p}{\partial \xi^2} + \mathbf{m}_{11}(\xi)\tilde{z}_p + \mathbf{m}_{12}(\xi)\tilde{z}_h + \mathbf{m}_{13}(\xi)\tilde{k} \\ \dfrac{\partial \tilde{z}_h}{\partial t} = -\mathbf{V}\dfrac{\partial \tilde{z}_h}{\partial \xi} + \mathbf{m}_{21}(\xi)\tilde{z}_p + \mathbf{m}_{22}(\xi)\tilde{z}_h + \mathbf{m}_{23}(\xi)\tilde{k} \\ \dfrac{d\tilde{k}}{dt} = \mathbf{m}_{31}(\xi)\tilde{z}_p + \mathbf{m}_{32}(\xi)\tilde{z}_h + \mathbf{m}_{33}(\xi)\tilde{k} \end{cases} \tag{4.26}$$

With the following new initial and boundary conditions

$$\begin{aligned} \frac{\partial \tilde{z}_p}{\partial \xi}|_{\xi=0} = 0 \quad \text{and} \quad \frac{\partial \tilde{z}_p}{\partial \xi}|_{\xi=l} = 0 \quad \text{and} \quad \tilde{z}_h(\xi=0) = z_h(\xi=0) - z_{h,ss}(\xi=0) \\ \tilde{z}_p(\xi,0) = z_{p,0}(\xi) - z_{p,ss}(\xi) \text{ and } \tilde{z}_h(\xi,0) = z_{h,0}(\xi) - z_{h,ss}(\xi) \text{ and } \tilde{k}(0) = k_0 - k_{ss} \end{aligned} \tag{4.27}$$

Where $\tilde{z}_p = z_p - z_{p,ss}$ and $\tilde{z}_h = z_h - z_{h,ss}$ and $\tilde{k} = k - k_{ss}$ are the state variables in deviation form. The functions $\mathbf{m}_{ij}, 0 \le i,j \le 3$ are the Jacobians of the nonlinear terms evaluated at the system steady state.

$$\mathbf{m}_{11}(\xi) = \frac{\partial \mathbf{f}(z_p, z_h, k)}{\partial z_p}|_{ss}, \qquad \mathbf{m}_{12}(\xi) = \frac{\partial \mathbf{f}(z_p, z_h, k)}{\partial z_h}|_{ss}, \qquad \mathbf{m}_{13}(\xi) = \frac{\partial \mathbf{f}(z_p, z_h, k)}{\partial k}|_{ss}$$

$$\mathbf{m}_{21}(\xi) = \frac{\partial \mathbf{g}(z_p, z_h, k)}{\partial z_p}|_{ss}, \qquad \mathbf{m}_{22}(\xi) = \frac{\partial \mathbf{g}(z_p, z_h, k)}{\partial z_h}|_{ss}, \qquad \mathbf{m}_{23}(\xi) = \frac{\partial \mathbf{g}(z_p, z_h, k)}{\partial k}|_{ss}$$

$$\mathbf{m}_{31}(\xi) = \frac{\partial \mathbf{h}(z_p, z_h, k)}{\partial z_p}|_{ss}, \qquad \mathbf{m}_{32}(\xi) = \frac{\partial \mathbf{h}(z_p, z_h, k)}{\partial z_h}|_{ss}, \qquad \mathbf{m}_{33}(\xi) = \frac{\partial \mathbf{h}(z_p, z_h, k)}{\partial k}|_{ss}.$$

From the other hand and to clarify more we have that:

$$\mathbf{m}_{12} = \begin{bmatrix} \frac{\partial \mathbf{f}(z_p,z_h,k)}{\partial z_{h1}}|_{ss} & \frac{\partial \mathbf{f}(z_p,z_h,k)}{\partial z_{h2}}|_{ss} & \frac{\partial \mathbf{f}(z_p,z_h,k)}{\partial z_{h3}}|_{ss} & \frac{\partial \mathbf{f}(z_p,z_h,k)}{\partial z_{h4}}|_{ss} & \frac{\partial \mathbf{f}(z_p,z_h,k)}{\partial z_{h5}}|_{ss} \end{bmatrix}$$

$$\mathbf{m}_{21}(\xi) = \begin{bmatrix} \frac{\partial \mathbf{g_1}(z_p,z_h,k)}{\partial z_p}|_{ss} \\ \frac{\partial \mathbf{g_2}(z_p,z_h,k)}{\partial z_p}|_{ss} \\ \frac{\partial \mathbf{g_3}(z_p,z_h,k)}{\partial z_p}|_{ss} \\ \frac{\partial \mathbf{g_4}(z_p,z_h,k)}{\partial z_p}|_{ss} \\ \frac{\partial \mathbf{g_5}(z_p,z_h,k)}{\partial z_p}|_{ss} \end{bmatrix} \qquad \mathbf{m}_{23}(\xi) = \begin{bmatrix} \frac{\partial \mathbf{g_1}(z_p,z_h,k)}{\partial k}|_{ss} \\ \frac{\partial \mathbf{g_2}(z_p,z_h,k)}{\partial k}|_{ss} \\ \frac{\partial \mathbf{g_3}(z_p,z_h,k)}{\partial k}|_{ss} \\ \frac{\partial \mathbf{g_4}(z_p,z_h,k)}{\partial k}|_{ss} \\ \frac{\partial \mathbf{g_5}(z_p,z_h,k)}{\partial k}|_{ss} \end{bmatrix}$$

$$\mathbf{m}_{22} = \begin{bmatrix} \frac{\partial \mathbf{g_1}(z_p,z_h,k)}{\partial z_{h1}}|_{ss} & \frac{\partial \mathbf{g_1}(z_p,z_h,k)}{\partial z_{h2}}|_{ss} & \frac{\partial \mathbf{g_1}(z_p,z_h,k)}{\partial z_{h3}}|_{ss} & \frac{\partial \mathbf{g_1}(z_p,z_h,k)}{\partial z_{h4}}|_{ss} & \frac{\partial \mathbf{g_1}(z_p,z_h,k)}{\partial z_{h5}}|_{ss} \\ \frac{\partial \mathbf{g_2}(z_p,z_h,k)}{\partial z_{h1}}|_{ss} & \frac{\partial \mathbf{g_2}(z_p,z_h,k)}{\partial z_{h2}}|_{ss} & \frac{\partial \mathbf{g_2}(z_p,z_h,k)}{\partial z_{h3}}|_{ss} & \frac{\partial \mathbf{g_2}(z_p,z_h,k)}{\partial z_{h4}}|_{ss} & \frac{\partial \mathbf{g_2}(z_p,z_h,k)}{\partial z_{h5}}|_{ss} \\ \frac{\partial \mathbf{g_3}(z_p,z_h,k)}{\partial z_{h1}}|_{ss} & \frac{\partial \mathbf{g_3}(z_p,z_h,k)}{\partial z_{h2}}|_{ss} & \frac{\partial \mathbf{g_3}(z_p,z_h,k)}{\partial z_{h3}}|_{ss} & \frac{\partial \mathbf{g_3}(z_p,z_h,k)}{\partial z_{h4}}|_{ss} & \frac{\partial \mathbf{g_3}(z_p,z_h,k)}{\partial z_{h5}}|_{ss} \\ \frac{\partial \mathbf{g_4}(z_p,z_h,k)}{\partial z_{h1}}|_{ss} & \frac{\partial \mathbf{g_4}(z_p,z_h,k)}{\partial z_{h2}}|_{ss} & \frac{\partial \mathbf{g_4}(z_p,z_h,k)}{\partial z_{h3}}|_{ss} & \frac{\partial \mathbf{g_4}(z_p,z_h,k)}{\partial z_{h4}}|_{ss} & \frac{\partial \mathbf{g_4}(z_p,z_h,k)}{\partial z_{h5}}|_{ss} \\ \frac{\partial \mathbf{g_5}(z_p,z_h,k)}{\partial z_{h1}}|_{ss} & \frac{\partial \mathbf{g_5}(z_p,z_h,k)}{\partial z_{h2}}|_{ss} & \frac{\partial \mathbf{g_5}(z_p,z_h,k)}{\partial z_{h3}}|_{ss} & \frac{\partial \mathbf{g_5}(z_p,z_h,k)}{\partial z_{h4}}|_{ss} & \frac{\partial \mathbf{g_5}(z_p,z_h,k)}{\partial z_{h5}}|_{ss} \end{bmatrix}$$

$$\mathbf{m}_{32} = \begin{bmatrix} \frac{\partial \mathbf{h}(z_p,z_h,k)}{\partial z_{h1}}|_{ss} & \frac{\partial \mathbf{h}(z_p,z_h,k)}{\partial z_{h2}}|_{ss} & \frac{\partial \mathbf{h}(z_p,z_h,k)}{\partial z_{h3}}|_{ss} & \frac{\partial \mathbf{h}(z_p,z_h,k)}{\partial z_{h4}}|_{ss} & \frac{\partial \mathbf{h}(z_p,z_h,k)}{\partial z_{h5}}|_{ss} \end{bmatrix}$$

To get the steady states many simulations have been done using different input values of gas temperature/concentrations. Using finite difference method in MATLAB at the optimal boundary conditions of SCR. The simulations of steady states are shown in the figures 4.2-4.3.

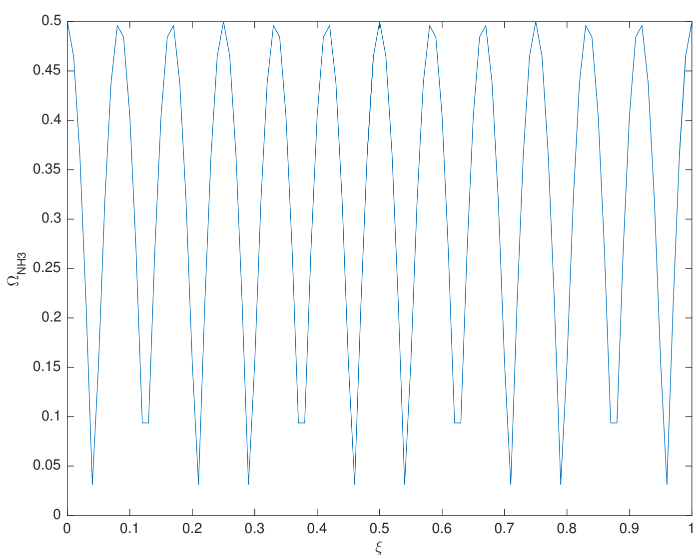

Figure 4.1: Concentration of Ω_{NH3} at steady state

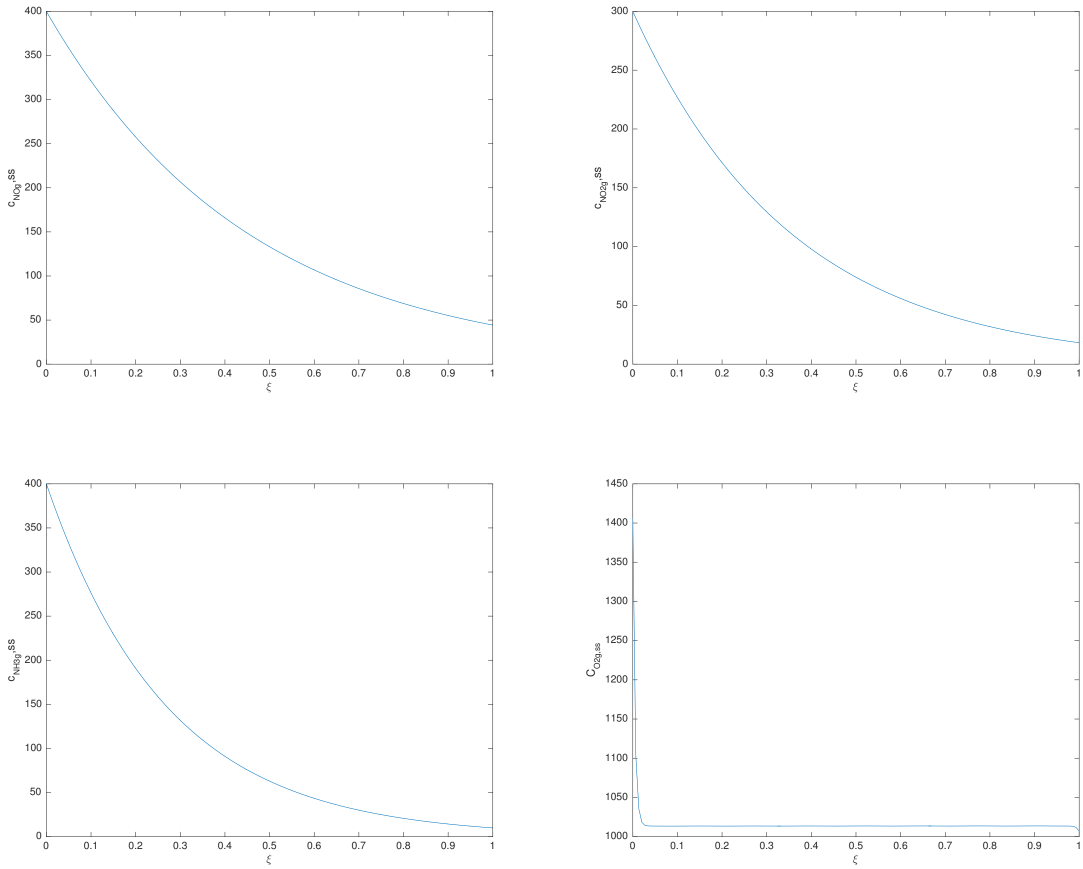

Figure 4.2: Concentrations of gas components at steady state

We use those values of steady states to get the functions $\mathbf{m}_{ij}$. The functions $\mathbf{m}_{ij}$ are given as follows:

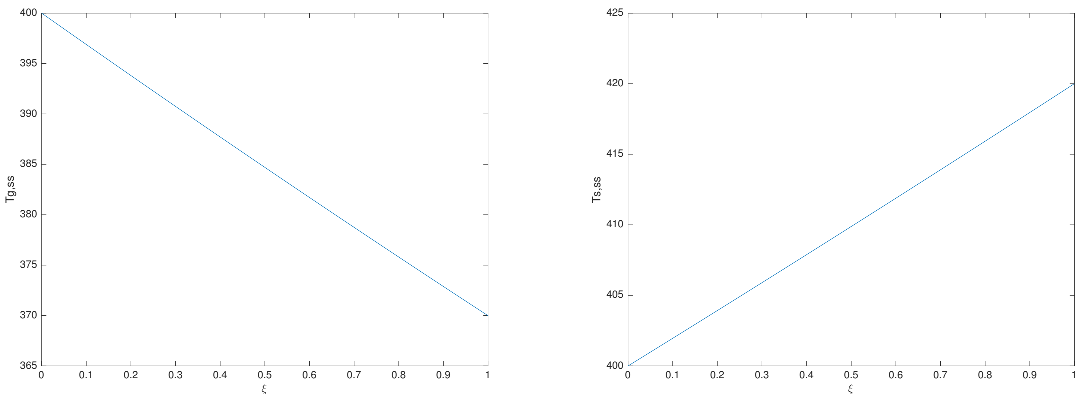

Figure 4.3: Gas and Surface temperatures at steady state

$$
\begin{cases}
\mathbf{m}_{11} = -\frac{h_{m,ss}a}{\rho^s c_p(1-\epsilon)} - \frac{h_{ext}a_{ext}}{\rho^s c_p(1-\epsilon)} - \frac{a(3007r_{1,ss}+7151r_{2,ss}+8507r_{3,ss}+15034r_{4,ss}+14503r_{5,ss})}{\rho^s c_p(1-\epsilon)T_{s,ss}^2} \\
\mathbf{m}_{12} = \begin{bmatrix} -\frac{a[(0.1748-2*18.318*10^{-6}T_{g,ss})(T_{s,ss}-T_{g,ss})-h_{m,ss}]}{\rho^s c_p(1-\epsilon)} & 0 & 0 & 0 & 0 \end{bmatrix} \\
\mathbf{m}_{13} = -\frac{1.32*10^7 a\Delta H_4 e^{\frac{-15034}{T_{s,ss}}}}{\rho^s c_p(1-\epsilon)} \\
\mathbf{m}_{21} = \begin{bmatrix} \frac{h_{m,ss}a}{\rho^g c_p^g \epsilon} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \\
\mathbf{m}_{22} = \begin{bmatrix}
\frac{a[(0.1748-2*18.318*10^{-6}T_{g,ss})(T_{s,ss}-T_{g,ss})-h_{m,ss}]}{\rho^s c_p^s \epsilon} & 0 & 0 & 0 & 0 \\
\frac{4.8*10^{-6}a(c_{NO}^s-c_{NO}^{g,ss})(T^{g,ss})^{0.75}}{\epsilon} & -\frac{k_{m,ss}^{NO}a}{\epsilon} & 0 & 0 & 0 \\
\frac{3.871*10^{-6}a(c_{NO2}^s-c_{NO2}^{g,ss})(T^{g,ss})^{0.75}}{\epsilon} & 0 & -\frac{k_{m,ss}^{NO2}a}{\epsilon} & 0 & 0 \\
\frac{5.18*10^{-6}a(c_{NH3}^s-c_{NH3}^{g,ss})(T^{g,ss})^{0.75}}{\epsilon} & 0 & 0 & -\frac{k_{m,ss}^{NH3}a}{\epsilon} & 0 \\
\frac{4.2*10^{-6}a(c_{O2}^s-c_{O2}^{g,ss})(T^{g,ss})^{0.75}}{\epsilon} & 0 & 0 & 0 & -\frac{k_{m,ss}^{O2}a}{\epsilon}
\end{bmatrix}
\end{cases}
$$

$$
\left\{
\begin{aligned}
\mathbf{m}_{23} &= \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \\
\mathbf{m}_{31} &= \frac{\Omega_{NH3,ss}[47.7*10^9(1-0.310\Omega_{NH3,ss})e^{\frac{-12992(1-0.310\Omega_{NH3,ss})}{T_{s,ss}}}+19.84*10^{10}ae^{\frac{-15043}{T_{s,ss}}}]}{\Omega^{cap}_{NH3}*T^2_{s,ss}} \\
\mathbf{m}_{32} &= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \end{bmatrix} \\
\mathbf{m}_{33} &= -\frac{0.82c^s_{NH3}+(\frac{1.48*10^{10}\Omega_{NH3,ss}}{T_{s,ss}}+3.67*10^6)e^{\frac{-12992(1-0.310\Omega_{NH3,ss})}{T_{s,ss}}}+1.32a*10^7e^{\frac{-15034}{T_{s,ss}}}}{\Omega^{cap}_{NH3}}
\end{aligned}
\right.
$$

Let us assume that the new state is by $z = \begin{bmatrix} \tilde{z}_p & \tilde{z}_h & \tilde{k} \end{bmatrix}^T$ and the new input is given by $w = \tilde{z}_{h_4}|_{\xi=0} = \begin{bmatrix} 0 & 0 & 0 & I|_{\xi=0} & 0 \end{bmatrix} \tilde{z}_h = M\tilde{z}_h$. Then, the above linear system can be formulated as an abstract boundary control problem on the Hilbert space H ([23]),

$$
\begin{cases} \dfrac{dz(t)}{dt} = \mathfrak{A}z(t) \qquad z(0) = z_0 \\ \mathcal{B}z(t) = w(t) \end{cases} \tag{4.28}
$$

Where $\mathfrak{A}$ is the linear operator defined by

$$
\mathfrak{A} = \begin{bmatrix} \mathbf{d}\dfrac{\partial^2}{\partial\xi^2} + \mathbf{m}_{11}(\xi) & \mathbf{m}_{12}(\xi) & \mathbf{m}_{13}(\xi) \\ \mathbf{m}_{21}(\xi) & -\mathbf{V}\dfrac{\partial}{\partial\xi} + \mathbf{m}_{22}(\xi) & \mathbf{m}_{23}(\xi) \\ \mathbf{m}_{31}(\xi) & \mathbf{m}_{32}(\xi) & \mathbf{m}_{33}(\xi) \end{bmatrix}
$$

and:

$$
D(\mathfrak{A}) = \left\{ z \in H : \tilde{z}_p, \tilde{z}_h, \frac{d\tilde{z}_p}{d\xi} \text{ are absolutely continous}, \frac{d\tilde{z}_h}{d\xi} \times \frac{d\tilde{z}_p}{d\xi} \times \frac{d^2\tilde{z}_p}{d\xi^2} \in (L^2(0,1))^3 \text{ and } \frac{\partial\tilde{z}_p}{\partial\xi}|_{\xi=0} = 0), \text{ and } \frac{\partial\tilde{z}_p}{\partial\xi}|_{\xi=l} = 0 \right\}
$$

The input operator $\mathcal{B} : H \to \mathbb{R}$ is given by

$$
\mathcal{B} = \begin{bmatrix} 0 & M & 0 \end{bmatrix}
$$

The objective is to find an operator $B \in \mathcal{L}(\mathbb{R}, H)$ such that for all $w \in \mathbb{R}$, $Bw \in D(\mathfrak{A})$, the operator $\mathfrak{A}B$ is an element of $\mathcal{L}(\mathbb{R}, H)$ and $\mathcal{B}Bw = w$. If B is chosen as follows: $B = \begin{bmatrix} B_p(\xi)\cdot I \\ B_h(\xi)\cdot I \\ B_k(\xi)\cdot I \end{bmatrix}$, such that $B_h(\xi) = \begin{bmatrix} B_{h1}(\xi) \\ B_{h2}(\xi) \\ B_{h3}(\xi) \\ B_{h4}(\xi) \\ B_{h5}(\xi) \end{bmatrix}$, where $Bu \in D(\mathfrak{A})$.

To get B we need to use those two conditions:

First conditions is $Bu \in D(\mathfrak{A})$ which gives us the following :

$$\frac{d(B_p(\xi)w)}{d\xi}(\xi=0) = w\frac{dB_p}{d\xi}(\xi=0) = 0 \Leftrightarrow \frac{dB_p}{d\xi}(\xi=0) = 0 \tag{4.29}$$

and

$$\frac{d(B_p(\xi)w)}{d\xi}(\xi=l) = w\frac{dB_p}{d\xi}(\xi=l) = 0 \Leftrightarrow \frac{dB_p}{d\xi}(\xi=l) = 0 \tag{4.30}$$

Second condition is $\mathcal{B}Bw = w$ which is hold if:

$$MB_h(\xi)\cdot I = B_{h4_{|\xi=0}} w = w \Leftrightarrow B_{h4}(\xi=0) = 1 \tag{4.31}$$

Lets assume that $A : D(A) \to Z$ such that $Az = \mathfrak{A}z$, and $D(A) = D(\mathfrak{A}) \bigcap ker(\mathcal{B})$. By transform the state as we did in the pervious section into $v(t) = z(t) - Bw(t)$ where the new input is $u(t) = \dot{w}(t)$, we get the following abstract Cauchy problem:

$$\begin{cases} \dot{x}(t) = \hat{A}x(t) + \hat{B}u(t) \qquad x(0) = x_0 \\ y(t) = \hat{C}x(t) \end{cases} \tag{4.32}$$

Where the operators $\hat{A}, \hat{B}$ and $\hat{C}$ are given by

$$\hat{A} = \begin{bmatrix} 0 & 0 \\ \mathfrak{A}B & A \end{bmatrix}; \quad \hat{B} = \begin{bmatrix} I \\ -B \end{bmatrix}, \quad \hat{C} = C[B \quad I] \tag{4.33}$$

Such that $c_3 = diag(c_{ii}),\ 1 \le j \le 5$, where c_{ii} are scalars.

The operator $\mathfrak{A}B$ is given by

$$\mathfrak{A}B = \begin{bmatrix} (\mathfrak{A}B)_1 \\ (\mathfrak{A}B)_2 \\ (\mathfrak{A}B)_3 \end{bmatrix} = \begin{bmatrix} \mathbf{d}\frac{\partial^2}{\partial\xi^2} + \mathbf{m}_{11} & \mathbf{m}_{12} & \mathbf{m}_{13} \\ \mathbf{m}_{21} & -\mathbf{V}\frac{\partial}{\partial\xi} + \mathbf{m}_{22} & \mathbf{m}_{23} \\ \mathbf{m}_{31} & \mathbf{m}_{32} & \mathbf{m}_{33} \end{bmatrix} \begin{bmatrix} B_p \\ B_h \\ B_k \end{bmatrix} \cdot I$$

Due to the fact that the operator $\mathfrak{A}B$ acts on elements on R (space independent elements), then if we assume that the functions B_p , B_h and b_k are constants (In this case and according to Equation (4.31) b_{h4} should equal to 1, then the operator $\mathfrak{A}B$ can be simplified and becomes

$$\mathfrak{A}B = \begin{bmatrix} \mathbf{m}_{11}B_p + \mathbf{m}_{12}B_h + \mathbf{m}_{13}B_k \\ \mathbf{m}_{12}B_p + \mathbf{m}_{22}B_h + \mathbf{m}_{23}B_k \\ \mathbf{m}_{31}B_p + \mathbf{m}_{32}B_h + \mathbf{m}_{33}B_k \end{bmatrix} \cdot I := \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{bmatrix} \cdot I$$

By taking : $A_{11} = \mathbf{d}\frac{\partial^2}{\partial\xi^2} + \mathbf{m}_{11}$, $A_{22} = -\mathbf{V}\frac{\partial}{\partial\xi} + \mathbf{m}_{22}$ the extended operators $\hat{A}$ and $\hat{B}$ are given by: $\hat{A} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \gamma_1 & A_{11} & \mathbf{m}_{12} & \mathbf{m}_{13} \\ \gamma_2 & \mathbf{m}_{21} & A_{22} & \mathbf{m}_{23} \\ \gamma_3 & \mathbf{m}_{31} & \mathbf{m}_{32} & \mathbf{m}_{33} \end{bmatrix} \cdot I$, $\hat{B} = \begin{bmatrix} 1 \\ -B_p \\ -B_h \\ -B_k \end{bmatrix} \cdot I$

4.2 Eigenvalues Problem and Dynamical System Properties

4.2.1 Eigenvalues Problem

As we introduced in the pervious section of eigenvalues problem the same process is going to be apply on the new values of $\mathbf{m}_{11}$ in order to get eigenvalues and eigenfunctions . We have that $\mathbf{m}_{11}$ varies over the space as follows:

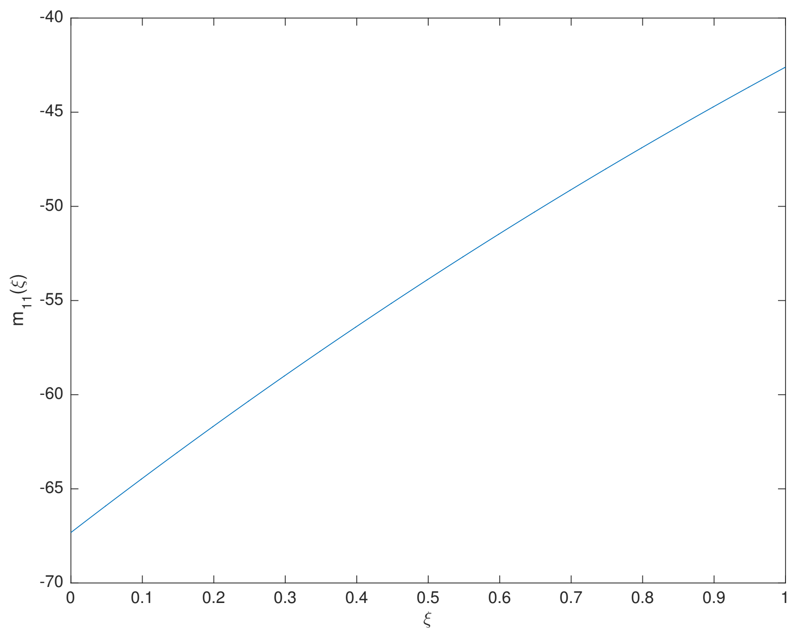

Figure 4.4: Variation of $\mathbf{m}_{11}$

ξ	[0, 0.2]	[0.2, 0.4]	[0.4, 0.6]	[0.6, 0.8]	[0.8, 1]
$\mathbf{m}_{11}(\xi)$	-65	-59	-54	-50	-45

To calculate the eigenvalues, it is assumed that the length of the reactor is divided into 5 equally spaces, and by applying our procedure as it is described in the pervious section we get The first five eigenvalues of the parabolic operator as follows:

$$\lambda_n^1 = \{-65.02, -65.42, -65.01, -67.02, -67.02, \dots\}$$

$$\lambda_n^2 = \{-59.08, -59.42, -59.01, -61.06, -61.06, \dots\}$$

$$\lambda_n^3 = \{-65.06, -56.06, -55.94, -56.24, -55.99, \dots\}$$

$$\lambda_n^4 = \{-50, -52.26, -50.34, -51.45, -53.65, \dots\}$$

$$\lambda_n^5 = \{-44.9, -54.77, -84.38, -133.73 - 203.13, \dots\}$$

The corresponding eigenfunctions are given by:

$$\phi_n^1 = \left\{\sqrt{2}\cos(1.4\xi), \sqrt{2}\cos(0.65\xi), \sqrt{2}\cos(-0.12\xi), \sqrt{2}\cos(1.43\xi), \sqrt{2}\cos(1.42\xi), \dots\right\}$$

$$\begin{aligned}\phi_n^2 &= \{1.5\cos(0.28\xi) + 0.13\sin(0.28\xi), 1.96\cos(0.65\xi) + 0.54\sin(0.65\xi),\\ &\quad 1.4\cos(1.4\xi) - 0.0025\sin(1.4\xi), 4.73\cos(1.43\xi) + 3.3\sin(1.43\xi),\\ &\quad 4.7\cos(1.42\xi) + 3.31\sin(1.42\xi), \dots\}\end{aligned}$$

$$\begin{aligned}\phi_n^3 &= \{10\cos(1.4\xi) + 8.59\sin(1.4\xi), -7.72\cos(1.42\xi) - 9.14\sin(1.42\xi),\\ &\quad 3.1\cos(1.39\xi) + 1.67\sin(1.39\xi), -1.2\cos(1.4\xi) - 2.62\sin(1.4\xi),\\ &\quad -1.17\cos(1.41\xi) - 2.6\sin(1.41\xi), \dots\}\end{aligned}$$

$$\begin{aligned}\phi_n^4 &= \{-13.37, -0.0037\cos(1.5\xi) - 1.418\sin(1.5\xi), -1.35\cos(0.58\xi) - 2.77\sin(0.58\xi),\\ &\quad 1.67\cos(-1.2\xi) + 0.25\sin(-1.2\xi), 0.22\cos(1.9\xi) - 1.2\sin(1.9\xi), \dots\}\end{aligned}$$

$$\phi_n^5 = \left\{\sqrt{2}, \sqrt{2}\cos(\pi\xi), \sqrt{2}\cos(2\pi\xi), \sqrt{2}\cos(3\pi\xi), \sqrt{2}\cos(4\pi\xi), \dots\right\}$$

4.2.2 Dynamical System Properties

Our approach to prove the exponential stabilizability and the exponential detectability is the same. Rather than dealing with v as scalar we have now a matrix V. So the following results hold by the same proofs.

Lemma 2. Let us consider the operator $\hat{A}$ defined by Equation (4.33), then $\hat{A}$ is the infinitesimal generator of a C_0 semigroup on $\mathcal{H}$.

The following result states that, under some technical conditions, the functions B_p and B_k can be chosen to guarantee the exponential stabilizability of the pair $(\hat{A}, \hat{B})$.

Proposition 3. Let us consider the operator pair (A, B), where A and B are given by Equations (4.38a) and (4.38b), respectively. Then, B_p and B_k can be always chosen to guarantee that there exists an operator $K \in \mathcal{L}(H, \mathbb{R})$ such that $A + BK$ generates an exponentially stable C_0-semigroup on H. Moreover, if $0 \in \rho(A)$ and $\forall s \in \overline{\mathbb{C}_0^+}$, $ker(sI \quad (\mathfrak{A}B)^*) \cap ker(0 \quad (sI - A^*)) \cap ker(I \quad - B^*) = \{0\}$, then the operator pair $(\hat{A}, \hat{B})$ generates an exponentially stabilizable C_0-semigroup on $\mathcal{H}$.

To guarantee the exponential stabilizability of $(\hat{A}, \hat{B})$ we need to verify that the choice of B_p and B_k give us that $\alpha_{22} < 0$ and in the same time give us $\frac{dB_p(\xi=0)}{d\xi} = \frac{dB_p(\xi=l)}{d\xi} = 0$ which are two conditons

$$\begin{cases} \alpha_{22} < 0 \quad (1) \\ \frac{dB_p(\xi=0)}{d\xi} = \frac{dB_p(\xi=l)}{d\xi} = 0 \quad (2) \end{cases}$$

By setting that $B_p = b_k = I$ the condition (2) holds. Concerning the condition (1) the figure (4.5) shows that the condition(1) also holds

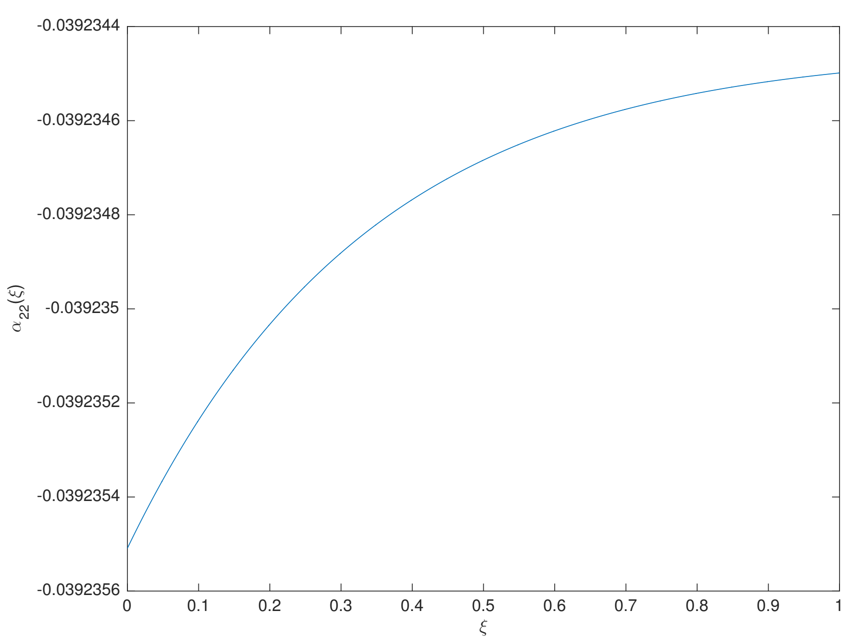

Figure 4.5: Variation of α_{22}

The exponential detectability of the operator pair $(\hat{C}, \hat{A})$ is stated in the following proposition.

Proposition 4. Let us consider the operator A and C given by Equations (4.38a) and (4.38c), respectively. If C_2 has full rank, then there exists an operator $L \in \mathcal{L}(H)$ such that $A + LC$ generates an exponentially stable C_0-semigroup on H. Moreover, if $0 \in \rho(A)$, then the operator pair $(\hat{C}, \hat{A})$ generates an exponentially stabilizable C_0-semigroup on $\mathcal{H}$.

Proof. Let us consider L under the following form

$$L = \begin{bmatrix} L_1 & 0 & 0 \\ L_2 & 0 & 0 \\ L_3 & L_4 & L_5 \end{bmatrix}$$

The operator $A + LC$ is

$$\begin{bmatrix} d\frac{\partial^2}{\partial \xi^2} + \mathbf{m}_{11} + L_1 C_1 & \mathbf{m}_{12} & \mathbf{m}_{13} \\ \mathbf{m}_{21} + L_2 C_1 & -V\frac{\partial}{\partial \xi} + \mathbf{m}_{22} & \mathbf{m}_{23} \\ \mathbf{m}_{31} + L_3 C_1 & \mathbf{m}_{32} + L_4 C_2 & \mathbf{m}_{33} + L_5 C_3 \end{bmatrix}$$

Let us choose $L_1 = -\mathbf{m}_{11} C_1^{-1}, L_2 = \mathbf{m}_{21} C_1^{-1}, L_3 = \mathbf{m}_{31} C_1^{-1} (C_1 \neq 0), L_4 = \mathbf{m}_{32} C_2^{-1}$ and L_5 can be chosen (always possible) $\mathbf{m}_{33} + L_5 C_3 = -\eta$ for some $\eta > 0$. In this case, the operator $A + LC$ becomes

$$A + LC = \begin{bmatrix} d\frac{\partial^2}{\partial \xi^2} & \mathbf{m}_{12} & \mathbf{m}_{13} \\ 0 & -V\frac{\partial}{\partial \xi} + \mathbf{m}_{22} & \mathbf{m}_{23} \\ 0 & 0 & -\eta \end{bmatrix}$$

The resulting operator is triangular and all its diagonal entries generates an exponentially stable C_0-semigroup and so is the operator $A + LC$. The exponential detectability of $(\hat{C}, \hat{A})$ is an immediate consequence of [23, Exercise 5.25]. □

4.3 Optimal Control Design

In this section, the aim is to design an optimal linear-quadratic (LQ) state feedback controller for the linearized system $\Sigma(\hat{A}, \hat{B}, \hat{C})$ given by Equations (4.32)-(4.33). Our objective is to find a control law to minimize the following cost functional:

$$J(x_0, u) = \int_0^\infty (\langle y(s), \mathbf{P} y(s) \rangle + \langle u(s), \mathbf{R} u(s) \rangle) ds \tag{4.34}$$

Where the operator $\mathbf{P} = P \cdot I = \begin{bmatrix} p_{11} & p_{12} & p_{13} & p_{14} \\ p_{21} & p_{22} & p_{23} & p_{24} \\ p_{31} & p_{32} & p_{33} & p_{34} \\ p_{41} & p_{42} & p_{43} & p_{44} \end{bmatrix} \cdot I$

Such that $(p_{13})_{1\times5} = p^*_{31}$, $(p_{23})_{1\times5} = p^*_{32}$, $(p_{43})_{1\times5} = p^*_{34}$, $(p_{33})_{5\times5}$.

The matrix P is symmetric and positive semi-definite and $\mathbf{R} = r \cdot I$ such that $\mathbf{r} > 0$. It has been shown in the previous section that the pair $(\hat{A}, \hat{B})$ is exponentially stabilizable and the pair $(\mathbf{P}^{1/2}\hat{C}, \hat{A})$ is exponentially detectable. It is well-known that, under those conditions, the solution of the LQ-control problem can be obtained via the corresponding Operator Riccati Equation (ORE) ([23]).

$$[\hat{A}^*\mathbf{Q} + \mathbf{Q}\hat{A} + \hat{C}^*\mathbf{P}\hat{C} - \mathbf{Q}\hat{B}\mathbf{R}\hat{B}^*\mathbf{Q}]x = 0 \quad \forall x \in D(\hat{A}) \text{ and } \mathbf{Q}(D(\hat{A})) \subset D(\hat{A}^*) \tag{4.35}$$

which admits a unique non-negative self adjoint solution and for any $x_0 \in H$, the quadratic cost (4.34) is minimized by the unique control u given for any $t \geq 0$ by

$$u(t) = \mathbf{K}x(t) := -\mathbf{R}^{-1}\hat{B}^*\mathbf{Q}x(t), \quad x(t) = e^{(\hat{A}+\hat{B}\mathbf{K})t}x_0 \tag{4.36}$$

Moreover, the C_0-semigroup $e^{(\hat{A}+\hat{B}\mathbf{K})t}$ generated by the closed-loop system is exponentially stable on H. Let us assume the operator Riccati equation (4.35) admits a diagonal solution of the following form:

$$\mathbf{Q} = \begin{bmatrix} Q_1 & 0 & 0 & 0 \\ 0 & Q_2 & 0 & 0 \\ 0 & 0 & Q_3 & 0 \\ 0 & 0 & 0 & Q_4 \end{bmatrix} \tag{4.37}$$

To guarantee that $\mathbf{Q}$ is positive we need just to make sure that $(Q_1)_{1\times1}$, $(Q_2)_{1\times1}$, $(Q_3)_{5\times5}$, $(Q_4)_{1\times1}$ are non-negative and self-adjoint operators.
Let's take Q_3 as follows:

$$Q_3 = \begin{bmatrix} q_{11} & q_{12} & q_{13} & q_{14} & q_{15} \\ q_{12} & q_{22} & q_{23} & q_{24} & q_{25} \\ q_{13} & q_{23} & q_{33} & q_{34} & q_{35} \\ q_{14} & q_{24} & q_{34} & q_{44} & q_{45} \\ q_{15} & q_{25} & q_{35} & q_{45} & q_{55} \end{bmatrix}$$

Equation (4.35) gives the following system of equations:

$$T_{11}^i = c_1^* p_{11}^i c_1 - Q_1^i r^i Q_1^i \tag{4.38a}$$

$$T_{12}^i = \gamma_1^* Q_2^i + c_1^* p_{12}^i c_2 + Q_1^i r^i B_p^* Q_2^i \tag{4.38b}$$

$$T_{13}^i = \gamma_2^* Q_3^i + c_1^* p_{13}^i c_3 + Q_1^i r^i B_h^* Q_3^i \tag{4.38c}$$

$$T_{14}^i = \gamma_3^* Q_4^i + c_1^* p_{14}^i c_4 + Q_1^i r^i B_k^* Q_4^i \tag{4.38d}$$

$$T_{22}^i = A_{11}^* Q_2^i + Q_2^i A_{11} + c_2^* p_{22}^i c_2 - Q_2^i B_p r^i B_p^* Q_2^i \tag{4.38e}$$

$$T_{23}^i = \mathbf{m}_{21}^* Q_3^i + Q_2^i \mathbf{m}_{12} + c_2^* p_{23}^i c_3 - Q_2^i B_p r^i B_h^* Q_3^i \tag{4.38f}$$

$$T_{24}^i = \mathbf{m}_{31}^* Q_4^i + Q_2^i \mathbf{m}_{13} + c_2^* p_{24}^i c_4 - Q_2^i B_p r^i B_k^* Q_4^i \tag{4.38g}$$

$$T_{33}^i = A_{22}^* Q_3^i + Q_3^i A_{22} + c_3^* p_{33}^i c_3 - Q_3^i B_h r^i B_h^* Q_3^i \tag{4.38h}$$

$$T_{34}^i = \mathbf{m}_{32}^* Q_4^i + Q_3^i \mathbf{m}_{23} + c_3^* p_{34}^i c_4 - Q_3^i B_h r^i B_k^* Q_4^i \tag{4.38i}$$

$$T_{44}^i = \mathbf{m}_{33}^* Q_4^i + Q_4^i \mathbf{m}_{33} + c_4^* p_{44}^i c_4 - Q_4^i B_k r^i B_k^* Q_4^i \tag{4.38j}$$

Note that the operators B_p, B_k and the components of the operator B_h are operators defined from $\mathbb{R}$ to $L^2(0,1)$ under the form $B_c u = B(z)u$. The adjoint operator of B_c is defined from $L^2(0,1) \to \mathbb{R}$ and is given by

$$B_c^* x = \int_0^1 B(z)x(z)dz$$

which represents the average value of the function Bx on the interval $[0,1]$ as we stated in the previous section. In our case we have a solution of Riccati equation on each subdivision With this fact, the Riccati equation is to become a set of integro-differential equations that are not easy to solve. To avoid this problem, the output of the adjoint operators B_p^*, B_h^* and B_k^* are to be substituted by the distributed functions instead of the average values. However, the average values will be used to calculate the optimal input which is defined in Equation (4.36) and can be found by the following expression:

$$u(t) = -r^{-1}\left[Q_1 x_1(t) - B_p \int_0^1 Q_2(z)x_2(t,z)dz \right.$$
$$\left. - \sum_{i=1}^{5} B_{h_i} \int_0^1 \left[Q_3(z)x_3(t,z)\right]_i dz - B_k \int_0^1 Q_4(z)x_4(t,z)dz\right] \tag{4.39}$$

where Q_1, Q_2, Q_3, Q_4 are the unique solutions of Equations (4.38a), (4.38e), (4.38h) and (4.38j), respectively. Now, we can solve these four equations separately and use the matrix P to force the other equations to be satisfied.

Q^i_1, Q^i_2, Q^i_3, Q^i_4 are the unique solutions of Equations:

$$\begin{aligned} T^i_{11}x &= 0 \\ T^i_{22}x &= 0 \\ T^i_{33}x &= 0 \\ T^i_{44}x &= 0 \end{aligned} \tag{4.40}$$

respectively. The same procedure is going to be followed in order to get the solution **Q**. In order to make this system hold

$$T^i_{kh}x = 0 \quad (1 \leq k, h \leq 4,\ k \neq h) \tag{4.41}$$

We use the matrix P to force all off-diagonals of (4.35) to be zeros.

Solution Q^i_1:

For each subdivision Q^i_1 is the solution of the equation $T^i_{11}x = 0$, so it is given as follows:

$$Q^i_1 = \sqrt{\frac{c_1 p^i_{11} c_1}{r^i}} \tag{4.42}$$

Solution Q^i_2:

In order to get Q^i_2 we need to solve the equation $T^i_{22}x = 0$.

By following the same method as the previous section we get Q^i_2 by the following expression :

$$Q^i_2 x = \sum_{n=0}^{\infty} \frac{\lambda^i_n + \sqrt{(\lambda^i_n)^2 + \beta^i_{nn}\alpha^i_{nn}}}{\alpha^i_{nn}} < x, \phi^i_n > \phi^i_n \tag{4.43}$$

Such that:

$c_2 p^i_{22} c_2 = \beta^i$, $B_p r^i B_p = \alpha^i$, $\beta^i_{mn} =< \beta^i \phi^i_m, \phi^i_n >$, $Q^i_{2,mn} =< Q^i_2 \phi^i_m, \phi^i_n >$ $\quad i = 1, 2 \cdots s$

Solution Q^i_3:

Solving $T_{33}^i x = 0$ in order to get Q_3^i on each subdivision, we will start by solving $T_{33}^1 = 0$

$$T_{33}^1 x = 0 \to A_{22}^* Q_3^1 x + Q_3^1 A_{22} x + c_3 p_{33}^1 c_3 x - Q_3^1 B_h r^1 b_h^* Q_3^1 x = 0$$

We have that $A_{22}^1 = -V\frac{d}{d\xi} + \mathbf{m}_{22}$. Assuming that the length of each subdivision is L. Changing the length to 1 by substituting ξ by $\frac{\xi}{L}$, so we get that $A_{22}^1 = -VL\frac{d}{d\xi} + \mathbf{m}_{22}$ with $D(A_{22}^1) = (h \in \mathcal{L}(0,1)/h, a.c\ and\ h(0) = 0)$

We have that V is a diagonal matrix, so $(VL)^* = (VL)$, then $(A_{22}^1)^* = VL\frac{d}{d\xi} + \mathbf{m}_{22}^*$ Where $D((A_{22}^1)^*) = (h \in \mathcal{L}(0,1)/h, a.c\ and\ h(1) = 0)$.
Substituting those operators terms into $T_{33}^1 x = 0$ we get that:

$$VL\frac{d(Q_3^1 x)}{d\xi} + \mathbf{m}_{22}^* Q_3^1 x + Q_3^1(-VL\frac{dx}{d\xi} + \mathbf{m}_{22} x) - Q_3^1 B_h r^1 b_h^* Q_3^1 x + c_3 p_{33}^1 c_3 x = 0$$

$$VL\frac{dQ_3^1}{d\xi} + m_{22}^* Q_3^1 + Q_3^1 \mathbf{m}_{22} - Q_3^1 B_h r^1 b_h^* Q_3^1 + c_3 p_{33}^1 c_3 = 0$$

On the other hand we have that $Q_3^1 x \in D((A_{22}^1)^*)$ then $(Q_3^1 x)(1) = 0$. We conclude that we get Q_3^1 by solving this equation

$$\begin{cases} VL\frac{dQ_3^1}{d\xi} + m_{22}^* Q_3^1 + Q_3^1 \mathbf{m}_{22} - Q_3^1 B_h r^1 b_h^* Q_3^1 + c_3 p_{33}^1 c_3 = 0 \\ Q_3^1(1) = 0 \end{cases} \tag{4.44}$$

Concerning others terms Q_3^i we get the same equation except in the boundary condition we have to ensure the continuity of the Q_3 so we get the following equation

$$\begin{cases} VL\frac{dQ_3^i}{d\xi} + m_{22}^* Q_3^i + Q_3^i \mathbf{m}_{22} - Q_3^i B_h r^i b_h^* Q_3^i + c_3 p_{33}^i c_3 = 0 \\ Q_3^i(\frac{(i-1)*L}{s}) = Q_3^{i-1}(\frac{(i-1)*L}{s}) \quad i \geq 2 \end{cases} \tag{4.45}$$

According to [1, Corollary 6.7.36], the following result holds.

Proposition 5. *If we assume that $V, p_{33}^i > 0$, then Equations (4.44) – (4.45) have a unique non-negative solution*

Remark 1. *The condition $V > 0$ is usually satisfied in chemical processes applications.*

Let's put that: $p_{33}^i = \begin{bmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} & \alpha_{14} & \alpha_{15} \\ \alpha_{12} & \alpha_{22} & \alpha_{23} & \alpha_{24} & \alpha_{25} \\ \alpha_{13} & \alpha_{23} & \alpha_{33} & \alpha_{34} & \alpha_{35} \\ \alpha_{14} & \alpha_{24} & \alpha_{34} & \alpha_{44} & \alpha_{45} \\ \alpha_{15} & \alpha_{25} & \alpha_{35} & \alpha_{45} & \alpha_{55} \end{bmatrix}$, so the system of equations (4.44) – (4.45) gives the following 15 Odes :

$$\begin{cases} v\frac{dq_{11}^i}{d\xi} + 2r_1^i - D_1^i r D_1^i + c_{11}\alpha_{11}c_{11} = 0 \\ v\frac{dq_{12}^i}{d\xi} + r_2^i - \frac{k_{m,ss}^{NO} a q_{12}^i}{E} - D_1^i r D_2^i + c_{11}\alpha_{12}c_{22} = 0 \\ v\frac{dq_{13}^i}{d\xi} + r_3^i - \frac{k_{m,ss}^{NO2} a q_{13}^i}{E} - D_1^i r D_3^i + c_{11}\alpha_{13}c_{33} = 0 \\ v\frac{dq_{14}^i}{d\xi} + r_4^i - \frac{k_{m,ss}^{NH_3} a q_{14}^i}{E} - D_1^i r D_4^i + c_{11}\alpha_{14}c_{44} = 0 \\ v\frac{dq_{15}^i}{d\xi} + r_5^i - \frac{k_{m,ss}^{O_2} a q_{15}^i}{E} - D_1^i r D_5^i + c_{11}\alpha_{15}c_{55} = 0 \\ v\frac{dq_{22}^i}{d\xi} - \frac{2k_{m,ss}^{NO} a q_{22}^i}{E} - D_2^i r D_2^i + c_{22}\alpha_{22}c_{22} = 0 \\ v\frac{dq_{23}^i}{d\xi} - \frac{k_{m,ss}^{NO} a q_{23}^i}{E} - \frac{k_{m,ss}^{NO_2} a q_{23}^i}{E} - D_2^i r D_3^i + c_{22}\alpha_{23}c_{33} = 0 \\ v\frac{dq_{24}^i}{d\xi} - \frac{k_{m,ss}^{NO} a q_{24}^i}{E} - \frac{k_{m,ss}^{NH_3} a q_{24}^i}{E} - D_2^i r D_4^i + c_{22}\alpha_{24}c_{44} = 0 \\ v\frac{dq_{25}^i}{d\xi} - \frac{k_{m,ss}^{NO} a q_{25}^i}{E} - \frac{k_{m,ss}^{O_2} a q_{25}^i}{E} - D_2^i r D_5^i + c_{22}\alpha_{25}c_{55} = 0 \\ v\frac{dq_{33}^i}{d\xi} - \frac{2k_{m,ss}^{NO_2} a q_{33}^i}{E} - D_3^i r D_3^i + c_{33}\alpha_{33}c_{33} = 0 \\ v\frac{dq_{34}^i}{d\xi} - \frac{k_{m,ss}^{NO_2} a q_{34}^i}{E} - \frac{k_{m,ss}^{NH_3} a q_{34}^i}{E} - D_3^i r D_4^i + c_{33}\alpha_{34}c_{44} = 0 \\ v\frac{dq_{35}^i}{d\xi} - \frac{k_{m,ss}^{NO_2} a q_{35}^i}{E} - \frac{k_{m,ss}^{O_2} a q_{35}^i}{E} - D_3^i r D_5^i + c_{33}\alpha_{35}c_{55} = 0 \\ v\frac{dq_{44}^i}{d\xi} - \frac{2k_{m,ss}^{NH_3} a q_{44}^i}{E} - D_4^i r D_4^i + c_{44}\alpha_{44}c_{44} = 0 \\ v\frac{dq_{45}^i}{d\xi} - \frac{k_{m,ss}^{NH_3} a q_{45}^i}{E} - \frac{k_{m,ss}^{O_2} a q_{45}^i}{E} - D_4^i r D_5^i + c_{44}\alpha_{45}c_{55} = 0 \\ v\frac{dq_{55}^i}{d\xi} - \frac{2k_{m,ss}^{O_2} a q_{44}^i}{E} - D_5^i r D_5^i + c_{55}\alpha_{55}c_{55} = 0 \\ q_{mn}^1(1) = 0,\ q_{mn}^i(\frac{(i-1)*L}{s}) = q_{mn}^{i-1}(\frac{(i-1)*L}{s}), (i > 1 and 1 \le m \le n \le 5) \end{cases} \tag{4.46}$$

Such that :

$$\begin{cases} D_1^i = q_{11}^i B_{h_1} + q_{12}^i B_{h_2} + q_{13}^i B_{h_3} + q_{14}^i B_{h_4} + q_{15}^i B_{h_5} \\ D_2^i = q_{12}^i B_{h_1} + q_{22}^i B_{h_2} + q_{23}^i B_{h_3} + q_{24}^i B_{h_4} + q_{25}^i B_{h_5} \\ D_3^i = q_{13}^i B_{h_1} + q_{23}^i B_{h_2} + q_{33}^i B_{h_3} + q_{34}^i B_{h_4} + q_{35}^i B_{h_5} \\ D_4^i = q_{14}^i B_{h_1} + q_{24}^i B_{h_2} + q_{34}^i B_{h_3} + q_{44}^i B_{h_4} + q_{45}^i B_{h_5} \\ D_5^i = q_{15}^i B_{h_1} + q_{25}^i B_{h_2} + q_{35}^i B_{h_3} + q_{45}^i B_{h_4} + q_{55}^i B_{h_5} \end{cases}$$

$$\begin{cases} r_1^i = a_{11}q_{11}^i + a_{21}q_{12}^i + a_{31}q_{13}^i + a_{41}q_{14}^i + a_{51}q_{15}^i \\ r_2^i = a_{11}q_{12}^i + a_{21}q_{22}^i + a_{31}q_{23}^i + a_{41}q_{24}^i + a_{51}q_{25}^i \\ r_3^i = a_{11}q_{13}^i + a_{21}q_{23}^i + a_{31}q_{33}^i + a_{41}q_{34}^i + a_{51}q_{35}^i \\ r_4^i = a_{11}q_{14}^i + a_{21}q_{24}^i + a_{31}q_{34}^i + a_{41}q_{44}^i + a_{51}q_{45}^i \\ r_5^i = a_{11}q_{15}^i + a_{21}q_{25}^i + a_{31}q_{35}^i + a_{41}q_{45}^i + a_{51}q_{55}^i \end{cases}$$

$$\begin{cases} a_{11} = \frac{a[(0.1748-2*18.318*10^{-}6T_{g,ss})(T_{s,ss}-T_{g,ss})-h_{m,ss}]}{\rho^s c_p^s \epsilon} \\ a_{21} = \frac{4.8*10^{-}6a(c^s_{NO}-c^{g,ss}_{NO})(T^{g,ss})^{0.75}}{\epsilon} \\ a_{31} = \frac{3.871*10^{-}6a(c^s_{NO2}-c^{g,ss}_{NO2})(T^{g,ss})^{0.75}}{\epsilon} \\ a_{41} = \frac{5.18*10^{-}6a(c^s_{NH3}-c^{g,ss}_{NH3})(T^{g,ss})^{0.75}}{\epsilon} \\ a_{51} = \frac{4.2*10^{-}6a(c^s_{O2}-c^{g,ss}_{O2})(T^{g,ss})^{0.75}}{\epsilon} \end{cases}$$

Solution Q_4^i:

Finally in order to get Q_4^i we need to solve $T_{44}^i x = 0$

$$T_{44}^i x = 0 \rightarrow A_{33}^* Q_4^i x + Q_4^i A_{33} x + c_4 p_{44}^i c_4 x - Q_4 B_k r^i B_k Q_4 x = 0$$

in our case we have that A_{33} is a scaler function and we assume that $B_k r^i B_k = r_k^i$ so in to get Q_4^i we need just to solve this second order equation :

$$2\mathbf{m}_{33} Q_4^i + c_4 p_{44} c_4 - r_k^i (Q_4^i)^2 = 0 \tag{4.47}$$

The variation of m_{33} is shown in the following figure : its obvious that the variation

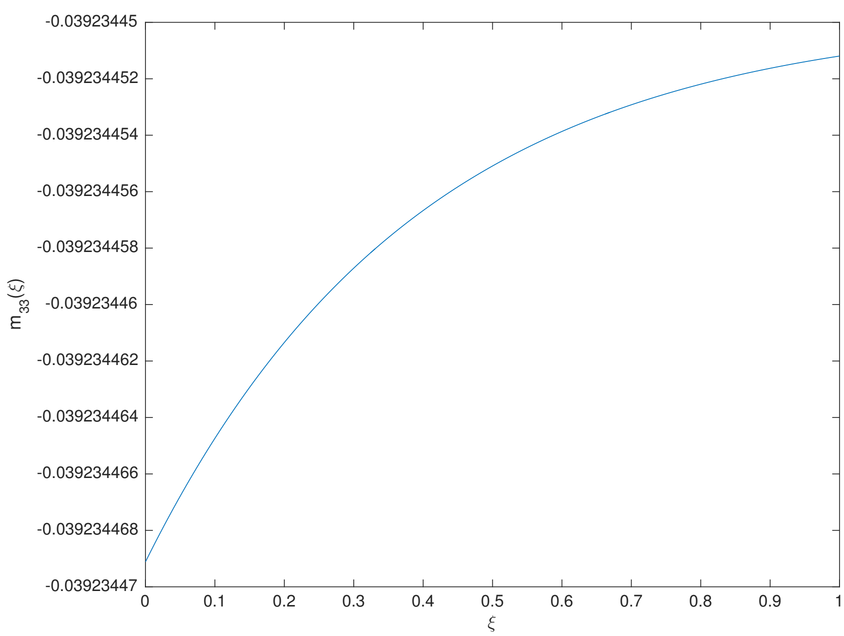

Figure 4.6: Variation of m_{33}

of m_{33} is very small, that's why it's acceptable to take $m_{33} = -0.0392$

so we are going to choose the appropriate p_{44} to make this equation has two solutions and finally we choose the positive one Q_4 on this form :

$$Q_4^i = \frac{\mathbf{m}_{33} + \sqrt{m_{33}^2 + r_k^i c_4 p_{44}^i c_4}}{r_k^i} \tag{4.48}$$

Algorithm to solve ORE (4.35):

- Choose p_{11}^i,p_{22}^i,p_{33}^i,p_{44}^i and r^i to find Q_1^i,Q_2^i,Q_3^i,Q_4^i such that Q is positive
- solve the off diagonal equations (4.41) to get (p_{ij}^i $i \neq j$) and check if this results in a positive P^i. If P^i is not positive then
- Choose a new p_{11}^i,p_{22}^i,p_{33}^i,p_{44}^i and r^i to find new Q_1^i,Q_2^i,Q_3^i,Q_4^i and solve (4.41) until we get $det(P_k^i) > 0 \quad (1 \leq k \leq n)$ such that n is the size of the matrix P^i

State-feedback control: In order to implement the state-feedback control given by Equation (4.39), we need to rewrite it in terms of the original variables. For this purpose, let us substitute $u = \dot{w}$ and $x_1 = w$, $x_2 = \tilde{z}_p - B_p w$ $x_3 = \tilde{z}_h - B_h w$ and $x_4 = \tilde{k} - B_k w$ in Equation (4.39)

$$\begin{aligned}
-r\dot{w}(t) = Q_1 w(t) - B_p \int_0^1 Q_2(z)(\tilde{z}_p - b_p w)dz \\
- \sum_{i=1}^{5} B_{h_i} \int_0^1 \left[Q_3(z)(\tilde{z}_h - B_h w)\right]_i dz - B_k \int_0^1 Q_4(z)(\tilde{k} - B_k w)dz
\end{aligned}$$

$$\begin{aligned}
-r\dot{w}(t) = \left[Q_1 + \int_0^1 \left(B_p^2 Q_2(z) + \sum_{i=1}^{5} B_{h_i}\left[Q_3(z)b_h\right]_i + B_k^2 Q_4(z)\right) dz\right] w(t) \\
- \int_0^1 \left(B_p Q_2(z)\tilde{z}_p(z) + \sum_{i=1}^{5} b_{h_i}\left[Q_3(z)\tilde{z}_h\right]_i + B_k Q_4(z)\tilde{k}\right) dz
\end{aligned}$$

$$\begin{aligned}
-r\dot{w}(t) = \left[Q_1 + \sum_{i=1}^{5} \int_{(i-1)h}^{ih} \left(B_p^2 Q_2^i(z) + \sum_{i=1}^{5} B_{h_i}\left[Q_3^i(z)b_h\right]_i + B_k^2 Q_4^i(z)\right) dz\right] w(t) \\
- \sum_{i=1}^{5} \int_{(i-1)h}^{ih} \left(B_p Q_2^i(z)\tilde{z}_p(z) + \sum_{i=1}^{5} b_{h_i}\left[Q_3^i(z)\tilde{z}_h\right]_i + B_k Q_4^i(z)\tilde{k}\right) dz
\end{aligned}$$

Then the function w satisfies the following linear differential equation

$$\dot{w}(t) + \tau w(t) = \gamma(t), \quad w(0) = 0 \tag{4.49}$$

where τ is a constant given by the following expression

$$\tau = r^{-1}\left[Q_1 + \sum_{i=1}^{5}\int_{(i-1)h}^{ih}\left(B_p^2 Q_2^i(z) + \sum_{i=1}^{5} B_{h_i}\left[Q_3^i(z)b_h\right]_i + B_k^2 Q_4^i(z)\right)dz\right]$$

and γ is a function of the SCR states and given by

$$\gamma(\tilde{z}_p, \tilde{z}_h, \tilde{k}) = r^{-1}\sum_{i=1}^{5}\int_{(i-1)h}^{ih}\left(B_p Q_2^i(z)\tilde{z}_p(z) + \sum_{i=1}^{5} b_{h_i}\left[Q_3^i(z)\tilde{z}_h\right]_i + B_k Q_4^i(z)\tilde{k}\right)dz$$

Consequently, the optimal (to be injected ammonia) state feedback control is given by

$$C^g_{NH3}(0) = w(t) + z_{h,0}(0) = e^{-\tau t}\left[\int e^{\tau t}\gamma(\tilde{z}_p(t), \tilde{z}_h(t), \tilde{k}(t))dt - G(0)\right] + z_{h,0}(0) \tag{4.50}$$

where G is the anti-deriavtive function of $e^{\tau t}\gamma(t)$.

4.4 Simulations

4.4.1 Calculations of Q_1, Q_2, Q_3, Q_4 in each subdivision

After applying our algorithm we get the following results in each subdivision:

1-**Solution over** $[\mathbf{0} \quad \mathbf{0.2}]$

For $\xi \in [0 \quad 0.2]$ we have that the appropriate values are :

$$\begin{cases} p_{11}^1 = 100 \\ p_{22}^1 = 5 \\ p_{33}^1 = 10^7 \begin{bmatrix} 3 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 3 \end{bmatrix} \\ p_{44}^1 = 0.01 \\ r^1 = 0.1 \end{cases}$$

we get that :

$$Q_1^1 = 63.826 \tag{4.51}$$

$$Q_2^1 x = 0.0384 < x, \phi_1^1 > \phi_1^1 + 0.382 < x, \phi_1^2 > \phi_1^2 + 0.0385 < x, \phi_1^3 > \phi_1^3 \tag{4.52}$$

$$+0.0372 < x, \phi_1^4 > \phi_1^4 + 0.0373 < x, \phi_1^5 > \phi_1^5$$

Concerning Q_3^1 we solve the ODEs systems numerically with MATLAB using ode45 function, and to make it easy to check the positivity of the matrix, the average has been taken by using mean function in MATLAB for all coefficients. the solution Q_3^1 are given as follows:

$$Q_3^1 = 10^7 \begin{bmatrix} 4.7 & 0.005 & 0.00033 & 0.00025 & 0.0002 \\ 0.0005 & 0.033 & 0.0006 & 0.0005 & 0.0004 \\ 0.00033 & 0.0006 & 2.761 & 0.00075 & 0.0006 \\ 0.00025 & 0.0005 & 0.00075 & 0.32 & 0.0008 \\ 0.0002 & 0.0004 & 0.0006 & 0.0008 & 0.101 \end{bmatrix} \tag{4.53}$$

To check the positivity we need just to make sure that all eigenvalues of this matrix are positive.

Eigenvalues are :

$$\sigma(Q_3^1) = 10^7 \, [0.0323, \; 0.1001, \; 0.320003, \; 2.761, \; 4.701]$$

.

$$Q_4^1 = 0.0587 \tag{4.54}$$

To guarantee that those values work we get the matrix P^1 as following:

$$P^1 = \begin{bmatrix} 3 & -0.007 & 35 & -4440 & -2213 & -2861 & -4355 & -0.1 \\ -0.007 & 5 & -4 & -0.02 & -0.02 & -0.02 & -0.02 & 0 \\ 35 & -4.2 & 3*10^7 & 0 & 0 & 0 & 0 & 1.2 \\ -4440 & -0.02 & 0 & 3*10^7 & 0 & 0 & 0 & 1.2 \\ -2213 & -0.02 & 0 & 0 & 3*10^7 & 0 & 0 & 1.2 \\ -2861 & -0.02 & 0 & 0 & 0 & 3*10^7 & 0 & 1.2 \\ -4355 & -0.02 & 0 & 0 & 0 & 0 & 3*10^7 & 1.2 \\ -0.1 & 0 & 1.2 & 1.2 & 1.2 & 1.2 & 1.2 & 0.01 \end{bmatrix}$$

Eigenvalues are :

$$\sigma(P^1) = \left[24.12, 17.85, 0.0087, 3*10^7, 3*10^7, 3*10^7, 2.89*10^7, 2.8*10^7\right]$$

because all eigenvalues are positives we conclude that P is a positive matrix

2-**Solution over** $[\mathbf{0.2} \quad \mathbf{0.4}]$

For $\xi \in [0.2 \quad 0.4]$ we have that the appropriate values are :

$$\begin{cases} p_{11}^2 = 100 \\ p_{22}^2 = 10000 \\ p_{33}^2 = 10^7 \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix} \\ p_{44}^2 = 100 \\ r^2 = 0.1 \end{cases}$$

we get that :

$$Q_1^2 = 63.826 \tag{4.55}$$

$$Q_2^2 x = 84.63 < x, \phi_2^1 > \phi_2^1 + 84.14 < x, \phi_2^2 > \phi_2^2 + 84.73 < x, \phi_2^3 > \phi_2^3 \tag{4.56}$$

$$+81.87 < x, \phi_2^4 > \phi_2^4 + 81.87 < x, \phi_2^5 > \phi_2^5$$

$$Q_3^2 = 10^7 \begin{bmatrix} 3 & 0.000018 & 0.00001 & 0.0000087 & 0.000007 \\ 0.000017 & 0.0024 & 0.000023 & 0.000017 & 0.000014 \\ 0.00001 & 0.000023 & 0.045 & 0.000026 & 0.00002 \\ 0.0000086 & 0.000017 & 0.000026 & 0.0019 & 0.000027 \\ 0.000007 & 0.000014 & 0.00002 & 0.000027 & 0.00005 \end{bmatrix} \tag{4.57}$$

$$\sigma(Q_3^2) = [486.6, \ 19288.6, \ 23755.04, \ 453591.9, \ 30000291.54] > 0$$

$$Q_4^2 = 1.47 \tag{4.58}$$

The matrix P^2 is given as follows:

$$P^2 = \begin{bmatrix} 100 & -9 & 2655 & -1872 & -940 & -1211 & -1836 & -11 \\ -9 & 10000 & -172676 & 0.0001 & 0.0001 & 0.0001 & 0.0001 & -0.02 \\ 2655 & -172676 & 2*10^7 & 0 & 0 & 0 & 0 & -1234.5 \\ -1872 & 0.0001 & 0 & 2*10^7 & 0 & 0 & 0 & -0.12 \\ -940 & 0.0001 & 0 & 0 & 2*10^7 & 0 & 0 & -0.12 \\ -1211 & 0.0001 & 0 & 0 & 0 & 2*10^7 & 0 & -0.12 \\ -1836 & 0.0001 & 0 & 0 & 0 & 0 & 2*10^7 & -0.12 \\ -11 & -0.02 & -1234.5 & -0.12 & -0.12 & -0.12 & -0.12 & 100 \end{bmatrix}$$

Eigenvalues are :

$$\sigma(P^2) = \left[56.72, 92.88, 8515.57, 1.98*10^7, 2*10^7, 2*10^7, 2*10^7, 2*10^7\right] > 0$$

3-**Solution over** $[\mathbf{0.4} \quad \mathbf{0.6}]$

For $\xi \in [0.4 \quad 0.6]$ we have that the appropriate values are :

$$\begin{cases} p_{11}^3 = 100 \\ p_{22}^3 = 2 \\ p_{33}^3 = 10^5 \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \\ p_{44}^3 = 1 \\ r^3 = 0.1 \end{cases}$$

we get that :

$$Q_1^3 = 63.826 \tag{4.59}$$

$$Q_2^3 x = 0.0153 < x, \phi_3^1 > \phi_3^1 + 0.017 < x, \phi_3^2 > \phi_3^2 + 0.018 < x, \phi_3^3 > \phi_3^3 \tag{4.60}$$

$$+0.0177 < x, \phi_3^4 > \phi_3^4 + 0.0179 < x, \phi_3^5 > \phi_3^5$$

$$Q_3^3 = \begin{bmatrix} 15*10^4 & 18.34 & 12.22 & 9.17 & 7.33 \\ 18.34 & 1265 & 24.45 & 18.34 & 1467 \\ 12.22 & 24.45 & 12000 & 27.51 & 22 \\ 9.17 & 18.34 & 2751 & 50000 & 2934 \\ 7.33 & 14.67 & 22 & 29.34 & 7625 \end{bmatrix} \tag{4.61}$$

Eigenvalues are :

$$\sigma(Q_3^3) = [1264.90,\ 7624.90,\ 12000.14,\ 50000.04,\ 150000] > 0$$

$$Q_4^3 = 2.76 \tag{4.62}$$

to guarantee that those values work we get the matrix P^3 as following:

$$P^3 = \begin{bmatrix} 10^5 & -0.1 & 7393 & -27281 & -2661.5 & -9826 & -26336 & -276 \\ -0.1 & 2 & -15 & -0.04 & -0.04 & -0.04 & -0.04 & 0.02 \\ 7393 & -15 & 10^5 & 0 & 0 & 0 & 0 & 20 \\ -2728 & -0.04 & 0 & 10^5 & 0 & 0 & 0 & 61 \\ -2661.5 & -0.04 & 0 & 0 & 10^5 & 0 & 0 & 61 \\ -9826 & -0.04 & 0 & 0 & 0 & 10^5 & 0 & 61 \\ -2634 & -0.04 & 0 & 0 & 0 & 0 & 10^5 & 61 \\ -276 & 0.02 & 20 & 61 & 61 & 61 & 61 & 1 \end{bmatrix}$$

Eigenvalues are :

$$\sigma(P^3) = \left[0.175, 2, 60000, 10^5, 10^5, 10^5, 10^5, 1.4 * 10^5\right] > 0$$

1-**Solution over [0.6 0.8]**

For $\xi \in [0.6 \quad 0.8]$ we have that the appropriate values are :

$$\begin{cases} p_{11}^4 = 100 \\ p_{22}^4 = 0.001 \\ p_{33}^4 = 10^8 \begin{bmatrix} 9 & 0 & 0 & 0 & 0 \\ 0 & 9 & 0 & 0 & 0 \\ 0 & 0 & 9 & 0 & 0 \\ 0 & 0 & 0 & 9 & 0 \\ 0 & 0 & 0 & 0 & 9 \end{bmatrix} \\ p_{44}^4 = 0.9 \\ r^4 = 0.1 \end{cases}$$

we get that :

$$Q_1^4 = 63.826 \tag{4.63}$$

$$Q_2^4 x = 10^-5 < x, \phi_4^1 > \phi_2^1 + 9.56 * 10^-6 < x, \phi_4^2 > \phi_4^2 + 9.93 * 10^-6 < x, \phi_4^3 > \phi_4^3 \tag{4.64}$$

$+9.72 * 10^-6 < x, \phi_4^4 > \phi_4^4 + 9.32 * 10^-6 < x, \phi_4^5 > \phi_4^5$

$$Q_3^3 = \begin{bmatrix} 1.4 * 10^9 & -1027.33 & -216.93 & -1921.7 & 202.14 \\ -1027.33 & 5 * 10^6 & -1044.4 & -355.84 & -25.4 \\ -216.93 & -1044.4 & 3 * 10^8 & 1377.61 & 418.88 \\ -1921.7 & -355.84 & 1377.61 & 304372 & 1253.46 \\ 202.14 & -25.4 & 418.88 & 1253.46 & 12 * 10^6 \end{bmatrix} \tag{4.65}$$

Eigenvalues are :

$$\sigma(Q_3^4) = \left[1.4 * 10^9,\ 3 * 10^8,\ 3 * 10^5,\ 5 * 10^6,\ 12 * 10^6\right] > 0$$

$$Q_4^4 = 16.83 \tag{4.66}$$

to guarantee that those values work we get the matrix P^4 as following:

$$P^4 = 10^6 \begin{bmatrix} 9 & 13e^{-11} & 43 & -58 & -7.7 & -22 & -56 & 0.0016 \\ 13e^{-11} & 9 & -0.009 & 0 & 0 & 0 & 0 & 2.5e^{-12} \\ 43 & -0.009 & 9 & 0 & 0 & 0 & 0 & -0.007 \\ -58 & 0 & 0 & 9 & 0 & 0 & 0 & -0.007 \\ -7.7 & 0 & 0 & 0 & 9 & 0 & 0 & -0.007 \\ -22 & 0 & 0 & 0 & 0 & 9 & 0 & -0.007 \\ -56 & 0 & 0 & 0 & 0 & 0 & 9 & -0.007 \\ 0.016 & 2.5e^{-12} & -76e^{-6} & -0.007 & -0.007 & -0.007 & -0.007 & 0.9e^{-6} \end{bmatrix}$$

Such that: $e^{-p} = 10^{-p} \quad p \in Z$

Eigenvalues are :

$$\sigma(P^4) = \left[0.000048, 0.52, 12.12 * 10^5, 9 * 10^8, 9 * 10^8, 9 * 10^8, 9 * 10^8\right] > 0$$

5-**Solution over $[\mathbf{0.8} \quad \mathbf{1}]$**

For $\xi \in [0.8 \quad 1]$ we have that the appropriate values are :

$$\begin{cases} p_{11}^5 = 100 \\ p_{22}^5 = 0.06 \\ p_{33}^5 = 10^7 \begin{bmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 4 \end{bmatrix} \\ p_{44}^5 = 0.001 \\ r^5 = 0.1 \end{cases}$$

we get that :

$$Q_1^5 = 63.826 \tag{4.67}$$

$$Q_2^5 x = 0.00067 < x, \phi_5^1 > \phi_5^1 + 0.00054 < x, \phi_5^2 > \phi_5^2 + 0.00035 < x, \phi_5^3 > \phi_5^3 \tag{4.68}$$

$$+0.00022 < x, \phi_5^4 > \phi_5^4 + 0.00015 < x, \phi_4^5 > \phi_5^5$$

$$Q_3^5 = \begin{bmatrix} 1060.28 & -154.15 & -32.55 & -288.36 & 30.33 \\ -154.15 & 1456.5 & -156.71 & -53.4 & -3.8 \\ -32.55 & -156.71 & 993.2 & 206.7 & 62.85 \\ -288.36 & -53.4 & 206.7 & 1716.3 & 188 \\ 30.33 & -3.8 & 62.85 & 188 & 1745.4 \end{bmatrix} \tag{4.69}$$

Eigenvalues are:

$$\sigma(Q_3^5) = [2002.7,\ 1631.5,\ 1540.9,\ 891.14,\ 905.5] > 0$$

$$Q_4^5 = 0.0054 \tag{4.70}$$

to guarantee that those values work we get the matrix P^2 as following:

$$P^5 = \begin{bmatrix} 300 & -0.0009 & 6301 & -62262 & -28134 & -38065 & -60952 & 0.1 \\ -0.0009 & 0.06 & -63 & 0 & 0 & 0 & 0 & 0 \\ 6301 & -63 & 4*10^7 & 0 & 0 & 0 & 0 & -2 \\ -62262 & 0 & 0 & 4*10^7 & 0 & 0 & 0 & -2 \\ -28134 & 0 & 0 & 0 & 4*10^7 & 0 & 0 & -2 \\ -38065 & 0 & 0 & 0 & 0 & 4*10^7 & 0 & -2 \\ -60952 & 0 & 0 & 0 & 0 & 0 & 4*10^7 & -2 \\ 0.1107 & 0 & -2 & -2 & -2 & -2 & -2 & 0.001 \end{bmatrix}$$

Eigenvalues are :

$$\sigma(P^5) = \left[0.00081, 0.06, 53.2, 4*10^7, 4*10^7, 4*10^7, 4*10^7\right] > 0$$

Finally we substitute those values in equation (4.50) to get the optimal input $C_{NH3}^g(0)$.

4.4.2 Implementation and discussions

:

The developed controller has been applied to the non-linear system and numerical simulations have been performed on the closed-loop non-linear system. Indeed, the expression of optimal amount of ammonia to be injected ($Equation$(4.50)) is implemented in the closed-loop system. Finite difference discretization method is adopted here by using the Crank-Nicholson scheme in MATLAB.

- Figure [4.7] shows the optimal input trajectory

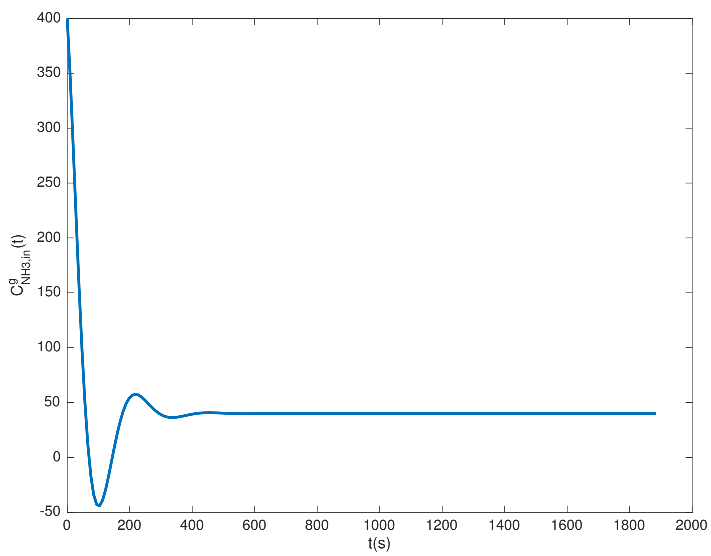

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Figure 4.7: Optimal input trajectory

- Figure [4.8] shows that surface temperature increases until it converges to the steady states. Almost our controller needs 500 second to drive this trajectory to the steady state

- Figure [4.9] describes the closed-loop trajectory for the gas temperature, it shows that gas temperature decreases for the first time, then it stats increasing until it converges to steady states. Our controller takes almost 500 second to reach to desired level

- Figures ([4.10], [4.11]) are the same. Those figures show that NO and NO_2 in bulk of gas decrease until they reach to our steady states which guarantees that

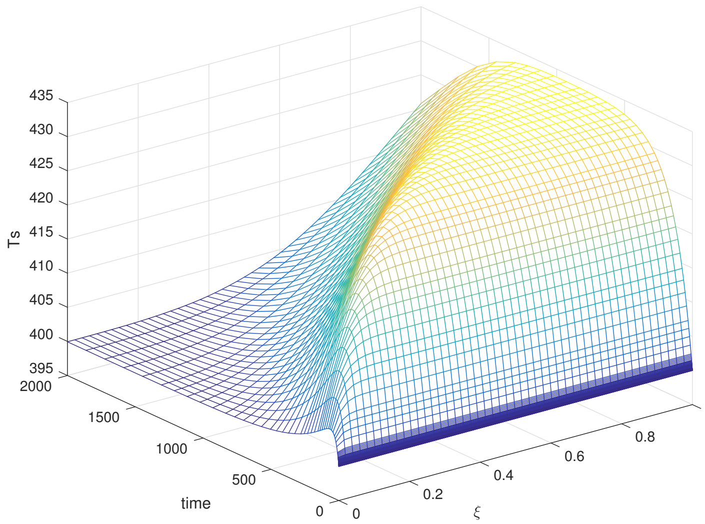

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Figure 4.8: Surface temperature of the closed loop

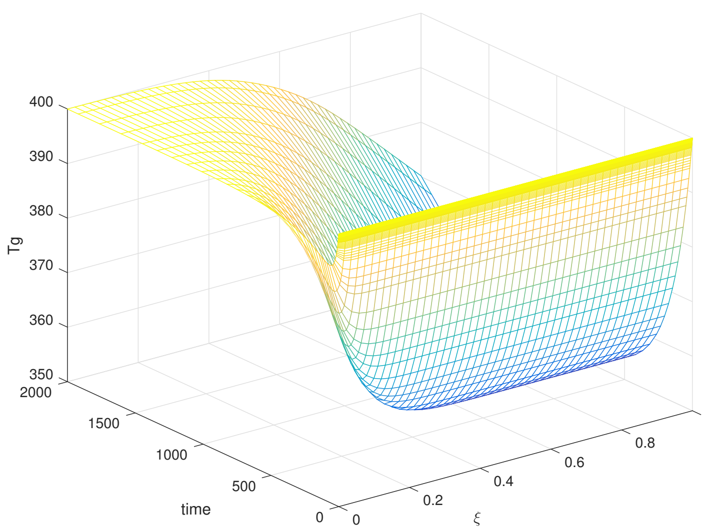

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Figure 4.9: Gas temperature of the closed loop

the performance of our controller is good, It is obvious that after 400 second the gas concentration of NO and NO_2 at the inlet is less than 50 ppm which is our objective

- Finally Figure 4.12 is the gas concentration of ammonia slip. This figure shows that NH_3 converges very fast comparing with others components, and this is a

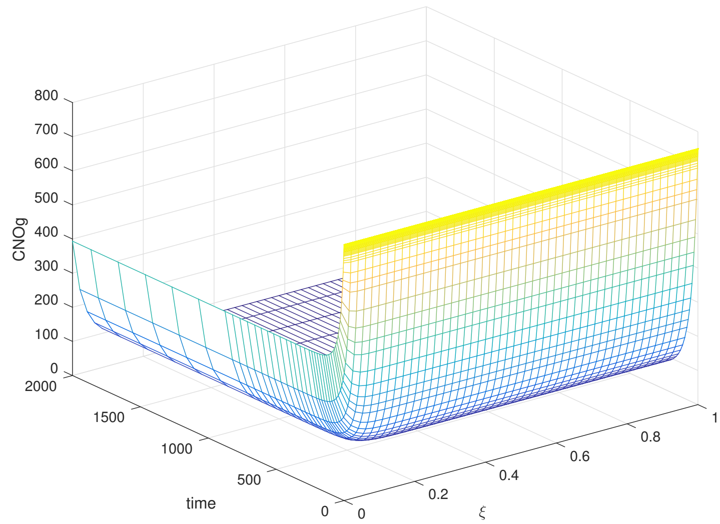

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Figure 4.10: Gas concentration of NO in the closed loop

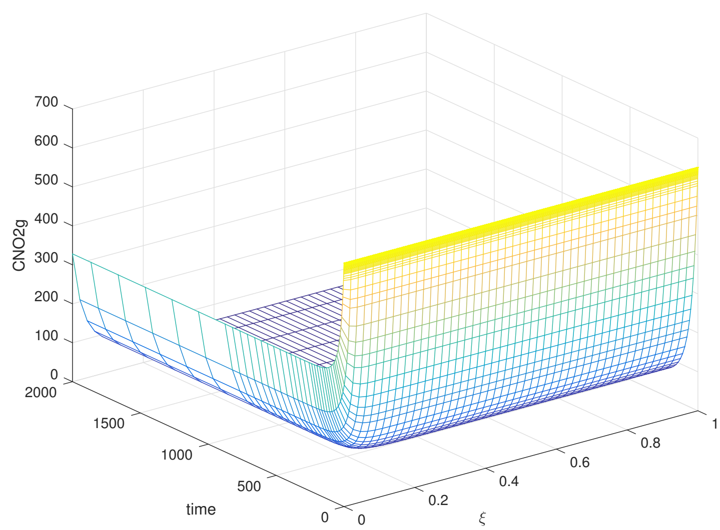

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Figure 4.11: Gas concentration of NO2 in the closed loop

good results because ammonia slip is the most dangerous one, it can seen that ammonia converge to the steady state after just 50 second

- Figure (4.13) shows the L^2-norm of the errors between the process states and the corresponding steady-states at time t. This confirms the reliability of the developed algorithm.

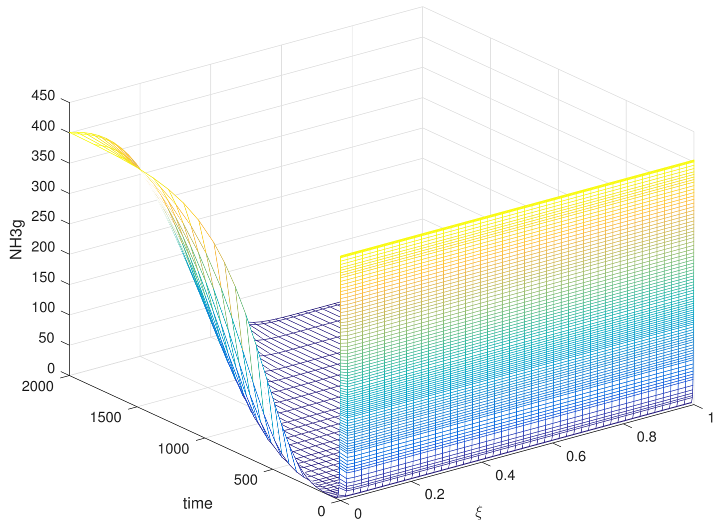

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Figure 4.12: Gas concentration of NH3 in the closed loop

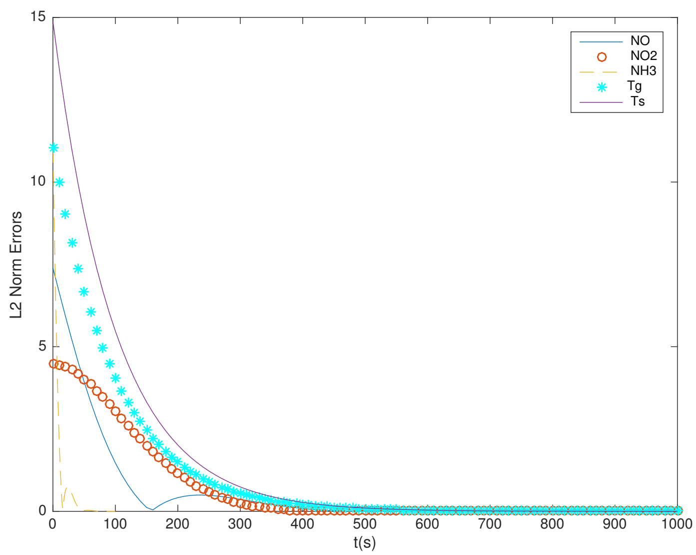

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Figure 4.13: trajectories of tracking errors

4.5 Conclusions

4.5.1 Summary

The objective of this thesis is to design a Linear Optimal Control of a coupled Parabolic-hyperbolic PDEs and ODE and apply it to the SCR . An Introduction to

Infinite-Dimensional Linear Systems is described as mathematic tools for the control of PDEs. Many concepts are introduced to use later in designing our controller. The fact of having the control input at the boundary makes the problem challenging, since in this case an augmented state space approach is needed to write the infinite-dimensional representation. After linearization of the Non-linear general model around steady states, the abstract boundary control problem approach is used to rewrite the problem in the standard form. Because of this approach the system is extended. Solving eigenvalues and eigenfunctions problem for parabolic Operator is needed in order to write this operator in Reisz-Spectral basis and solving Operator Reccati Equation (ORE).The exponential stabilizability and detectability has been proved to guarantee the existence and the uniqueness of optimal control input. Assuming that the solution of ORE is diagonal enables us to decouple the system of ORE and to make it easier to solve. An algorithm is developed in order to get the optimal control input. In order to test the performances of our controller, a Monolithic Catalyst Reactor(MCR) has been studied as the case study. Models for a MCR are a combination of coupled hyperbolic and parabolic PDEs, and ODE.The parabolic PDE represents the solid temperature. The hyperbolic PDE represents gas temperature. The last equation which is an ODE represents housing temperature. By considering that manipulated variable is gas temperature at the inlet ($u = T^g(t, 0)$) our controller has been tested on this model and it has been shown that the performances of our controller are very good, and our optimal input drives the closed loop to steady states very fast.

The main focus of this study is to test the controller described above on the SCR models. Models for a SCR consist of coupled hyperbolic and parabolic PDEs and ODE. The hyperbolic PDEs represent the concentrations of the gas phase components and the gas phase temperature. The parabolic PDE represents the solid temperature. ODE represent the coverage of stored ammonia. The main difference between the SCR models and the general case is that instead of having one hyperbolic PDE, we have multiple hyperbolic equations. The same proofs are stated for SCR, just substituting v scalar with V matrix. Also, getting the exact solution of hyperbolic operator is not realizable as in the scalar case, so a system of ODEs equations are stated and solved numerically in order to get Q_3.

Good results have been found when we apply our controller, and the closed loop converges to the steady states at a good real time. The results have also been confirmed by the errors between the closed loop and the steady states.

4.5.2 Directions for Future Work

There are many options for the future work to improve the performances of this optimal control. Design an optimal controller in a discretize the system to make it technically trivial to apply , and also to avoid the problem of unboundedness of operators. Also we know that the measurements of the reaction rates and heat and mass transfer coefficients cannot be made without affecting the systems that's why in our future work we need to add some uncertainties to the SCR model. To control our output matrix, a Kalman Filter is one of the best approaches that we can use it to estimate all states, especially concentrations which are hard to measure them along SCR. Analysis of the closed-loop CSR system is another direction of future research (see [9]).

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