Optimal Control of a Tubular Reactor via Cayley-Tustin Time Discretization

by

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Abstract

Boundary value problems involving continuous flow reactors have been considered in which tubular reactors have been modeled with an axial dispersion model. Concentration distribution in tubular reactors can have variety of consequences. It can have negative effects on the conversion and selectivity of the desired reaction. Consequently, it will affect the productivity and energy efficiency of the plant. It is therefore important to design efficient controllers that are able to track the optimal pre-defined trajectories of the operating conditions to ensure optimal operation of the reactor. The governing transport phenomena occurring in a tubular reactor is modeled by parabolic partial differential equations (PDEs). In this work, infinite dimensional optimal control of a tubular reactor is studied which is discretized exactly over time, without any discretization over space. The discrete case is derived from the continuous case and the process is shown theoretically. Numerical simulations are performed for formulated optimal controller and its performance is studied.

To Behdokht and Iradj

Acknowledgments

I would like to thank my supervisor, Dr. Stevan S. Dubljević for the guidance and support in the past two years. I appreciate the discussions that helped me explore this field and move in this path.
I am grateful for the support my family who always encouraged me.
To my friends, thank you for being there whenever I needed you.

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Introduction

1.1 Motivation

Tubular reactors have vast applications in chemical and petrochemical industries. They can be regarded as one of the most important parts of a chemical plant. In a chemical plant, usually the reactors are followed by other unit operations such as separation processes or stirred tanks. Therefore, the operational performance of the ensuing processes strongly depends on the quality and state of the products from the reactors. Thus, optimal operation of reactors in each plant is of great economical and operational importance. If the concentration of the reactant in the reactor does not follow the desired process, it can have negative repercussions on the conversion and selectivity of the desired reaction. Consequently, it will affect the productivity and energy efficiency of the plant. Therefore, the desired concentration must be maintained through an off-line dynamic optimization problem. These trajectories are used as the set-point variables for the controllers. It is therefore important to design efficient controllers that are able to track the pre-defined trajectories of the operating conditions.

In control theory, systems similar to a tubular reactor are regarded as distributed parameter systems (DPS) where the dependent variables are functions of time and space; opposite to lumped parameter systems where the dependent variables are only functions of time (e.g., a well-mixed stirred pot). Other examples of DPS in chemical engineering are heat exchangers, fluidized beds, and continuous flow stirred tank reactors (CSTR). Traditionally, most of control methods have been developed for lumped parameter systems. Therefore, the DPS are commonly approximated with lumped parameter systems and controlled using algorithms for such lumped systems. As a result of the boundless existence of DPS and economic advantages of precise control of these systems, developing controllers that use the most punctilious model of these systems can have superabundant performance benefit. Motivated by this, this thesis is focused on formulation of an optimal controller for tubular reactors. In the following sections the available studies on the topic of DPS and the outline of the thesis will be recapitulated.

1.2 Background

As stated before, the most conventional approaches for control of DPS use lumping techniques to approximate the partial differential equations (PDEs) model of the system by a set of coupled ordinary differential equations (ODEs). Methods such as finite differences may be used for spatial discretization, resulting in model approximations that consist of ODEs. However, such approximations may not be proper for high performance control schemes, as the dimensionality of the produced sets of ODEs can be very high when trying to ensure high performance control. Besides, this high dimensionality requires powerful and expensive computing tools which may not be usually available. Also controllability and observability of the system will depend on the number and location of the discretization points, see [8]. Another method for controlling DPS is to develop the control algorithm based on the PDEs and discretize the resulting controller during the implementation. The advantage of this approach is that the controller synthesis is based on the original model of the system which represent all the dynamical properties of the system without any approximation. Over the recent years, research on the control of DPS is oriented towards development of algorithms that deal with infinite dimensional nature of these systems.

Mathematical theory of optimal control of DPS began in late 1960s in the work of Lions [20] and followed by other researchers (e.g., [4], [18], and [9]).

In a functional analysis frame of reference, systems modeled by PDEs can be formulated in a state-space form similar to that for lumped parameter systems by introducing a suitable infinite-dimensional system representation and operators instead of usual matrices in lumped parameter systems, see [9]. The type of PDE system (e.g. hyperbolic, parabolic or elliptic) determines the approach followed for the solution of the control problem [8]. Based on the governing phenomenon in a chemical process, convection or diffusion, the model equations can be hyperbolic or parabolic.

For hyperbolic systems, Callier and Winkin in [7] studied the linear quadratic (LQ) control problem using spectral factorization for the case of finite rank bounded observation and control operators. Aksikas in [1] extended this approach for the more general case of exponentially stable linear systems with bounded observation and control operators. In his work, this method was applied to a non-isothermal plug flow reactor to regulate the temperature and the reactant concentration in the reactor. The optimal control problem for a particular class of hyperbolic PDEs is solved via the infamous Riccati equation, which is developed in a series of papers by Aksikas and co-workers. (e.g., [1], [2], [3], etc); however, the approach taken in this work addresses only a particular class of hyperbolic PDEs and does not address the case of parabolic systems, which models widespread number of chemical engineering processes.

The conventional approach for dealing with parabolic systems is modal decomposition, see [25]. The main characteristic of parabolic systems is that their spectrum can be partitioned into a finite slow part and an infinite fast complement (slow modes and fast modes). This feature has been used by many researchers to perform model reduction and synthesize finite dimensional models representing the distributed parameter system with arbitrary accuracy (see [8], [11], [17] and references therein). The low dimensional model is used to formulate predictive controllers for the infinite dimensional system. Although the model reduction method is computationally efficient for diffusion dominant systems, it can result in a high dimensional system for convection dominant parabolic systems.

The control action in a DPS can be distributed over the spatial domain of the system, or can be applied at the boundary. For example, in the case of a tubular reactor, the manipulated variable can be inlet concentration (i.e., boundary control) or the concentration profile of the reactor (i.e. distributed control). Boundary control systems are mathematically more complex than systems with distributed control inputs.

Boundary control of DPS has been explored by few studies. Curtain and Zwart in [9], Emirsjlow and Townley in [12], Yapari in [28], and Mohammadi in [22] address the transformation of the boundary control problem into a well-posed abstract control problem. Byrnes et al in [6] studied the boundary feedback control of parabolic systems using zero dynamics. The proposed algorithm is designed for parabolic systems with self-adjoint operator $\mathcal{A}$.

The topic of parabolic systems with non-self-adjoint operators was introduced by Amundson in [24]; however, due to mathematical complexity, boundary control approach through abstract control problem has not yet been investigated much. An applicable proposed solution is via backstepping method with some less theoretical complexity (see [19], [16], and references therein).

The topic of optimal control of infinite dimensional systems is explored by many researchers ([2], [28], [22], and etc.), but time discretization issue was not discussed too much. The novel idea of this thesis is that the optimality notion of the controller is studied by exact time discretization. Exact time discretization for a class of parabolic PDEs is studied by [27]. In this thesis, optimality in controller design is added to the

method proposed by [14] and [27].
Although the emphasis of this thesis is on tubular reactors, the general idea and developed controllers are capable of controlling any system that is modeled by the studied class of DPS in this work.

1.3 Outline and Contributions

In this thesis, the control of a tubular reactor is demonstrated through the application of linear quadratic (LQ) controller. The system to be controlled is given in the form of a parabolic partial differential equation (PDE) which describes the spatiotemporal dynamics of the concentration of the reactant, [23].
In Chapter 2, the governing PDE is first put into an abstract boundary control problem and then discretized exactly in time via symplectic Euler's method. Then, a gain-based full-state feedback controller is designed to show the original behavior of the system. Exact time discretization is applied to this controller. In this chapter, three different numerical schemes are studied and the effect of each one on the stability of a parabolic system is inspected also. It is shown that the symplectic method used in this work does not have any effects on the stability and preserves the system stability status.
In Chapter 3, linear quadratic (LQ) controller is designed for the governing PDE, both in continuous and discrete space. The optimal gain K of the controller is calculated and the stability of the LQ controller is studied.
Finally, Chapter 4 consists of the concluding remarks and summarizes possibilities for future research direction.

Chapter 2

Tubular Reactors and Self-Adjoint Operators

In this chapter the approach proposed to solve the eigenvalue problem for a parabolic PDE is spectral decomposition used by [25]. Using the spectral properties of the system, stability of the system is studied and the gained-based full-state feedback controller is designed. The model studied in this work is parabolic PDE.

In the nature, pure hyperbolic systems are found seldom. Normally, hyperbolic equations result from ignoring the effect of diffusion phenomenon within the process. In most chemical engineering systems, more specifically in most tubular reactors, transport may not be ignored and as a result, the model of the system should be represented by one or a set of parabolic PDEs. Here, system described by one parabolic PDE is studied.

The only difference between a first order hyperbolic PDE and a parabolic PDE is presence of the second order derivative with respect to the space variable. This difference results in completely different dynamical behavior and mathematical properties.

Parabolic systems can be characterized by their set of eigenvalues and eigenfunctions. The spectral property of these systems is the tool that is generally used to deal with parabolic systems ([25], [23], and [24]).

Control of transport systems, which are described by parabolic PDEs has studied by many researchers (e.g. [8], [11], [17] and references therein). In these works, modal decomposition is used to derive finite dimensional system that captures the dominant dynamics of the original PDE and is subsequently used for low dimensional optimal controller design. The potential drawback of this approach is that for diffusion-convection-reaction systems the number of modes that should be used to derive the ODE system may be very large, which leads to computationally demanding controllers which requires powerful and expensive computing tools that may not be available usu-

ally.
Boundary control of parabolic systems have been explored in few studies. Curtain and Zwart in [9], Emirsjlow and Townley in [12], Yapari in [28], and Mohammadi in [22] introduced transformation of the boundary control problem to a well-posed abstract control problem using an exact transformation. Byrnes et al in [6] studied the boundary feedback control of parabolic systems using zero dynamics. The proposed algorithm is designed for parabolic systems with self-adjoint operator $\mathcal{A}$.
Parabolic systems with non-self-adjoint operators was introduced by Amundson in [24]; however, due to mathematical complexity, boundary control approach through abstract control problem has not yet been done. Proposed solution are via backstepping method with less theoretical complexity (see [19], [16], and references therein).
The topic of optimal control of infinite dimensional systems is explored by many researchers ([2], [28], [22], and etc.), but time discretization issue was not discussed too much. The novel idea of this work is that the optimality notion of the controller is studied by exact time discretization. Exact time discretization for a class of parabolic PDEs is studied by [27]. In this work optimal controller design is added to this method.
Although the emphasis of this thesis is on tubular reactors, the general idea and developed controllers are capable of controlling any system that is modeled by the studied class of DPS in this work.

2.1 Problem Statement

In this section, some background will be provided for infinite dimensional representation of parabolic partial differential equations. The introduced concepts will be used throughout this thesis to formulate the infinite dimensional controller and analyze the stabilizability of the parabolic systems. The following transport equation will be used.
The problem is consisted of a tubular lead in which homogeneous first order reaction ($A \rightarrow Product$) occurs. The entire reactor is held at a constant temperature.

Axial dispersion model is applied to the reactor, so that the differential equation that governs the concentration c of the reactant A is given by

$$D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - kc = \frac{\partial c}{\partial t} \qquad 0 < x < l \tag{2.1}$$

The boundary condition at the inlet ($x = 0$) is

$$-D\frac{\partial c}{\partial x}(0^+, t) + vc(0^+, t) = vc_f \tag{2.2}$$

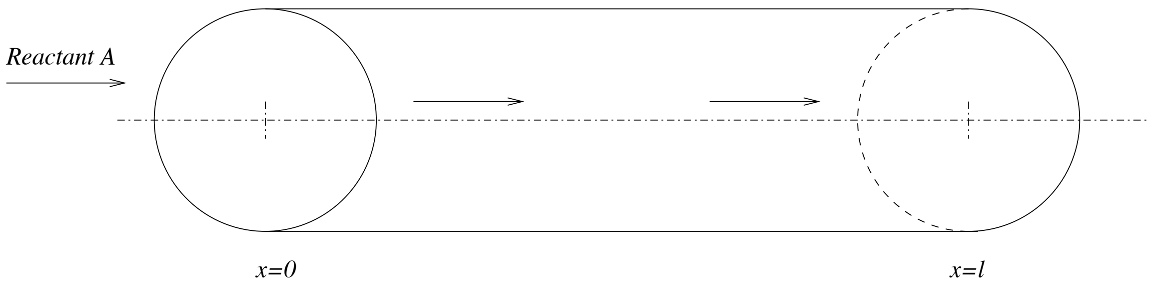


Figure 2.1: Tubular reactor

where c_f denotes the concentration at section $-\infty < x < 0$ which is a function of time only.
The initial condition is

$$c(x,0) = F(x) \tag{2.3}$$

Non-dimensionalizing the variables

$$\xi \equiv \frac{x}{l}; \qquad \tau \equiv \frac{Dt}{l^2}; \qquad \mathrm{Pe} \equiv \frac{lv}{D};$$

$$u(\xi,\tau)\mathrm{e}^{1/2\ \mathrm{Pe}\ \xi} \equiv \frac{c(x,t)}{c_f(0)}; \qquad u_f(\tau) \equiv \frac{c_f(\tau)}{c_f(0)}; \qquad \alpha \equiv \frac{kl^2}{D};$$

$$\beta \equiv \frac{V}{\mathrm{A}l}; \qquad f(\xi) \equiv \frac{1}{c_f(0)}F(x)\mathrm{e}^{1/2\ \mathrm{Pe}\ \xi}$$

Employing all of the dimensionless parameters above, the boundary value problem becomes as

$$-\frac{\partial^2 u}{\partial \xi^2} + \left(\alpha + \frac{\mathrm{Pe}^2}{4}\right)u = -\frac{\partial u}{\partial \tau}, \qquad 0 < \xi < 1 \tag{2.4}$$

$$-\frac{\partial u}{\partial \xi}(0^+,\tau) + \frac{1}{2}\mathrm{Pe}u(0^+,\tau) = \mathrm{Pe}u_f \tag{2.5}$$

$$\frac{1}{\beta}\frac{\partial u}{\partial \xi}(1^-,\tau) = 0 \tag{2.6}$$

$$u(\xi,0) = f(\xi) \tag{2.7}$$

So, Equations 2.4 and 2.5 can be written in the following form

$$\mathcal{F}u = \frac{\partial u}{\partial \tau}$$

and

$$\mathcal{B}u = \mathrm{Pe}\ u_f$$

where $u(.,t) = \{u(\xi,t), 0 < \xi < 1\}$ is the state variable in the Hilbert space $\mathcal{H} := \mathcal{L}_2([0,1];t)$ [9], and $u_f(t) \in \mathbb{R}$ is the boundary actuation. $\mathcal{F}$ is the spatial derivative operator defined as:

$$\mathcal{F}\Phi(\xi) = \left[\frac{\partial^2}{\partial\xi^2} - \gamma\right]\Phi(\xi) \quad \text{where} \quad \gamma = \alpha + \frac{\mathrm{Pe}^2}{4} \tag{2.8}$$

with the domain $\mathcal{D}(\mathcal{F}) = \big\{\Phi(\xi) \in \mathcal{L}_2(0,1) : \Phi(\xi), \Phi'(\xi) \text{ are abs. cont.}, \mathcal{F}\Phi(\xi) \in \mathcal{L}_2(0,1), \Phi'(0) = \frac{\mathrm{Pe}}{2}\Phi(0), \Phi'(1) = 0\big\}$. Here $\mathcal{L}_2(0,1)$ denotes the Hilbert space of measurable, square-integrable, real-valued functions.

The boundary operator $\mathcal{B} : \mathcal{L}_2(0,1) \mapsto \mathbb{R}$ can be defined as follows

$$\mathcal{B}\Phi(\xi) = \left[-\frac{\partial}{\partial\xi} + \frac{1}{2}\mathrm{Pe}\right]\Phi(0) \tag{2.9}$$

Our PDE equation is not well posed, due to the fact that the controlled input appears in the boundary condition. Therefore, one define a new operator $\mathcal{A}$ such that

$$\mathcal{A}\Phi(\xi) = \mathcal{F}\Phi(\xi) \text{ and } \mathcal{D}(\mathcal{A}) = \mathcal{D}(\mathcal{F}) \cap \ker(\mathcal{B}) \tag{2.10}$$

This is based on the assumption that $u_f \in \mathbf{C}^2([0,t];V)$ is sufficiently smooth, and one can find function $B(\xi)$ such that $\forall u_f(\tau)$, $B(\xi)u_f(\tau) \in \mathcal{D}(\mathcal{F})$, and

$$\mathcal{B}B(\xi)u_f(\tau) = \mathrm{Pe}u_f(\tau), \qquad u_f \in V \tag{2.11}$$

Now having Equations 2.4 and 2.5, one can lift the boundary actuation into the domain by having the following state transformation

$$u(\xi,\tau) = p(\xi,\tau) + B(\xi)u_f(\tau) \tag{2.12}$$

So, Equations 2.4 and 2.5 become the following well posed abstract system of differential equations

$$\begin{aligned} \frac{\mathrm{d}u_f}{\mathrm{d}\tau} &= \tilde{u}_f \\ \frac{\partial p}{\partial\tau} &= \mathcal{A}p(\xi,\tau) + \mathcal{A}B(\xi)u_f(\tau) - B\tilde{u}_f \end{aligned} \tag{2.13}$$

with

$$p(\xi,0) = p_0(\xi) \tag{2.14}$$

Now from the boundary conditions it is known that $\mathcal{B}B(\xi) = \mathrm{Pe}$ which can be written as

$$-\frac{\partial B(0)}{\partial\xi} + \frac{1}{2}\mathrm{Pe}B(0) = \mathrm{Pe} \tag{2.15}$$

So, one can write

$$-\frac{\partial p(0,\tau)}{\partial \xi} + \frac{1}{2}\mathrm{Pe}p(0,\tau) = 0 \tag{2.16}$$

Besides, from the boundary condition imposed over u at $\xi = 1$, one can say $\dfrac{\partial u(1,\tau)}{\partial \xi} = 0$ which leads us to

$$\frac{\partial p(1,\tau)}{\partial \xi} + \frac{\partial B(1)}{\partial \xi} u_f(\tau) = 0$$

Since $B(\xi)$ is an arbitrary function, one can define $B(\xi)$ such that

$$\frac{\partial B(1)}{\partial \xi} = 0 \tag{2.17}$$

Based on Equations 2.15 and 2.17 and the assumption that $\mathcal{A}$ is the infinitesimal generator of a C_0-semigroup on $\mathcal{L}_2$, one can easily suggest a function for $B(\xi)$ which in this case would be $B(\xi) = 2$; a constant scalar function over space.
By taking Laplace transformation of Equation 2.13 it can be said

$$sp(\xi,s) - p_0(\xi) = \frac{\partial^2 p(\xi,s)}{\partial \xi^2} - \gamma p(\xi,s) - 2\gamma u_f(s) - 2\tilde{u}_f(s) \tag{2.18}$$

So, it can be said

$$\frac{\partial}{\partial \xi}\begin{bmatrix} p(\xi,s) \\ \dfrac{\partial p(\xi,s)}{\partial \xi} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ s+\gamma & 0 \end{bmatrix}\begin{bmatrix} p(\xi,s) \\ \dfrac{\partial p(\xi,s)}{\partial \xi} \end{bmatrix} + \begin{bmatrix} 0 \\ -1 \end{bmatrix} p_0(\xi) + \begin{bmatrix} 0 \\ 2 \end{bmatrix}\Big(\gamma u_f(s) + \tilde{u}_f(s)\Big) \tag{2.19}$$

The solution to this first order system is

$$\begin{aligned}\begin{bmatrix} p(\xi,s) \\ \dfrac{\partial p(\xi,s)}{\partial \xi} \end{bmatrix} &= \begin{bmatrix} \cosh(\sqrt{s+\gamma}\,\xi) & \dfrac{1}{\sqrt{s+\gamma}}\sinh(\sqrt{s+\gamma}\,\xi) \\ \sqrt{s+\gamma}\sinh(\sqrt{s+\gamma}\,\xi) & \cosh(\sqrt{s+\gamma}\,\xi) \end{bmatrix}\begin{bmatrix} p(0,s) \\ \dfrac{\partial p(0,s)}{\partial \xi} \end{bmatrix} \\ &\quad - \int_0^{\xi} \begin{bmatrix} \dfrac{1}{\sqrt{s+\gamma}}\sinh\Big(\sqrt{s+\gamma}(\xi - x)\Big) \\ \cosh\Big(\sqrt{s+\gamma}(\xi - x)\Big) \end{bmatrix} p_0(x)\mathrm{d}x \\ &\quad + 2\int_0^{\xi} \begin{bmatrix} \dfrac{1}{\sqrt{s+\gamma}}\sinh\Big(\sqrt{s+\gamma}(\xi - x)\Big) \\ \cosh\Big(\sqrt{s+\gamma}(\xi - x)\Big) \end{bmatrix}\Big(\gamma u_f(s) + \tilde{u}_f(s)\Big)\mathrm{d}x\end{aligned} \tag{2.20}$$

In addition, the following boundary condition is known for $p(\xi, s)$

$$
\begin{aligned}
0 = &\frac{\partial p(1,s)}{\partial \xi}\\
&= \sqrt{s+\gamma}\sinh(\sqrt{s+\gamma})p(0,s) + \cosh(\sqrt{s+\gamma})\frac{\partial p(0,s)}{\partial \xi}\\
&- \int_0^1 \cosh\left(\sqrt{s+\gamma}(1-x)\right)p_0(x)\mathrm{d}x + 2\int_0^1 \cosh\left(\sqrt{s+\gamma}(1-x)\right)\left(\gamma u_f(s) + \tilde{u}_f(s)\right)\mathrm{d}x
\end{aligned}
\tag{2.21}
$$

Besides, it is known that

$$\frac{\partial p(0,s)}{\partial \xi} = \frac{1}{2}\mathrm{Pe}p(0,s)$$

So, putting above boundary condition into Equation 2.21 one will have

$$
\begin{aligned}
0 = &\sqrt{s+\gamma}\sinh(\sqrt{s+\gamma})p(0,s) + \cosh(\sqrt{s+\gamma})\frac{1}{2}\mathrm{Pe}p(0,s)\\
&- \int_0^1 \cosh\left(\sqrt{s+\gamma}(1-x)\right)p_0(x)\mathrm{d}x + 2\int_0^1 \cosh\left(\sqrt{s+\gamma}(1-x)\right)\left(\gamma u_f(s) + \tilde{u}_f(s)\right)\mathrm{d}x
\end{aligned}
\tag{2.22}
$$

Thus

$$p(0,s) = \frac{\int_0^1 \cosh\left(\sqrt{s+\gamma}(1-x)\right)p_0(x)\mathrm{d}x - \frac{2}{\sqrt{s+\gamma}}\sinh(\sqrt{s+\gamma})\Big(\gamma u_f(s) + \tilde{u}_f(s)\Big)}{\sqrt{s+\gamma}\sinh(\sqrt{s+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{s+\gamma})} \tag{2.23}$$

and ($\tilde{u}_f(s) = su_f - u_f(0)$, where $u_f(0) = 0$ is assumed without loss of generality)

$$
\begin{aligned}
&p(\xi,s) =\\
&\left[\cosh(\sqrt{s+\gamma}\xi) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{s+\gamma}}\sinh(\sqrt{s+\gamma}\xi)\right]\frac{\int_0^1 \cosh\left(\sqrt{s+\gamma}(1-x)\right)p_0(x)\mathrm{d}x}{\sqrt{s+\gamma}\sinh(\sqrt{s+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{s+\gamma})}\\
&- \int_0^\xi \frac{1}{\sqrt{s+\gamma}}\sinh\left(\sqrt{s+\gamma}(\xi-x)\right)p_0(x)\mathrm{d}x\\
&+ \Bigg[2\Big[\cosh(\sqrt{s+\gamma}) - 1\Big]\\
&- \left[\cosh(\sqrt{s+\gamma}\xi) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{s+\gamma}}\sinh(\sqrt{s+\gamma}\xi)\right]\frac{\frac{2}{\sqrt{s+\gamma}}\sinh(\sqrt{s+\gamma})(\gamma+s)}{\sqrt{s+\gamma}\sinh(\sqrt{s+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{s+\gamma})}\Bigg]u_f(s)\\
&+ 2\int_0^\xi \frac{1}{\sqrt{s+\gamma}}\sinh\left(\sqrt{s+\gamma}(\xi-x)\right)(s+\gamma)u_f(s)\mathrm{d}x
\end{aligned}
\tag{2.24}
$$

In other words, it can be written

$$p(\xi, s) = \bar{\mathbb{A}}(\xi, s)p(\xi, 0) + \bar{\mathbb{B}}(\xi, s)u_f(s) \tag{2.25}$$

2.2 Time Discretization

Now, having built up the foundation, one will have a look at linear system time discretization. If a system is represented as

$$\dot{X}(\zeta, t) = \mathbb{A}X(\zeta, t) + \mathbb{B}U(t) \tag{2.26}$$

we will have its solution in Laplace space in the following form

$$X(\zeta, s) = (sI - \mathbb{A})^{-1}X(\zeta, 0) + (sI - \mathbb{A})^{-1}\mathbb{B}U(s) \tag{2.27}$$

In addition, given a discretization parameter $\Delta t > 0$, a slightly non-standard time discretization of Equation 2.26 of Crank-Nicolson type is given by [14] as

$$\frac{X(\zeta, k+1) - X(\zeta, k)}{\Delta t} \approx \mathbb{A}\frac{X(\zeta, k+1) + X(\zeta, k)}{2} + \mathbb{B}U(k) \tag{2.28}$$

Re-arranging Equation 2.28 gives us

$$X(\zeta, k+1) \approx (\frac{2}{\Delta t} - \mathbb{A})^{-1}(\frac{2}{\Delta t} + \mathbb{A})X(\zeta, k) + (\frac{2}{\Delta t} - \mathbb{A})^{-1}\mathbb{B}U(k) \tag{2.29}$$

Here, Equation 2.29 is the discrete version of Equation 2.27. Comparing these two equations, one can conclude that in order to discretize a continuous equation in Laplace space, one can simply replace s by $\frac{2}{\Delta t}$ and one will have the discrete version as well [14].

There is an extensive discussion over the stability of the numerical methods given in §2.5.

Discretization Procedure for a Simple Case

Consider the simple ordinary differential equation (ODE) given by

$$\dot{x} = ax$$

$$x(0) = x_0 \tag{2.30}$$

it can be discretized with the following schemes.

- **Explicit Euler** method discretizes the ODE as

$$\frac{x^{n+1} - x^n}{\Delta t} = ax^n$$
$$x^{n+1} = (\Delta t + a)x^n$$

- **Implicit Euler** method discretizes the ODE as

$$\frac{x^{n+1} - x^n}{\Delta t} = ax^{n+1}$$
$$x^{n+1} = (a - \Delta t)^{-1}x^n$$

- **Crank-Nicolson** method discretizes the ODE as

$$\frac{x^{n+1} - x^n}{\Delta t} = a\frac{x^{n+1} + x^n}{2}$$
$$x^{n+1} = (1 - \frac{a\Delta t}{2})^{-1}(1 + \frac{a\Delta t}{2})x^n$$
$$x^{n+1} = \frac{1 + \frac{a\Delta t}{2}}{1 - \frac{a\Delta t}{2}}x^n$$
$$x^{n+1} = (\frac{2}{\Delta t} - a)^{-1}(\frac{2}{\Delta t} + a)x^n$$

As shown above, in Crank-Nicolson method the coefficient of x^n is the first order approximation for the exponential expression.

Applying the discretization method, the discrete expression for p over time is then found.

$$
\begin{aligned}
&p(\xi, k+1) = \\
&\quad \Bigg[\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)\Bigg] \\
&\quad \times \frac{\int_0^1 \cosh\Big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\Big)p(x,k)\mathrm{d}x}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
&\quad - \int_0^\xi \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\Big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\Big)p(x,k)\mathrm{d}x \\
&\quad + \Bigg(2\Bigg[\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}) - 1\Bigg] \\
&\quad - \Bigg[\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)\Bigg] \\
&\quad \times \frac{\frac{2}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})(\gamma+\frac{2}{\Delta t})}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
&\quad + 2\int_0^\xi \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\Big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\Big)(\frac{2}{\Delta t}+\gamma)\mathrm{d}x\Bigg)u_f(k) \qquad (2.31)
\end{aligned}
$$

For $k = 1$ the above equation holds which implies that one can build the state at any arbitrary k by starting from $k = 0$. It is utmost clear that $k = 0$ is given by the initial condition.
Therefore, based on what is shown in Equation 2.31, it can be said that $p(\xi, s)$ is consisted of two parts; initial condition contribution, and input contribution.

Assuming zero-input condition, leads us to

$$p(\xi,k+1)=$$
$$\left[\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)+\frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)\right]$$
$$\times\frac{\int_0^1\cosh\left(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\right)p(x,k)\mathrm{d}x}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})+\frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})}$$
$$-\int_0^\xi\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\left(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\right)p(x,k)\mathrm{d}x \quad (2.32)$$

which is a function of initial profile $p_0(\xi)$ as it is shown.
Now, assuming an initial profile for $p(\xi,\mathfrak{t})$, one can see the system evolution through time.
Hence, by taking $p_0(\xi)=2\pi\xi-\sin(2\pi\xi)$, one will have

$$p(\xi,1)=$$
$$\frac{\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)+\frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})+\frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})}$$
$$\times\int_0^1\cosh\left(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\right)(2\pi\xi\sin(2\pi x))\mathrm{d}x$$
$$-\int_0^\xi\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\left(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\right)(2\pi\xi-\sin(2\pi\xi))\mathrm{d}x \quad (2.33)$$

Implementing Equation 2.33 in MATLAB, one will see the behavior of the system with a prescribed initial condition $p_0(\xi)=2\pi\xi-\sin(2\pi\xi)$. State evolution is depicted in Figure 2.2.

Note that in this case since there is no input at the boundary ($u_f=0$), the evolution for both p and u would be the same.

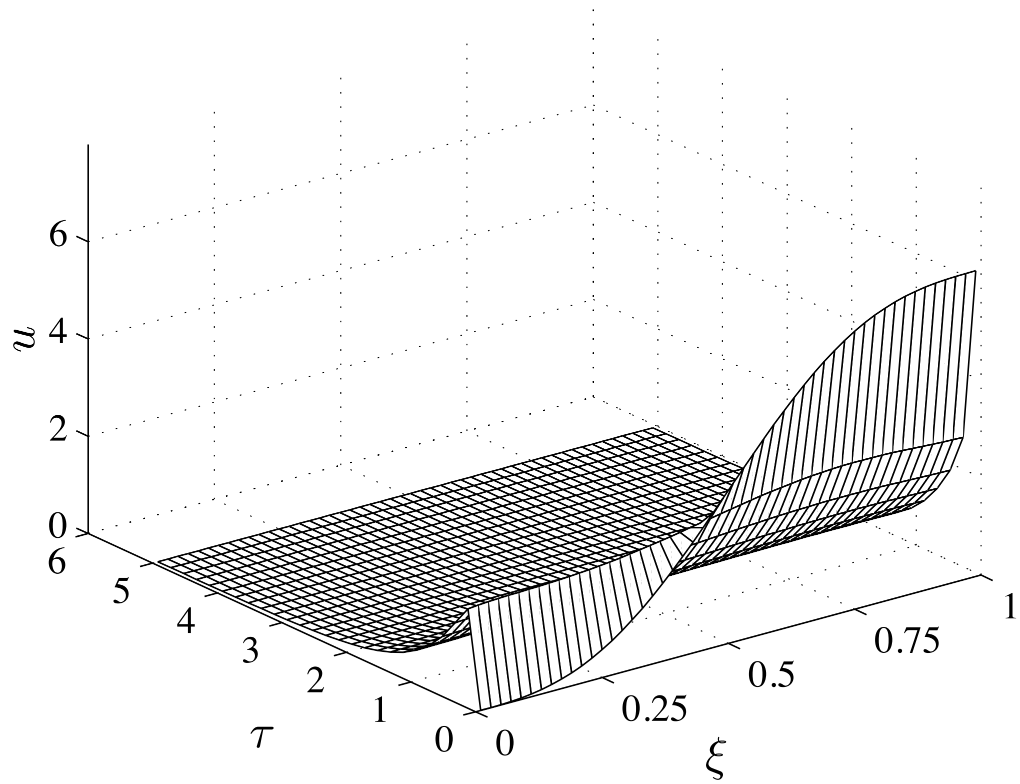


Figure 2.2: Discrete system evolution in time for $p_0(\xi) = 2\pi\xi - \sin(2\pi\xi)$.

Now, how the input affects the evolution of the system is considered. To do that, an arbitrary input function will be chosen and the system evolution would be governed by Equation 2.31.
Here, step input is chosen, i.e. $u(k) = \text{cte}$[1]. Therefore, the governing equation would be Equation 2.31 where $p_0(\xi) = 2\pi\xi - \sin(2\pi\xi)$ and $u(k) = \text{cte}$, and the system evolution in time is shown by Figure 2.3. Note that in this case, finally system reaches the profile of the input.

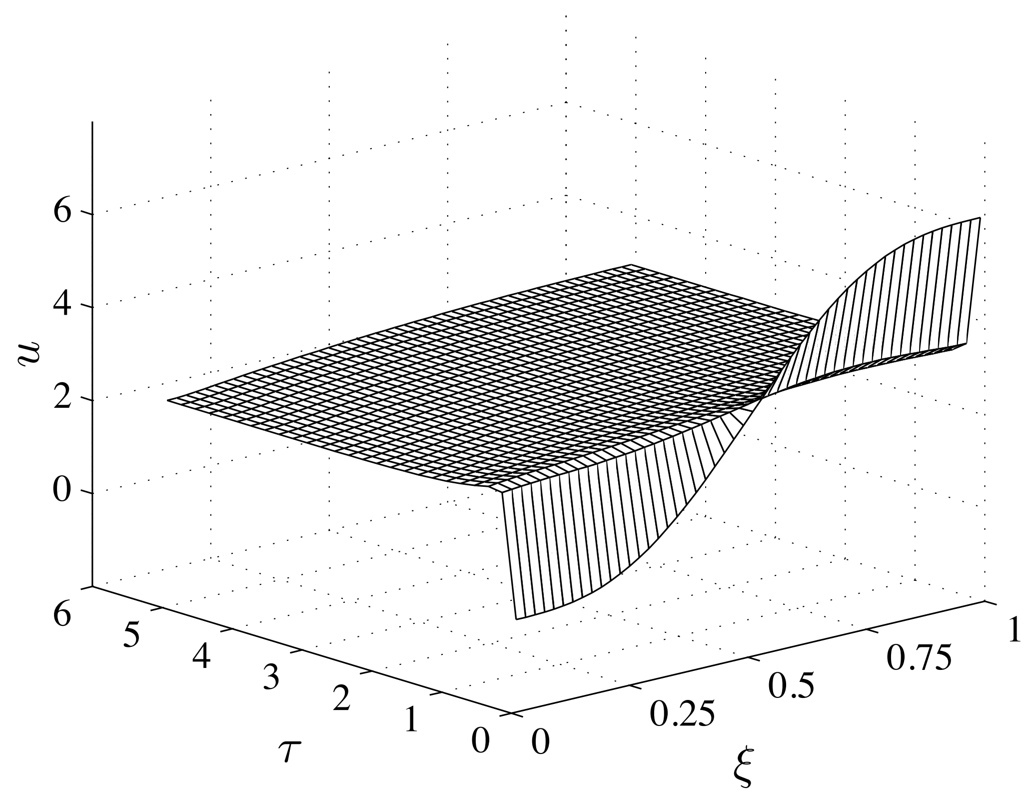


Figure 2.3: Discrete system evolution in time for $p_0(\xi) = 2\pi\xi - \sin(2\pi\xi)$ and step input $u_f(k) = \text{cte}$.

[1]denotes constant function

2.3 Eigenvalue Problem

Now, looking back at abstract boundary control problem in Equation 2.13.

$$\frac{\partial p}{\partial \tau} = \mathcal{A}p(\xi,\tau) + \mathcal{A}B(\xi)u_f(\tau) - B\tilde{u}_f$$

with

$$\frac{\partial p(0,\tau)}{\partial \xi} = \frac{1}{2}\mathrm{Pe}p(0,\tau), \qquad \frac{\partial p(1,\tau)}{\partial \xi} = 0$$

This PDE can be reformulated on extended state space $\mathcal{L}_2^e := \mathcal{L}_2 \oplus V$, yielding

$$\dot{x}^e(\xi,\tau) = \begin{bmatrix} 0 & 0 \\ \mathcal{A}B & \mathcal{A} \end{bmatrix} \begin{bmatrix} u_f(\tau) \\ p(\xi,\tau) \end{bmatrix} + \begin{bmatrix} 1 \\ -B \end{bmatrix} \tilde{u}_f$$

$$x^e(\xi,0) = \begin{bmatrix} u_f(0) \\ p(\xi,0) \end{bmatrix} = x_0^e(\xi) \tag{2.34}$$

Here, the eigenvalue problem of interest is given by the following equation

$$\mathcal{A}^e\phi = \lambda\phi$$

where operator $\mathcal{A}^e$ is given by Equation 2.34 and

$$\mathcal{A}^e = \begin{bmatrix} 0 & 0 \\ \mathcal{A}B & \mathcal{A} \end{bmatrix} \tag{2.35}$$

We observe that the operator $\mathcal{A}^e$ is a lower triangular operator, therefore the set of eigenvalues consists of the eigenvalues of the elements on its diagonal, i.e.

$$\sigma(\mathcal{A}^e) = \{0\} \cup \sigma(\mathcal{A}) \tag{2.36}$$

Eigenvalues of Operator $\mathcal{A}$

The eigenvalues and corresponding eigenfunctions of $\mathcal{A}$ can be found through the separation of variables [9]. Furthermore, eigenfunctions of the adjoint operator $\mathcal{A}^*$ that satisfy the orthogonality condition $\langle \phi_i(\xi), \phi(\xi)_j^* \rangle = \delta_{ij}$, can also be computed [25]. For $\mathcal{A}$ it is known that

$$\mathcal{A}\phi(\xi) = \frac{\mathrm{d}^2\phi(\xi)}{\mathrm{d}\xi^2} - \gamma\phi(\xi) = -\lambda\phi(\xi)$$

So, introducing new operator L, the above equation be written as

$$L\phi(\xi) = \frac{\mathrm{d}^2\phi(\xi)}{\mathrm{d}\xi^2} + (\lambda - \gamma)\phi(\xi) \tag{2.37}$$

where

$$\frac{\mathrm{d}\phi(0)}{\mathrm{d}\xi} = \frac{\mathrm{Pe}}{2}\phi(0), \text{ and } \frac{\mathrm{d}\phi(1)}{\mathrm{d}\xi} = 0$$

Equation 2.37 is Sturm-Liouville operator, which is self-adjoint and can be put in the following general form of this type, i.e.

$$L(.) = a_2(\xi)\frac{\mathrm{d}^2(.)}{\mathrm{d}\xi^2} + a_1(\xi)\frac{\mathrm{d}(.)}{\mathrm{d}\xi} + a_0(\xi)(.)$$

and its adjoint looks like

$$L^*(.) = \frac{\mathrm{d}^2\Big(a_2(\xi)(.)\Big)}{\mathrm{d}\xi^2} + \frac{\mathrm{d}\Big(a_1(\xi)(.)\Big)}{\mathrm{d}\xi} + a_0(\xi)(.)$$

Now, it is known that $a_2(\xi) = 1$, $a_1(\xi) = 0$, and $a_0 = -\gamma$. Therefore, one can say that L is self-adjoint, i.e. $L = L^*$ or $\mathcal{A} = \mathcal{A}^*$.
Hence, $\mathcal{A}$ has a solution for its eigenfunctions of the following form

$$\phi_n(\xi) = A_n \cos(\sqrt{\lambda_n - \gamma}\xi) + B_n \sin(\sqrt{\lambda_n - \gamma}\xi) \tag{2.38}$$

Applying boundary conditions, one has

$$\frac{\mathrm{d}\phi(0)}{\mathrm{d}\xi} = \frac{\mathrm{Pe}}{2}\phi(0) \Rightarrow \sqrt{\lambda_n - \gamma}B_n = \frac{\mathrm{Pe}}{2}A_n$$

$$\frac{\mathrm{d}\phi(1)}{\mathrm{d}\xi} = 0 \Rightarrow A_n \sin(\sqrt{\lambda_n - \gamma}) = B_n \cos(\sqrt{\lambda_n - \gamma})$$

Therefore one can write

$$\sqrt{\lambda_n - \gamma}\sin(\sqrt{\lambda_n - \gamma}) = \frac{\mathrm{Pe}}{2}\cos(\sqrt{\lambda_n - \gamma}) \tag{2.39}$$

Equation 2.39 is to be solved numerically. Assuming $\mathrm{Pe} = 2$, $\gamma = 1$, and employing MATLAB to solve that, the following numerical values for λ_n are found:

$$\begin{cases} \lambda_1 = 1.7402 \\ \lambda_2 = 12.7349 \\ \lambda_3 = 42.4388 \\ \vdots \end{cases}$$

Based on the values found for λ_n, one can compute the coefficients A_n and B_n. Hence, eigenfunctions of $\mathcal{A}$ are found. Here, ϕ_n and λ_n are the eigenvalues and eigenfunctions of $\mathcal{A}$.
So, associated eigenvalues of $\mathcal{A}^e$ are given by

$$\sigma(\mathcal{A}^e) = \{0\} \cup \sigma(\mathcal{A}) = \{\bar{\lambda}_n\} \quad n = 0, 1, 2, \ldots \tag{2.40}$$

where $\bar{\lambda}_0 = 0$, and $\bar{\lambda}_n = \lambda_n$ for $n \geq 1$.

Note that if there are m boundary input variables, the zero eigenvalue will be repeated m times. Here, $m = 1$ as there is only one input variable.
Since the operator $\mathcal{A}$ is self-adjoint, biorthogonality holds over the spectrum of its domain [25], so

$$\langle \phi_n, \phi_n \rangle = \int_0^1 \phi_n^2 \mathrm{d}\xi = 1$$

Coefficients A_n and B_n are calculated numerically.
Therefore ϕ_n are given by

$$\begin{cases} \phi_1(\xi) = 0.8268 \cos(\sqrt{\lambda_1 - \gamma}\xi) + 0.9610 \sin(\sqrt{\lambda_1 - \gamma}\xi) \\ \phi_2(\xi) = 1.3110 \cos(\sqrt{\lambda_2 - \gamma}\xi) + 0.3827 \sin(\sqrt{\lambda_2 - \gamma}\xi) \\ \phi_3(\xi) = 1.3816 \cos(\sqrt{\lambda_3 - \gamma}\xi) + 0.2146 \sin(\sqrt{\lambda_3 - \gamma}\xi) \\ \vdots \end{cases}$$

If $\mathbf{\Phi}_n$ is defined as $\mathbf{\Phi}_n = \begin{bmatrix} F_{1,n} \\ F_{2,n} \end{bmatrix}$ as the eigenfunction of $\mathcal{A}^e$, one can say

$$\mathcal{A}^e \begin{bmatrix} F_{1,n} \\ F_{2,n} \end{bmatrix} = \sigma_n \begin{bmatrix} F_{1,n} \\ F_{2,n} \end{bmatrix} \tag{2.41}$$

For, $n \geq 1$ one can write $\mathbf{\Phi}_n = \begin{bmatrix} 0 \\ \phi_n \end{bmatrix}$.
For $n = 0$, it can be written

$$\mathcal{A}^e \begin{bmatrix} F_{1,0} \\ F_{2,0} \end{bmatrix} = 0 \begin{bmatrix} F_{1,0} \\ F_{2,0} \end{bmatrix}$$

So, $\mathbf{\Phi}_0 = \begin{bmatrix} 1 \\ -\mathcal{A}^{-1}(\mathcal{A}B) \end{bmatrix}$.
Therefore, by utilizing the definition of resolvent sets [9], associated eigenfunctions of $\mathcal{A}^e$ are given by

$$\mathbf{\Phi}_0 = \begin{bmatrix} 1 \\ \sum_{j=1}^{\infty} \frac{1}{\lambda_j} \langle \mathcal{A}B, \phi_j \rangle \phi_j \end{bmatrix}, \text{ and } \mathbf{\Phi}_n = \begin{bmatrix} 0 \\ \phi_n \end{bmatrix} \qquad n = 1, 2, \ldots \tag{2.42}$$

Eigenvalues of Operator $\mathcal{A}^{e^*}$

By doing the same procedure as the previous section, one obtains the following expression for $\mathbf{\Psi}_n$

$$\mathbf{\Psi}_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \text{ and } \mathbf{\Psi}_n = \begin{bmatrix} \frac{1}{\lambda_n} (\mathcal{A}B)^* \phi_n \\ \phi_n \end{bmatrix} \qquad n = 1, 2, \ldots \tag{2.43}$$

2.4 Gain-Based Full-State Feedback

In this part the state is inserted as the input to study the behavior of the model. So, one will have $\tilde{u}_f(k) = -Kx^e$ and in this part there is constant gain, i.e. $K = \text{cte}$. Hence, our extended state space will look like

$$\dot{x}^e(\xi,\tau) = \begin{bmatrix} 0 & 0 \\ \mathcal{A}B & \mathcal{A} \end{bmatrix} \begin{bmatrix} u_f(\tau) \\ p(\xi,\tau) \end{bmatrix} + \begin{bmatrix} 1 \\ -B \end{bmatrix} \begin{bmatrix} K_1 & K_2 \end{bmatrix} \begin{bmatrix} u_f(\tau) \\ p(\xi,\tau) \end{bmatrix}$$
$$\begin{bmatrix} \dot{u}_f(\tau) \\ \dot{p}(\xi,\tau) \end{bmatrix} = \begin{bmatrix} K_1 & K_2 \\ \mathcal{A}B - BK_1 & \mathcal{A} - BK_2 \end{bmatrix} \begin{bmatrix} u_f(\tau) \\ p(\xi,\tau) \end{bmatrix} \tag{2.44}$$

Now, a *new* extended state space arises where $\dot{x}^e = \bar{A}x^e$ and

$$\dot{x}^e = \bar{A}x^e = \begin{bmatrix} K_1 & K_2 \\ \mathcal{A}B - BK_1 & \mathcal{A} - BK_2 \end{bmatrix} x^e$$

Expanding our state by the eigenvalues, it can be said

$$\begin{bmatrix} 1 & 0 \\ 0 & \phi_i \end{bmatrix} \dot{x}_i^e = \begin{bmatrix} K_1 & K_2 \\ \mathcal{A}B - BK_1 & \mathcal{A} - BK_2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \phi_i \end{bmatrix} x_i^e \tag{2.45}$$

Projecting this onto

$$\begin{bmatrix} 1 & 0 \\ 0 & \phi_i^* \end{bmatrix} \tag{2.46}$$

we obtain

$$\dot{x}_i^e = \begin{bmatrix} \dot{u} \\ \dot{p}_i \end{bmatrix} = \begin{bmatrix} K_1 & K_2 \\ \langle \mathcal{A}B, \phi_i^* \rangle - \langle K_1 B, \phi_i^* \rangle & \lambda_i - \langle K_2 B, \phi_i^* \rangle \end{bmatrix} \begin{bmatrix} u \\ p_i \end{bmatrix} \tag{2.47}$$

Putting $i = 1$, it is shown (in §2.3) that $\lambda_1 = 1.7402$ and $\phi_1 = \phi_1^* = 0.8268\cos(\sqrt{\lambda_1 - \gamma}\xi) + 0.9610\sin(\sqrt{\lambda_1 - \gamma}\xi)$.
Therefore, it can be written

$$\dot{x}_1^e = \begin{bmatrix} \dot{u} \\ \dot{p}_1 \end{bmatrix} = \begin{bmatrix} K_1 & K_2 \\ \langle \mathcal{A}B, \phi_1 \rangle - \langle K_1 B, \phi_1 \rangle & \lambda_1 - \langle K_2 B, \phi_1 \rangle \end{bmatrix} \begin{bmatrix} u \\ p_1 \end{bmatrix}$$

So, the above equation turns into the following simple equation

$$\dot{x}_1^e = \begin{bmatrix} \dot{u} \\ \dot{p}_1 \end{bmatrix} = \begin{bmatrix} K_1 & K_2 \\ 2.2340(-\gamma - K_1) & \lambda_1 - 2.2340K_2 \end{bmatrix} \begin{bmatrix} u \\ p_1 \end{bmatrix} \tag{2.48}$$

Now one can find the eigenvalues of the above equation via $\det(\bar{\lambda}I - \bar{A}) = 0$, i.e.

$$\det(\bar{\lambda}I - \bar{A}) = \det \begin{bmatrix} \bar{\lambda} - K_1 & -K_2 \\ 2.2340(\gamma + K_1) & \bar{\lambda} - \lambda_1 + 2.2340K_2 \end{bmatrix} \tag{2.49}$$

which says that in order to have closed-loop system stability, one has to manipulate K_1 and K_2 such that it is always as $\Re(\bar{\lambda}) < 0$. In other words, if the system is

unstable, by proper choice of the coefficients in full-state feedback gains, one can simply stabilize the system.
Another method is to decompose x^e by the eigenfunctions of $\mathcal{A}^e$, i.e.

$$x^e = \sum_{i=0}^{\infty} x_i \mathbf{\Phi}_n$$

If K_i is at hand, Equation 2.44 becomes

$$\begin{aligned} \dot{x}_i \mathbf{\Phi}_i &= \begin{bmatrix} 0 & 0 \\ \mathcal{A}B & \mathcal{A} \end{bmatrix} x_i \mathbf{\Phi}_i + \begin{bmatrix} 1 \\ -B \end{bmatrix} K_i x_i \mathbf{\Phi}_i \\ \dot{x}_i^e &= \Big(\sigma_i + \langle B^e K_i, \mathbf{\Psi}_i \rangle \Big) x_i \end{aligned} \tag{2.50}$$

This way gives the same result, that is K_i must be manipulated such that it is always $\Re(\bar{\sigma}) < 0$. In other words, if the system is unstable, by proper choice of the coefficients in full-state feedback gains, one can simply stabilize the system.

2.4.1 Time Discretization

We know that

$$\begin{aligned} \tilde{u}_f = \dot{u}_f = \begin{bmatrix} K_1 & K_2 \end{bmatrix} \begin{bmatrix} u_f(\tau) \\ p(\xi,\tau) \end{bmatrix} &= K_1 u_f + K_2 p \\ \mathcal{L}\{\dot{u}_f\} = s u_f - u_f(0) &= K_1 u_f + K_2 p \\ u_f = \frac{K_2}{s-K_1} p + \frac{1}{s-K_1} &u_f(0) \end{aligned}$$

Without loss of generality, one can assume $u_f(0) = 0$, so u_f will look like this

$$u_f = \frac{K_2}{s-K_1} p \tag{2.51}$$

Therefore, taking Laplace's transformation of Equation 2.44, the evolution of p will be as

$$sp(\xi,s) - p_0(\xi) = \frac{\partial^2 p(\xi,s)}{\partial \xi^2} + (-\gamma - 2K_2) p(\xi,s) + (-2\gamma - 2K_1) \frac{K_2}{s-K_1} p(\xi,s) \tag{2.52}$$

So, it is

$$\frac{\partial}{\partial \xi} \begin{bmatrix} p(\xi,s) \\ \dfrac{\partial p(\xi,s)}{\partial \xi} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \mu & 0 \end{bmatrix} \begin{bmatrix} p(\xi,s) \\ \dfrac{\partial p(\xi,s)}{\partial \xi} \end{bmatrix} + \begin{bmatrix} 0 \\ -1 \end{bmatrix} p_0(\xi) \tag{2.53}$$

where $\mu = s + \gamma + 2K_2 + \dfrac{(2\gamma + 2K_1)K_2}{s-K_1}$.

Therefore, one has the following solution for Equation 2.53

$$\begin{bmatrix} p(\xi,s) \\ \\ \dfrac{\partial p(\xi,s)}{\partial \xi} \end{bmatrix} = \begin{bmatrix} \cosh(\sqrt{\mu}\xi) & \dfrac{1}{\sqrt{\mu}}\sinh(\sqrt{\mu}\xi) \\ \\ \sqrt{\mu}\sinh(\sqrt{\mu}\xi) & \cosh(\sqrt{\mu}\xi) \end{bmatrix} \begin{bmatrix} p(0,s) \\ \\ \dfrac{\partial p(0,s)}{\partial \xi} \end{bmatrix} - \int_0^{\xi} \begin{bmatrix} \dfrac{1}{\sqrt{\mu}}\sinh\Big(\sqrt{\mu}(\xi - x)\Big) \\ \\ \cosh\Big(\sqrt{\mu}(\xi - x)\Big) \end{bmatrix} p_0(x)\mathrm{d}x \quad (2.54)$$

Following the same procedure as was done early in this chapter, one has the following expression for evolution of $p(0,s)$

$$p(0,s) = \frac{\int_0^1 \cosh\Big(\sqrt{\mu}(1-x)\Big)p_0(x)\mathrm{d}x}{\sqrt{\mu}\sinh(\sqrt{\mu}) + \dfrac{\mathrm{Pe}}{2}\cosh(\sqrt{\mu})} \quad (2.55)$$

So, one can write $p(\xi,s)$ as

$$p(\xi,s) = \left[\cosh(\sqrt{\mu}\xi) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\mu}}\sinh(\sqrt{\mu}\xi)\right] \frac{\int_0^1 \cosh\Big(\sqrt{\mu}(1-x)\Big)p_0(x)\mathrm{d}x}{\sqrt{\mu}\sinh(\sqrt{\mu}) + \dfrac{\mathrm{Pe}}{2}\cosh(\sqrt{\mu})} - \int_0^{\xi} \frac{1}{\sqrt{\mu}}\sinh\Big(\sqrt{\mu}(\xi - x)\Big)p_0(x)\mathrm{d}x \quad (2.56)$$

Now, based on what was discussed in §2.2, one has the discrete expression for the above equation as

$$p(\xi,k+1) = \left[\cosh(\sqrt{\mu_d}\xi) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\mu_d}}\sinh(\sqrt{\mu_d}\xi)\right] \frac{\int_0^1 \cosh\Big(\sqrt{\mu_d}(1-x)\Big)p(x,k)\mathrm{d}x}{\sqrt{\mu_d}\sinh(\sqrt{\mu_d}) + \dfrac{\mathrm{Pe}}{2}\cosh(\sqrt{\mu_d})} - \int_0^{\xi} \frac{1}{\sqrt{\mu_d}}\sinh\Big(\sqrt{\mu_d}(\xi - x)\Big)p(x,k)\mathrm{d}x \quad (2.57)$$

where $\mu_d = \dfrac{2}{\Delta t} + \gamma + 2K_2 + \dfrac{(2\gamma + 2K_1)K_2}{\dfrac{2}{\Delta t} - K_1}$.

We see that another condition over the feedback gain arises; K_1 cannot be chosen equal to $\dfrac{2}{\Delta t}$. Hence, K_1 must satisfy the stability condition for Equation 2.49 and must hold $K_1 \neq \dfrac{2}{\Delta t}$. Besides, if gains are chosen in advance in order to stabilize the system, one can say that one is not allowed to take any arbitrary Δt. So, Δt must be chosen such it is always $\dfrac{2}{\Delta t} \neq K_1$.
One of these conditions must be met based on the design requirements.

Numerical Demonstration

Looking back at Equation 2.49, one can assign stabilizing and unstabilizing values to K_1 and K_2.

Similar to §2.2, the boundary condition must satisfy the original PDE. Therefore, the boundary condition is chosen as same as the way is chosen in that section (i.e. $p_0(\xi) = 2\pi\xi - \sin(2\pi\xi)$).

For the stabilizing gains, it is well demonstrated in Figures 2.4 and 2.5 that by changing gain values, the controller has different dynamics. By the proper choice of the gains system can have the desired dynamics; fast or slow dynamics. Simulations are conducted via MATLAB.

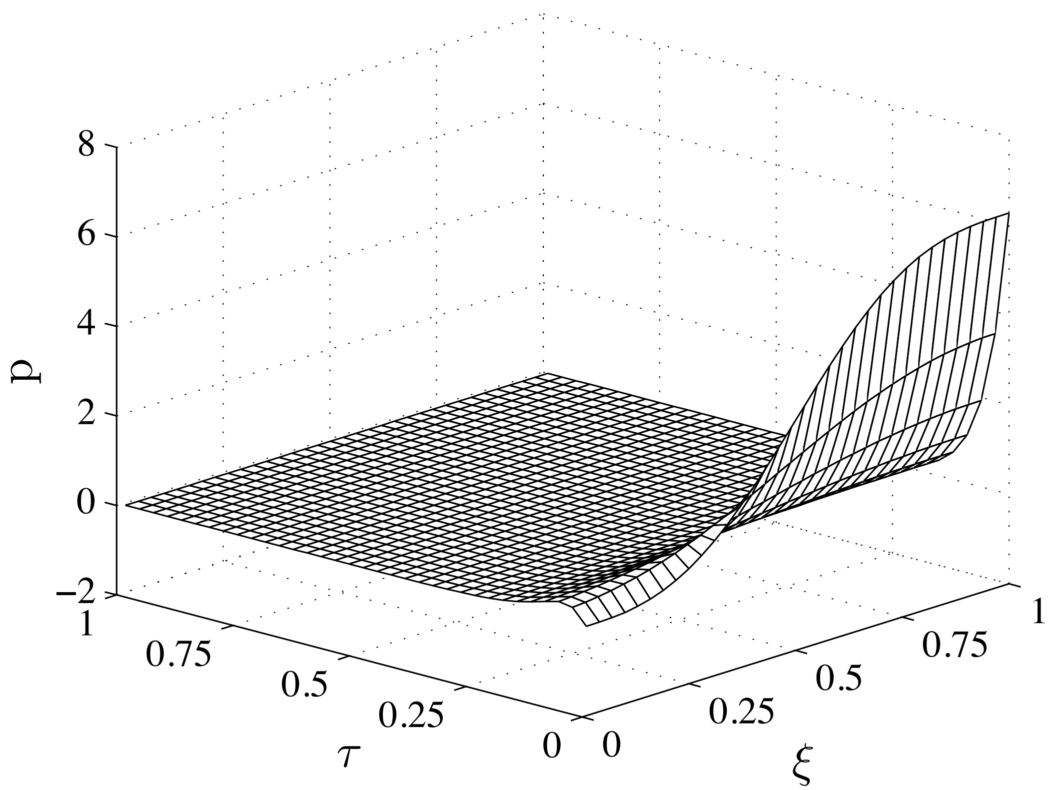


Figure 2.4: System converges and has stability, and has a relatively *fast* dynamics.

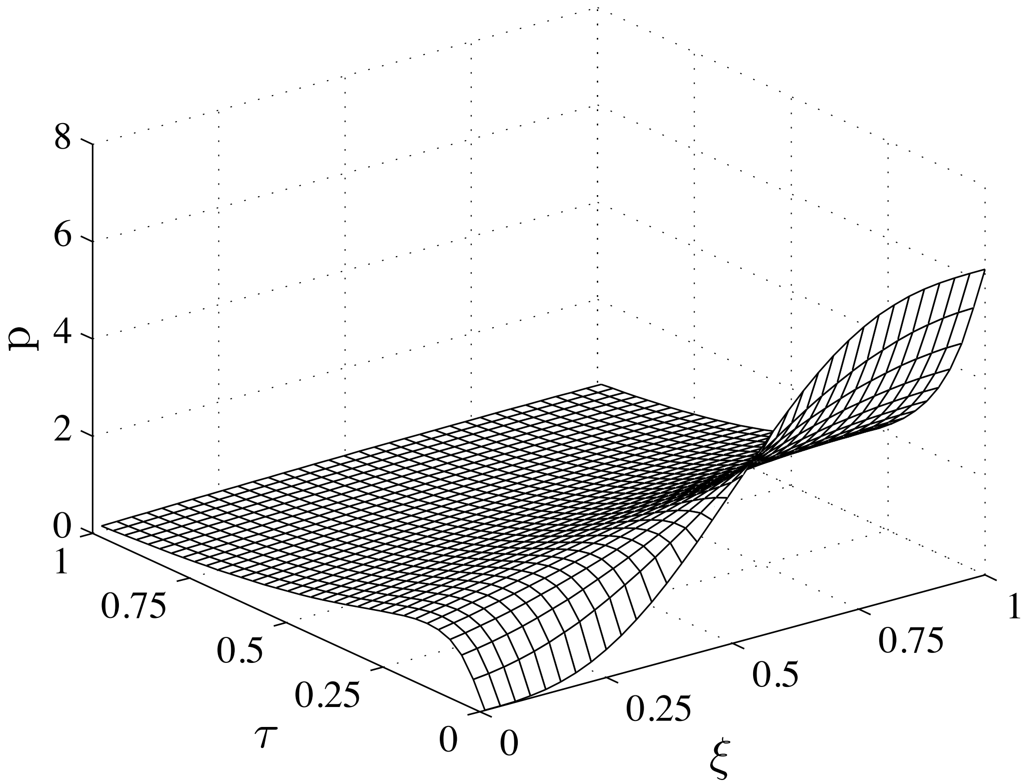


Figure 2.5: System converges and has stability, and has a relatively *slow* dynamics.

As shown in Figure 2.6, by poor choice of the gain values, the system diverges and does not have any stability whatsoever. In this case by simply just manipulating K_1 one is able to make the system unstable. It cannot be put $K_1 = \dfrac{2}{\Delta t}$ due to zero-division limit; however, by putting K_1 slightly greater than $\dfrac{2}{\Delta t}$, i.e. $K_1 = \dfrac{2}{\Delta t} + \epsilon$, the system becomes unstable.

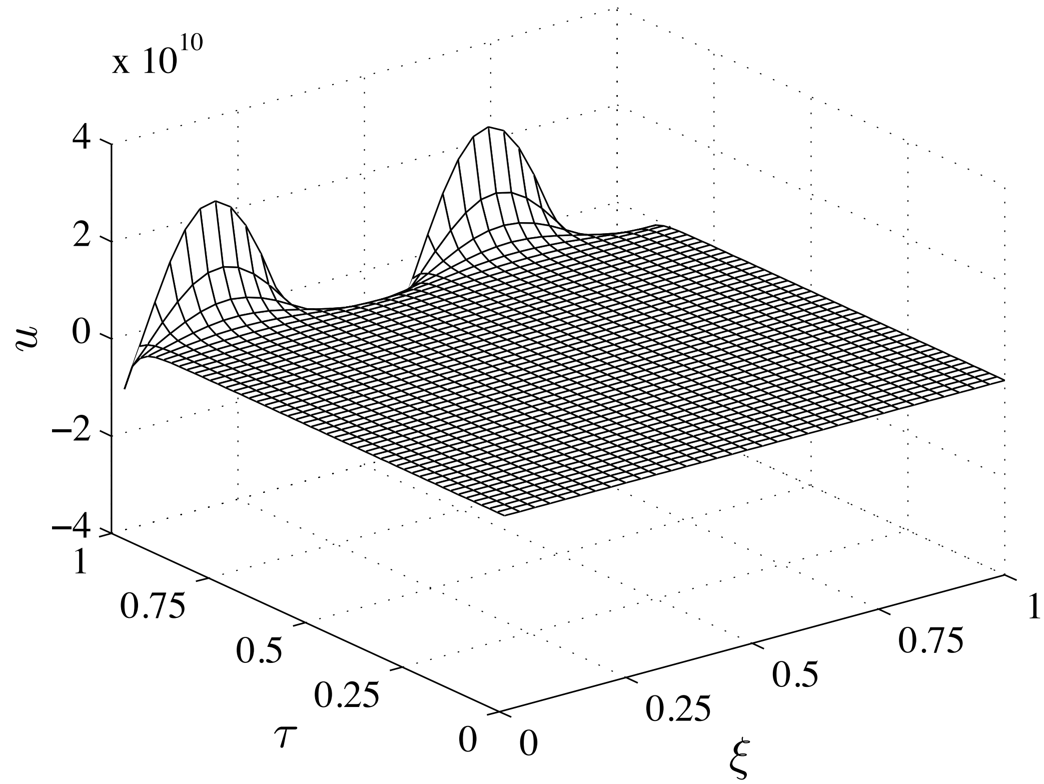


Figure 2.6: System diverges and does not have stability, since the controller gains are chosen poorly.

Trajectory of boundary input u_f for unstable full-state feedback systems are shown in Figure 2.7. It is clear that by choosing poor gain values, the system oscillates and there is no stability whatsoever.

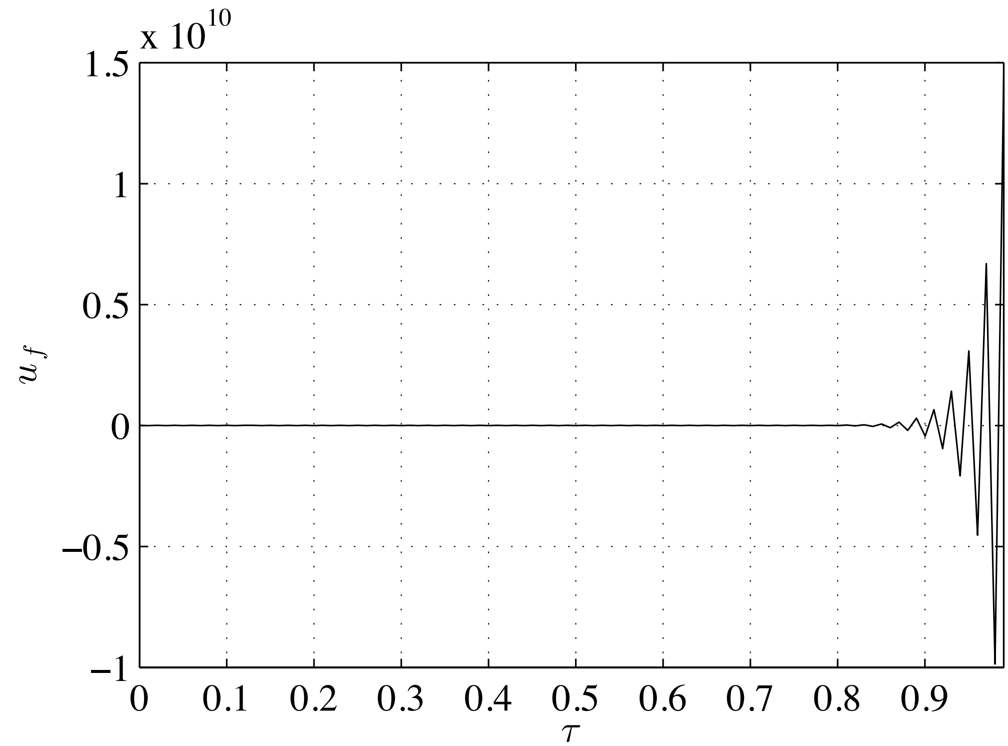


Figure 2.7: Trajectory of boundary input u_f for unstable gain value.

2.5 Numerical Methods

In this section, motivated by [5] and [14], the stability of a generalized, infinite-dimensional version of symplectic scheme used in this thesis is shown. The resulting numerical method can be used for input/output simulation of input/output stable linear dynamical systems that are governed by PDEs, specifically parabolic PDEs in this thesis, see [14].

The only difference between a first order hyperbolic PDE and a parabolic PDE is presence of the second order derivative with respect to the space variable. This difference results in completely different dynamical behavior and mathematical properties. However, this type of PDE is not studied in this work.

In this section, each Euler method is presented and inspected by a general parabolic PDE. The stability and convergence of the scheme is then theoretically studied. Numerical examples are given for each case too.

2.5.1 General Case

To have a coherence and a common frame of reference in studying each numerical scheme, let us assume the following parabolic PDE as our general system which is going to be solved via numerical methods.

$$\frac{\partial x(\zeta,t)}{\partial t} = \frac{\partial^2 x(\zeta,t)}{\partial \zeta^2} + \Psi x(\zeta,t) \tag{2.58}$$

with

$$\left.\frac{\partial x(\zeta,t)}{\partial \zeta}\right|_0 = 0 = \left.\frac{\partial x(\zeta,t)}{\partial \zeta}\right|_L$$

The stability of the above PDE is dependent on the sign of the parameter Ψ, i.e. for $\Psi < 0$ the system is stable and for $\Psi > 0$ the system is unstable.

2.5.2 Explicit Euler

An explicit Euler scheme, sometimes called a forward Euler, is perhaps the simplest scheme to be implemented. To construct the approximation, one must first deal with the time derivative in Equation 2.58. Recall that the derivative is defined by

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \lim_{h\to 0} \frac{y(t+h) - y(t)}{h}$$

The computer has no chance of understanding this quantity. Since we have discretized the time, no information about the solution on time scales less than Δt can be found. This suggests replacing the derivative with

$$\frac{\mathrm{d}y}{\mathrm{d}t} \approx \frac{y(t+\Delta t) - y(t)}{\Delta t}$$

The forward Euler scheme is as follows.
For $1 \leq n \leq N$

$$y(0) = y_0,$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = F(t,y)$$

is approximated by

$$y(0) = y_0,$$
$$\frac{y_{n+1} - y_n}{\Delta t} = F(t_n, y_n) \tag{2.59}$$

Let $\Omega = (0; L)$ be decomposed into a uniform grid $\{0 = \zeta_0 < \zeta_1 < \ldots < \zeta_{N+1} = L\}$ with $\zeta_i = ih$; $h = 1/N$, and time interval $(0; T)$ be decomposed into $\{0 = t_0 < t_1 < \ldots < t_M = T\}$ with $t_n = n\delta t = T/M$. The tensor product of these two grids gives a two dimensional rectangular grid for the domain (0;T). We now expand Equation 2.58 by second order central difference on grid points.

$$\frac{x_i^{n+1} - x_i^n}{\delta t} = \frac{x_{i+1}^n - 2x_i^n + x_{i-1}^n}{h^2} + \Psi_i^n \tag{2.60}$$

Equation 2.60 can be written in matrix form, so

$$\begin{bmatrix} x_1^{n+1} \\ x_2^{n+1} \\ \vdots \\ x_N^{n+1} \end{bmatrix} = \begin{bmatrix} 1-2\lambda & \lambda & 0 & \cdots & 0 & 0 & 0 \\ \lambda & 1-2\lambda & \lambda & \cdots & 0 & 0 & 0 \\ & \ddots & & \ddots & & \ddots & \\ 0 & 0 & 0 & \cdots & \lambda & 1-2\lambda & \lambda \\ 0 & 0 & 0 & \cdots & 0 & \lambda & 1-2\lambda \end{bmatrix} \begin{bmatrix} x_1^n \\ x_2^n \\ \vdots \\ x_N^n \end{bmatrix} + \delta t \begin{bmatrix} \Psi_1^n \\ \Psi_2^n \\ \vdots \\ \Psi_N^n \end{bmatrix} \tag{2.61}$$

where $\lambda = \delta t / h^2$.

Here, the first issue is on the stability in time. When $\Psi = 0$, i.e. PDE does not contain any source term, in the continuous level, the solution should decay exponentially. In the discrete level, one has $x_i^{n+1} = \mathbf{A}x_i^n$ and want to control the magnitude of x in certain norm.

Theorem 1 *When the time step $\delta t \leq h^2/2$, the forward Euler method is stable in the maximum norm in the sense that if $x_i^{n+1} = \mathbf{A}x_i^n$ then*

$$\|x^n\|_\infty \leq \|x^0\|_\infty \leq \|x_0\|_\infty$$

Proof. By the definition of the norm of a matrix

$$\|\mathbf{A}\|_\infty = \max_{i=1,\ldots,N} \sum_{j=1}^{N} |a_{ij}| = 2\lambda + |1 - 2\lambda|$$

if $\delta t \leq h^2/2$, then $\|\mathbf{A}\|_\infty = 1$ and consequently

$$\|x^n\|_\infty \leq \|\mathbf{A}\|_\infty \|x^{n-1}\|_\infty \leq \|x^{n-1}\|_\infty$$

■

Numerical Demonstration

Now, having the following stable PDE

$$\frac{\partial x(\zeta, t)}{\partial t} = \frac{\partial^2 x(\zeta, t)}{\partial \zeta^2} + \Psi x(\zeta, t), \qquad \Psi < 0$$

we will see that by manipulating the stability factor $b = \dfrac{\delta t}{h^2/2}$ such that $b > 1$, the simulation becomes unstable numerically. Although the PDE is stable intrinsically, the system diverges which is as expected.

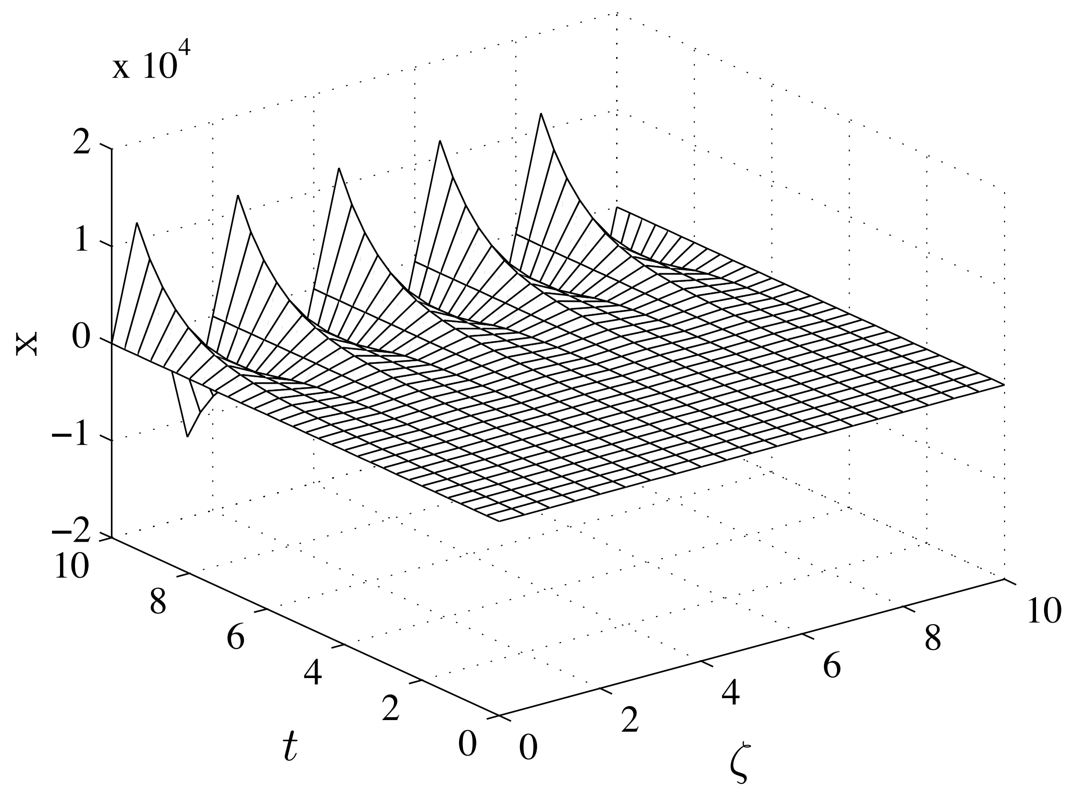


Figure 2.8: The PDE is stable, but the scheme is unstable, i.e. $b = 2.666 > 1$

2.5.3 Implicit Euler

An implicit Euler scheme is sometimes called a backward Euler.
The backward Euler scheme is as follows.
For $1 \le n \le N$

$$y(0) = y_0,$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = F(t, y)$$

is approximated by

$$y(0) = y_0,$$
$$\frac{y_{n+1} - y_n}{\Delta t} = F(t_{n+1}, y_{n+1}) \tag{2.62}$$

Now backward Euler is studied to remove the strong constraint of the time step for the stability. The method is simply using backward difference to approximate the time derivative. We list the system below:

$$\frac{x_i^n - x_i^{n-1}}{\delta t} = \frac{x_{i+1}^n - 2x_i^n + x_{i-1}^n}{h^2} + \Psi_i^n \quad 1 \le i \le N,\ 1 \le n \le M \tag{2.63}$$

In the matrix form, Equation 2.63 reads as

$$(I - \lambda\Delta_h)x^n = x^{n-1} + \delta t \Psi^n \tag{2.64}$$

Starting from x^0, to compute the value at the next time step, one needs to solve an algebraic equation to obtain

$$x^n = (I - \lambda\Delta_h)^{-1}(x^{n-1} + \delta t \Psi^n)$$

If there is no source term, i.e. $\Psi = 0$, our system would be $(I - \lambda\Delta_h)x^n = x^{n-1}$. Note that it has been defined

$$\Delta_h = \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ & \ddots & & \ddots & & \ddots & \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2 \end{bmatrix}$$

Theorem 2 *For the backward Euler method, we always have the stability.*

$$\|x^n\|_\infty \leq \|x^{n-1}\|_\infty \leq \|x_0\|_\infty$$

Proof. We shall rewrite the backward Euler scheme as

$$(1 + 2\lambda)x_i^n = x_i^{n-1} + \lambda x_{i-1}^n + \lambda x_{i+1}^n$$

Therefore, for any $1 \leq i \leq N$

$$(1 + 2\lambda)|x_i^n| \leq \|x^{n-1}\|_\infty + 2\lambda\|x^n\|_\infty$$

which implies

$$(1 + 2\lambda)\|x_i^n\|_\infty \leq \|x^{n-1}\|_\infty + 2\lambda\|x^n\|_\infty$$

and the desired result then follows. ■

Numerical Demonstration

The amplification factor here is $\epsilon = \dfrac{1}{1 + \dfrac{4\Delta t}{h^2(1+\Delta t\Psi)}\sin^2\left(\dfrac{kh}{2}\right)}$, which is clearly $|\epsilon| \leq 1$ for every Δt at each time step. Hence, the scheme is unconditionally stable. This scheme can turn an inherently unstable system into a stable discrete system. Assuming the following unstable PDE

$$\frac{\partial x(\zeta, t)}{\partial t} = \frac{\partial^2 x(\zeta, t)}{\partial \zeta^2} + \Psi x(\zeta, t), \qquad \Psi > 0$$

The result is shown in Figure 2.9.

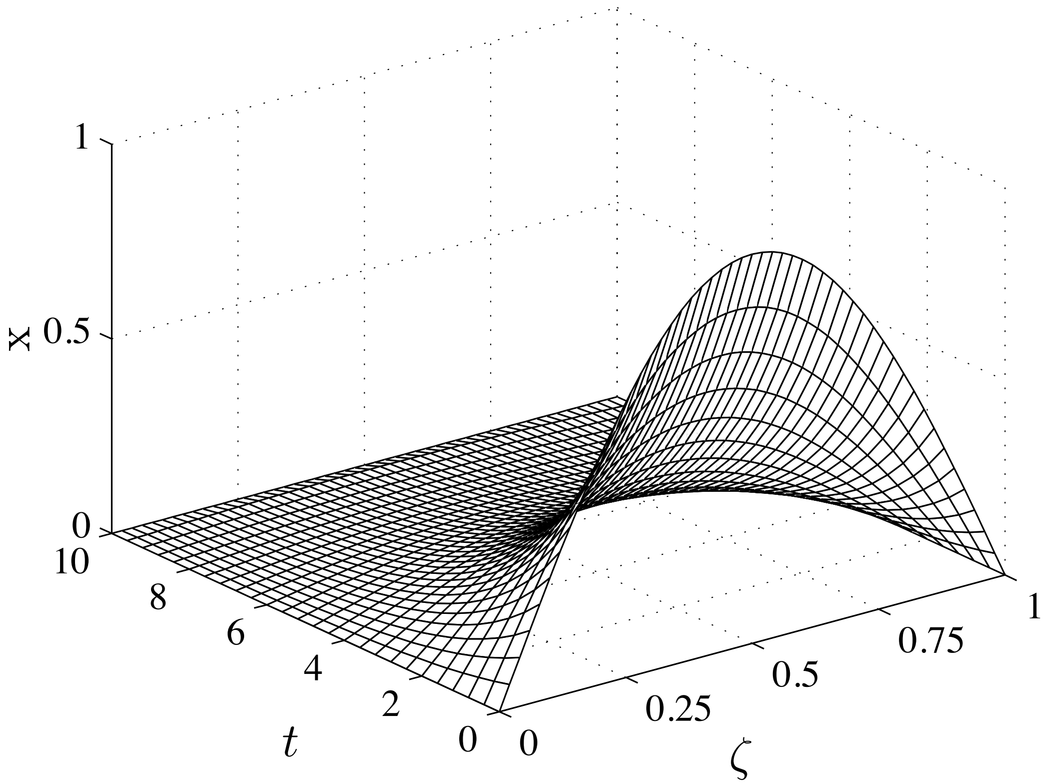


Figure 2.9: The PDE is unstable, but the scheme is stable.

2.5.4 Tustin's Method

Here, the approach used is Tustin's method which for any stable continuous system, returns continuous discrete system, see [14]. In other words, Tusin's method does not affect the stability of the system and that is the reason that this method is used to discretize the system in this work.

In numerical analysis, integration schemes that preserve energy equalities or more complex invariants of the system are called *Hamiltonian* or *symplectic*, respectively. The Tustin scheme (Equation 2.28) for linear systems is the lowest order symplectic integration scheme from the family of Gauss quadrature based Runge-Kutta methods. There exists an extensive literature of symplectic schemes given in [13].

To briefly show the stability region of the symplectic method, from [13] and [14] the following is given.

For $1 \leq n \leq N$

$$y(0) = y_0,$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = \lambda y$$

is approximated by

$$\frac{y_{n+1} - y_n}{\Delta t} = \frac{\lambda y_{n+1} + \lambda y_n}{2} \tag{2.65}$$

So it can be written

$$y_{n+1} = \frac{1 + \dfrac{h\lambda}{2}}{1 - \dfrac{h\lambda}{2}} y_n = G(h\lambda) \tag{2.66}$$

From [13], it is known that (m, n) Padé approximation for e^z is

$$\mathrm{e}^z \approx \frac{1 + a_1 z + \cdots + a_m z^m}{1 + a_1 z + \cdots + a_n z^n} \tag{2.67}$$

therefore, for $(1, 1)$ Padé approximation of e^z, the following holds

$$\mathrm{e}^z \approx G(z) = \frac{1 + \dfrac{z}{2}}{1 - \dfrac{z}{2}} \tag{2.68}$$

And it is known that for stability, it is required that $|G(h\lambda)| < 1$.
By using a conformal map as suggested by [13], it can be said

$$G(z) = \frac{1 + \dfrac{z}{2}}{1 - \dfrac{z}{2}} = \frac{2 + z}{2 - z} \Longrightarrow z = 2\frac{G - 1}{G + 1} \tag{2.69}$$

By assigning numerical values to G and using the mapping above, peer points in z-plane are found. The mapping is graphically shown in Figure 2.10.

$$O: \;\; G = 0 \Longrightarrow z = -2$$
$$A: \;\; G = 1 \Longrightarrow z = 0$$
$$B: \;\; G = i \Longrightarrow z = 2\frac{i - 1}{i + 1}$$
$$C: \;\; G = -1^{+} \Longrightarrow z \rightarrow i\infty$$
$$\bar{C}: \;\; G = -1^{-} \Longrightarrow z \rightarrow -i\infty$$
$$D: \;\; G = -i \Longrightarrow z = -2i$$

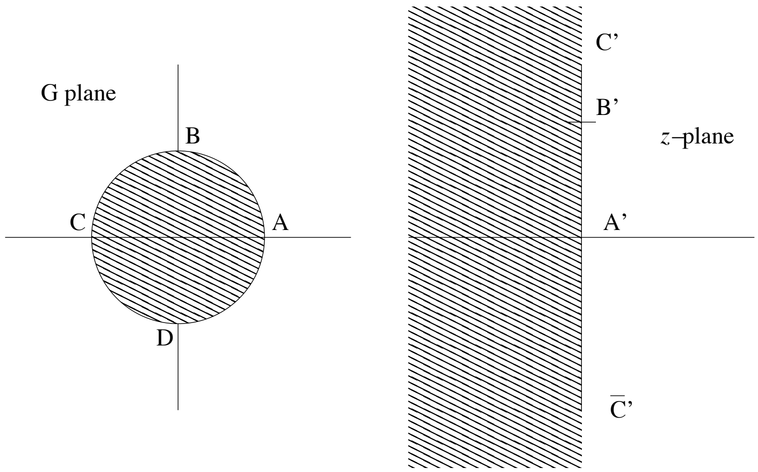
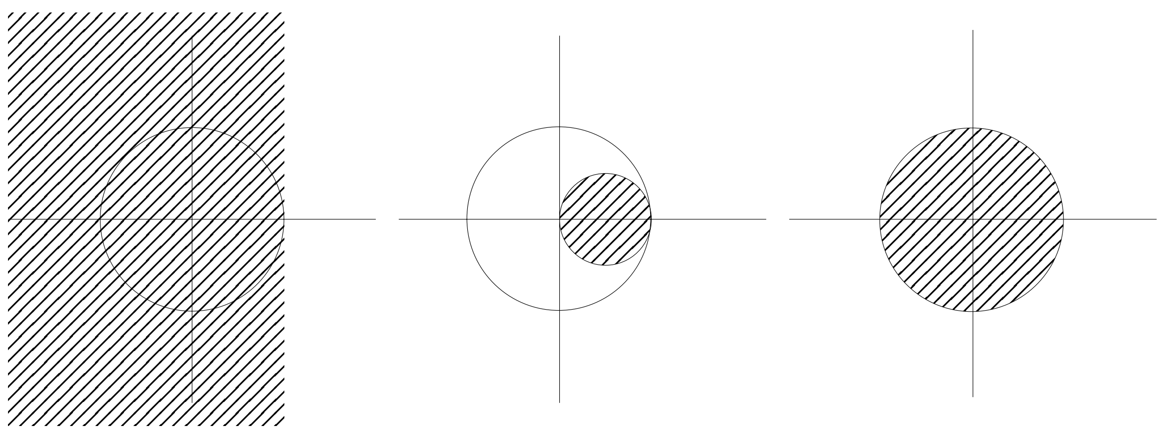


Figure 2.10: Mapping from discrete to continuous space via symplectic Euler

2.5.5 Conclusion

To have a conclusion over these schemes, one can have the following graph. The graph shows that the symplectic scheme preserves the stability status of the system as expected, while for the other methods stability is case-sensitive, see [14].



(a) (b) (c)

(a)	(b)	(c)
Discrete stable $\Longrightarrow$ Continuous stable	Discrete stable $\Longleftarrow$ Continuous stable	Discrete stable $\Longleftrightarrow$ Continuous stable
Can have continuous stable, discrete unstable.	Can have continuous unstable, discrete stable.	

Figure 2.11: (a) Forward Euler, (b) Backward Euler, (c) Symplectic Euler

Chapter 3

Optimal Controller Design

This chapter addresses the optimal control of tubular leads modeled by a parabolic PDEs.

Control of transport systems, which are described by parabolic PDEs has been studied by many researchers (e.g. [8], [11], [17] and references therein). In these works, modal decomposition is used to derive finite dimensional system that captures the dominant dynamics of the original PDE and is subsequently used for low dimensional optimal controller design. The potential drawback of this approach is that for diffusion-convection-reaction systems the number of modes that should be used to derive the ODE system *may* be very large, which leads to computationally demanding controllers, see [22].

Boundary control of parabolic systems have been explored in few studies. Curtain and Zwart in [9], Emirsjlow and Townley in [12], Yapari in [28], and Mohammadi in [22] introduced transformation of the boundary control problem to a well-posed abstract control problem using an exact transformation. Byrnes et al in [6] studied the boundary feedback control of parabolic systems using zero dynamics. The proposed algorithm is designed for parabolic systems with a self-adjoint spatial operator. Parabolic systems with non-self-adjoint spatial operators were introduced by Amundson in [24]; however, due to mathematical complexity, boundary control approach through abstract control problem has not been done much. One proposed solution is via backstepping method with some less theoretical complexity (see [19], [16], and references therein).

The topic of optimal control of infinite dimensional systems is explored by many researchers ([2], [28], [22], and etc.), but time discretization issue was not discussed too much. The novel idea of this work is that the optimality notion of the controller is studied by exact time discretization. Exact time discretization for a class of parabolic PDEs is studied by [27]. In this thesis, optimality of the controller design is added to this method.

Although the emphasis of this thesis is on tubular reactors, the general idea and developed controllers are capable of controlling any system that is modeled by the studied class of DPS in this work.

Current chapter focuses on the infinite dimensional control of a system represented by a parabolic PDE. The only difference between a first order hyperbolic PDE and a parabolic PDE is presence of the second order derivative with respect to the space variable. This difference results in completely different dynamical behavior and mathematical properties. Unlike hyperbolic systems, for parabolic systems the operator Riccati equation cannot be converted to a matrix Riccati equation. Therefore, one needs an alternative method to solve the operator Riccati equation. Here, method used by [9] is employed to solve the Riccati equation.

The boundary control problem is already transformed into a well-posed abstract boundary control problem by applying an exact transformation similar to the transformation introduced by [9]. The stabilizability of the resulting systems is also investigated. Stability of linear parabolic systems with constant coefficients is studied by [26], and [10] for the special case of a tubular reactor with two state variables. Finally, by using the spectral properties of the system, the operator Riccati equation is converted into a set of coupled algebraic equations, which can be solved numerically. It is solved via Newton's method in this case. The Riccati equation is solved for the continuous case and the result is then used for the discrete case.

In this work, our focus is on parabolic systems defined in one-dimensional spatial domain, but the approach can easily be extended to a more general form of parabolic systems with 2D or 3D domain in space, see [22].

3.1 Continuous Optimal Controller Design

In this section, a linear-quadratic optimal controller is formulated for a system described by 2.34. The state-feedback controller assumes that full state measurement is available. The existence of the solution for the LQ control problem requires that the linear system is exponentially stabilizable and detectable. These two properties will be investigated and in the following sections. Then, it will be proven that the infinite dimensional system in Equation 2.34 is a Riesz spectral system. In this section, one will use the spectral properties of Riesz spectral systems to solve the LQ control problem, see [9].

The linear quadratic control problem on an infinite-time horizon employs the cost

function:
$$J(x_0,u)=\int_0^\infty \langle x^e(s),Qx^e(s)\rangle+\langle u(s),Ru(s)\rangle \mathrm{d}s \tag{3.1}$$
where $u(s)$ and $x^e(s)$ are the input and state trajectories, respectively. Q is nonnegative operator in $\mathcal{L}(X)$ and R is a self-adjoint, coercive operator in $\mathcal{L}(U)$.
The control problem is to minimize the above cost functional over the trajectories of the state linear system $\Sigma(A^e,B^e,C^e)$.
It is well-known that the solution of this optimal control problem can be obtained by solving the following algebraic Riccati equation (ARE) by [9]:

$$\langle A^e x_1^e,\Pi x_2^e\rangle+\langle \Pi x_1^e,A^e x_2^e\rangle+\langle C^e x_1^e,C^eQx_2^e\rangle-\langle B^e\Pi x_1^e,R^{-1}B^{e^*}\Pi x_2^e\rangle=0 \tag{3.2}$$

When (A^e,B^e) is exponentially stabilizable and (C^e,A^e) is exponentially detectable, the algebraic Riccati equation 3.2 has a unique nonnegative self-adjoint $\Pi\in\mathcal{L}(\mathcal{H})$ and for any initial state $x_0^e\in\mathcal{H}$ the quadratic cost 3.1 is minimized by the unique control u_{opt} given by:

$$u_{opt}(s,x_0^e)=-R^{-1}B^{e^*}\Pi x^e_{opt}(s),\qquad x^e_{opt}(s)=T_{-B^eR^{-1}B^{e^*}\Pi}x_0^e \tag{3.3}$$

In addition, the optimal cost is given by $J(x_0^e,u_{opt})=\langle x_0^e,\Pi x_0^e\rangle$.
The ARE 3.2 is valid for any infinite dimensional system, but depending on the characteristics of the infinite dimensional system different approaches are needed to solve it. For Riesz spectral systems, the spectral properties of the system can be used to solve the ARE 3.2. It is known that $\mathbf{\Phi}_n$ are the normalized eigenfunctions of A^e. If x_1^e and x_2^e are taken as $x_1^e=\mathbf{\Phi}_n$ and $x_2^e=\mathbf{\Phi}_m$, then the Riccati equation 3.2 becomes:

$$\langle A^e\mathbf{\Phi}_n,\Pi\mathbf{\Phi}_m\rangle+\langle \Pi\mathbf{\Phi}_n,A^e\mathbf{\Phi}_m\rangle+\langle \mathbf{\Phi}_n,Q\mathbf{\Phi}_m\rangle-\langle B^e\Pi\mathbf{\Phi}_n,R^{-1}B^{e^*}\Pi\mathbf{\Phi}_m\rangle=0 \tag{3.4}$$

Assuming $R=I$ and a solution of this form $\Pi(.)=\sum_{n,m=0}^\infty \Pi_{nm}\langle\ .\ ,\mathbf{\Phi}_m\rangle\mathbf{\Phi}_n$ for Π, turns Equation 3.4 to the system of infinite number of coupled scalar equations:

$$(\sigma_n+\sigma_m)\Pi_{nm}+Q_{nm}-\sum_{k=0}^\infty\sum_{l=0}^\infty B_{kl}\Pi_{nl}\Pi_{km}=0 \tag{3.5}$$

where $B_{kl}=\langle B^eB^{e^*}\mathbf{\Phi}_n,\mathbf{\Phi}_m\rangle=\langle B^{e^*}\mathbf{\Phi}_n,B^{e^*}\mathbf{\Phi}_m\rangle$ and $Q_{nm}=\langle\mathbf{\Phi}_n,Q\mathbf{\Phi}_m\rangle$.
Using the spectral properties of the Riesz spectral systems, the operator Riccati equation 3.4 is converted to a set of coupled algebraic equations that can be solved by any numerical algorithm. Then the main step to solve the optimal control problem for these systems is to calculate the spectrum of the operator A^e, which is already done.
Note that since Π is a self-adjoint operator, $\Pi_{nm}=\Pi_{mn}$. As a result, Equation

3.5 gives $\dfrac{n(n+1)}{2}$ coupled algebraic equations that should be solved simultaneously where n is the number of modes that are used to formulate the controller. In this work, the first two modes were used for numerical simulation. The computed LQ controller was applied to the model of the reactor.

Employing two modes to calculate Π, there are three coupled quadratic equations, i.e. $n, m = 0, 1$. So, it can be said

$$\begin{aligned}
2\sigma_0\Pi_{00} + Q_{00} - B_{00}\Pi_{00}^2 - 2B_{01}\Pi_{01}\Pi_{00} - B_{11}\Pi_{01}^2 &= 0\\
2\sigma_1\Pi_{11} + Q_{11} - B_{00}\Pi_{01}^2 - 2B_{01}\Pi_{01}\Pi_{11} - B_{11}\Pi_{11}^2 &= 0\\
(\sigma_0+\sigma_1)\Pi_{01} + Q_{01} - B_{00}\Pi_{00}\Pi_{01} - B_{01}\Pi_{01}^2 - B_{01}\Pi_{00}\Pi_{11} - B_{11}\Pi_{01}\Pi_{11} &= 0
\end{aligned}$$

Therefore, using a preferred numerical method to solve the above coupled equations (here Newton's method) one has the following for each coefficient by assuming $Q = I$

$$\begin{cases}\Pi_{00} = 1\\ \Pi_{01} = \Pi_{10} = 0\\ \Pi_{11} = -0.227723\end{cases} \tag{3.6}$$

Hence, our Π will be equal to

$$\Pi(.) = \langle\ .\ , \mathbf{\Phi}_0\rangle\mathbf{\Phi}_0 - 0.227723\langle\ .\ , \mathbf{\Phi}_1\rangle\mathbf{\Phi}_1 \tag{3.7}$$

Recalling Equation 2.42, if $\mathcal{A}B$ is replaced with -2γ, for $\mathbf{\Phi}_0$ one can write

$$\mathbf{\Phi}_0 = \begin{bmatrix}1\\ \sum_{j=1}^{\infty}\dfrac{1}{\lambda_j}\langle\mathcal{A}B, \phi_j\rangle\phi_j\end{bmatrix} = \begin{bmatrix}1\\ \sum_{j=1}^{\infty}\dfrac{1}{\lambda_j}\langle -2\gamma, \phi_j\rangle\phi_j\end{bmatrix} = \begin{bmatrix}1\\ -2\gamma\sum_{j=1}^{\infty}\dfrac{1}{\lambda_j}\int_0^1\phi_j(\xi)\mathrm{d}\xi\phi_j\end{bmatrix}$$

Using first three modes to approximate the second element of $\mathbf{\Phi}_0$, it can be said:

$$\begin{aligned}
\mathbf{\Phi}_0 &= \begin{bmatrix}1\\ -2\gamma\sum_{j=1}^{3}\dfrac{1}{\lambda_j}\int_0^1\phi_j(\xi)\mathrm{d}\xi\phi_j\end{bmatrix}\\
&= \begin{bmatrix}1\\ -2\gamma\left(\dfrac{1}{\lambda_1}\int_0^1\phi_1(\xi)\mathrm{d}\xi\phi_1 + \dfrac{1}{\lambda_2}\int_0^1\phi_2(\xi)\mathrm{d}\xi\phi_2 + \dfrac{1}{\lambda_3}\int_0^1\phi_3(\xi)\mathrm{d}\xi\phi_3\right)\end{bmatrix}
\end{aligned} \tag{3.8}$$

Deriving Equation 3.5

Conversion of Equation 3.4 to Equation 3.5 is done through the following procedure. Recalling Equation 3.4, it is known that:

$$\langle A^e \mathbf{\Phi}_n, \Pi \mathbf{\Phi}_m \rangle \;+\; \langle \Pi \mathbf{\Phi}_n, A^e \mathbf{\Phi}_m \rangle \;+\; \langle \mathbf{\Phi}_n, Q \mathbf{\Phi}_m \rangle \;-\; \langle \Pi \mathbf{\Phi}_n, B^e B^{e^*} \Pi \mathbf{\Phi}_m \rangle \quad = \quad 0$$

Knowing that σ_n is an eigenvalue of the operator A^e and $\mathbf{\Phi}_n$ is the corresponding eigenvector, one has

$$\begin{aligned}
\langle A^e \mathbf{\Phi}_n, \Pi \mathbf{\Phi}_m \rangle + \langle \Pi \mathbf{\Phi}_n, A^e \mathbf{\Phi}_m \rangle &= \langle \sigma_n \mathbf{\Phi}_n, \Pi \mathbf{\Phi}_m \rangle + \langle \Pi \mathbf{\Phi}_n, \sigma_m \mathbf{\Phi}_m \rangle \\
&= \sigma_n \langle \mathbf{\Phi}_n, \Pi \mathbf{\Phi}_m \rangle + \sigma_m \langle \Pi \mathbf{\Phi}_n, \mathbf{\Phi}_m \rangle \\
&= \sigma_n \Pi_{nm} + \sigma_m \Pi_{mn} \\
&= (\sigma_n + \sigma_m) \Pi_{nm}
\end{aligned}$$

Now let us calculate the last term of the Riccati equation 3.4. From [9], it is known that any element in the space can be written uniquely in the Riesz basis; particularly, one claim that

$$B^e B^{e^*} \psi = \sum_{k=0}^{\infty} \langle B^e B^{e^*} \psi, \mathbf{\Phi}_k \rangle \mathbf{\Phi}_k$$

Therefore,

$$\begin{aligned}
\langle \Pi \mathbf{\Phi}_n, B^e B^{e^*} \Pi \mathbf{\Phi}_m \rangle &= \left\langle \Pi \mathbf{\Phi}_n, \sum_{k=0}^{\infty} \langle B^e B^{e^*} \Pi \mathbf{\Phi}_m, \mathbf{\Phi}_k \rangle \mathbf{\Phi}_k \right\rangle \\
&= \sum_{k=0}^{\infty} \langle B^e B^{e^*} \Pi \mathbf{\Phi}_m, \mathbf{\Phi}_k \rangle \langle \Pi \mathbf{\Phi}_n, \mathbf{\Phi}_k \rangle \\
&= \sum_{k=0}^{\infty} \langle \Pi \mathbf{\Phi}_m, B^e B^{e^*} \mathbf{\Phi}_k \rangle \Pi_{kn} \\
&= \sum_{k=0}^{\infty} \left\langle \Pi \mathbf{\Phi}_m, \sum_{l=0}^{\infty} \langle B^e B^{e^*} \mathbf{\Phi}_k, \mathbf{\Phi}_l \rangle \mathbf{\Phi}_l \right\rangle \Pi_{kn} \\
&= \sum_{k,l=0}^{\infty} \langle B^e B^{e^*} \mathbf{\Phi}_k, \mathbf{\Phi}_l \rangle \langle \Pi \mathbf{\Phi}_m, \mathbf{\Phi}_l \rangle \Pi_{kn} \\
&= \sum_{k,l=0}^{\infty} B_{kl} \Pi_{ml} \Pi_{kn} \\
&= \sum_{k,l=0}^{\infty} B_{kl} \Pi_{nl} \Pi_{km}
\end{aligned}$$

Hence, if Q_{nm} is defined as $Q_{nm} = \langle \mathbf{\Phi}_n, Q \mathbf{\Phi}_m \rangle$, Equation 3.5 is found.

It is utmost obvious that in order to implement a continuous system via computer, its discrete version should be provided or the continuous case must be somehow discretized. In this work, the exact discrete model in time is provided by the proposed method without the need of space discretization. Besides, the continuous case can be modeled through an approximation method (e.g. spectral decomposition, see [25]). Therefore, in order to have a frame of reference to compare the performance of the controller, both results are compared.

To model the continuous case optimal controller, one can use the spectral property of the extended state space method, i.e. to approximate the system by its eigenfunctions. To do so, one can write

$$\dot{x}^e(\xi,\tau) = \begin{bmatrix} 0 & 0 \\ \mathcal{A}B & \mathcal{A} \end{bmatrix} x^e(\xi,\tau) + \begin{bmatrix} 1 \\ -B \end{bmatrix} K x^e(\xi,\tau)$$

where $K = -R^{-1}B^*\Pi$.

From [25] it is known that $x^e(\xi,\tau) = \sum_{i=0}^{\infty} a_i(\tau)\mathbf{\Phi}_i(\xi)$. Therefore, by expanding the extended space and projecting the resulting equation onto adjoint space of operator $\mathcal{A}^e$, one can say

$$\dot{a}_i(\tau) = \Big(\sigma_i - \langle BB^*\Pi\mathbf{\Phi}_i(\xi), \mathbf{\Psi}_i\rangle\Big)a_i(\tau) \tag{3.9}$$

Now, by using finite number of eigenfunctions, one can approximate the evolution of a_i in Equation 3.9 over time. Hence, the evolution of p can be found.

3.2 Discrete Optimal Controller Design

Consider continuous-time state linear system $\Sigma(A, B, C)$ on the Hilbert space $\mathcal{H}$ and its related discrete-time system $\Sigma_d(A_d, B_d, C_d, D_d)$ with $-1 \in \rho(A_d)$. From previous section, it is known that the following relationship holds between discrete- and continuous-time spaces

$$A = (I + A_d)^{-1}(A_d - I), \tag{3.10}$$

$$B = \sqrt{2}(I + A_d)^{-1}B_d, \tag{3.11}$$

$$C = \sqrt{2}C_d(I + A_d)^{-1}, \tag{3.12}$$

$$D = D_d - C_d(I + A_d)^{-1}B_d \tag{3.13}$$

Note that even if our continuous-time space does not have D, our discrete-time system will always have D_d which is an important point. In other words, input has contribution in at least one of discrete or continuous cases.

From [29] and [9], it is known that the following discrete algebraic Riccati equation (DARE)

$$A_d^*\Pi A_d - \Pi + C_d^*C_d - \mathbf{K}^*(B_d^*\Pi B_d + D_d^*D_d)^{-1}\mathbf{K} = 0 \tag{3.14}$$

has a unique nonnegative solution $\Pi \in \mathcal{L}(\mathcal{H})$ if and only if the continuous ARE has a solution. And the solution for Π in continuous case would be the solution in discrete case as well. Here $\mathbf{K} = B_d^*\Pi A_d + D_d^*C_d$.

Besides, it is known that continuous-time ARE has the following form

$$\Pi A + A^*\Pi + C^*C - (\Pi B + C^*D)(D^*D)^{-1}(D^*C + B^*\Pi) = 0 \tag{3.15}$$

Now, based on what was found in previous section, one has the solution for DARE and therefore can design the discrete LQ controller.

First, for obtaining A_d, based on the definition of resolvent sets, one can write

$$A = (I + A_d)^{-1}(A_d - I)$$

$$A_d = (A + I)(I - A)^{-1}$$

$$A_d = (A + I)\sum_{i=1}^{\infty}\frac{1}{1 - \lambda_i}\langle ., \mathbf{\Psi_i}\rangle\mathbf{\Phi}_i \tag{3.16}$$

And B_d has the following form

$$B = \sqrt{2}(I + A_d)^{-1}B_d$$

$$B_d = \frac{\sqrt{2}}{2}(I + A_d)B$$

Furthermore, if $C = I$, one can say that

$$\begin{aligned} I &= \sqrt{2}C_d(I + A_d)^{-1} \\ C_d &= \frac{\sqrt{2}}{2} I(I + A_d) \\ C_d &= \frac{\sqrt{2}}{2}(I + A_d) \end{aligned} \tag{3.17}$$

Besides, it has been already assumed $D = 0$, so our D_d is achieved as follows

$$\begin{aligned} D_d &= C_d(I + A_d)^{-1}B_d \\ D_d &= \frac{\sqrt{2}}{2}(I + A_d)(I + A_d)^{-1}B_d \\ D_d &= \frac{\sqrt{2}}{2}B_d \end{aligned} \tag{3.18}$$

Note that even if our continuous-time space does not have D, our discrete-time system will always have D_d which is an important point. In other words, input has contribution in at least one of the discrete or continuous cases.

Hence, $\mathbf{K}$ would have the following structure

$$\mathbf{K} = B_d^* \Big(\Pi A_d + \frac{1}{2}(I + A_d) \Big) \tag{3.19}$$

Note that $\mathbf{K}$ is only used to simplify the equation and does not have anything to do with optimal gain.

Since the continuous case has a solution Π, our discrete case has the same solution and there is no need to solve the above DARE. However, the corresponding equations to solve DARE are brought too.

From [9], it is known that the unique control input for the discrete case would be

$$\tilde{u}_{opt}(k) = -R^{-1}B^{e^*}\Pi x^e(k) \tag{3.20}$$

Besides, here the evolution of $p(\xi, k)$ is of importance to us. Therefore, $K = R^{-1}B^{e^*}\Pi A^e$ and system can be simulated as well using the same approach as §2.4.

Recalling Equation 2.31, the discrete system looks like this

$$
\begin{aligned}
&p(\xi,k+1)= \\
&\frac{\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)+\frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})+\frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})}\int_0^1\cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\big)p(x,k)\mathrm{d}x \\
&\qquad -\int_0^\xi\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\big)p(x,k)\mathrm{d}x \\
&-2\frac{\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)+\frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})+\frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})}\int_0^1\cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\big)\big(\gamma u_f+\tilde{u}_f\big)\mathrm{d}x \\
&\qquad +2\int_0^\xi\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\big)(\gamma u_f+\tilde{u}_f)\mathrm{d}x
\end{aligned}
$$

where $\dot{u}_f=\tilde{u}_f$. So by assuming $u_f(0)=0$, it can be said $u_f=\frac{1}{s}\tilde{u}_f$. In discrete case one should write $u_f=\frac{\Delta t}{2}\tilde{u}_f$.
Now it can be said

$$
\begin{aligned}
\bar{A}_d(.)=&\left[\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)+\frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)\right] \\
&\times\frac{\int_0^1\cosh\Big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\Big)(.)\mathrm{d}x}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})+\frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
&-\int_0^\xi\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\Big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\Big)(.)\mathrm{d}x
\end{aligned}
\tag{3.21}
$$

and

$$\bar{B}_d(.) = -2\frac{\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})}$$
$$\times \int_0^1 \cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\mathrm{d}x(.)$$
$$+ 2\int_0^{\xi} \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\mathrm{d}x(.) \quad (3.22)$$

As shown in Appendix A, by employing the method used in [21], B_d^* is then calculated as

$$\bar{B}_d^*(.) = -2\frac{\cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-\xi)\big)\big(\gamma\frac{\Delta t}{2}+1\big)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})}$$
$$\times \int_0^1 \Big[\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}x) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}x)\Big]\mathrm{d}x(.)$$
$$+ 2\int_{\xi}^{1} \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(x-\xi)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\mathrm{d}x(.) \quad (3.23)$$

Applying proper initial conditions which must satisfy the original PDE, it can be written

$$p_0(\xi) = 2\pi\xi - \sin(2\pi\xi)$$

Note that here any boundary condition that satisfies the original PDE can be applied. The above boundary condition is implemented without loss of generality, and can be replaced by another condition of a choice.

Therefore, the simulation of full-state feedback optimal controller can be done with the above gain and state space model. Simulations are conducted via MATLAB.

Besides, to show the effect of Π approximation, trajectories of boundary control input for two different Πs are brought in Figure 3.3. It is obvious that by increasing the order of approximation for Π, the performance of the controller is improved. Besides, it must be noted that from a step ahead, increasing the approximation of Π will not have any significant effect on the performance of the controller and will only

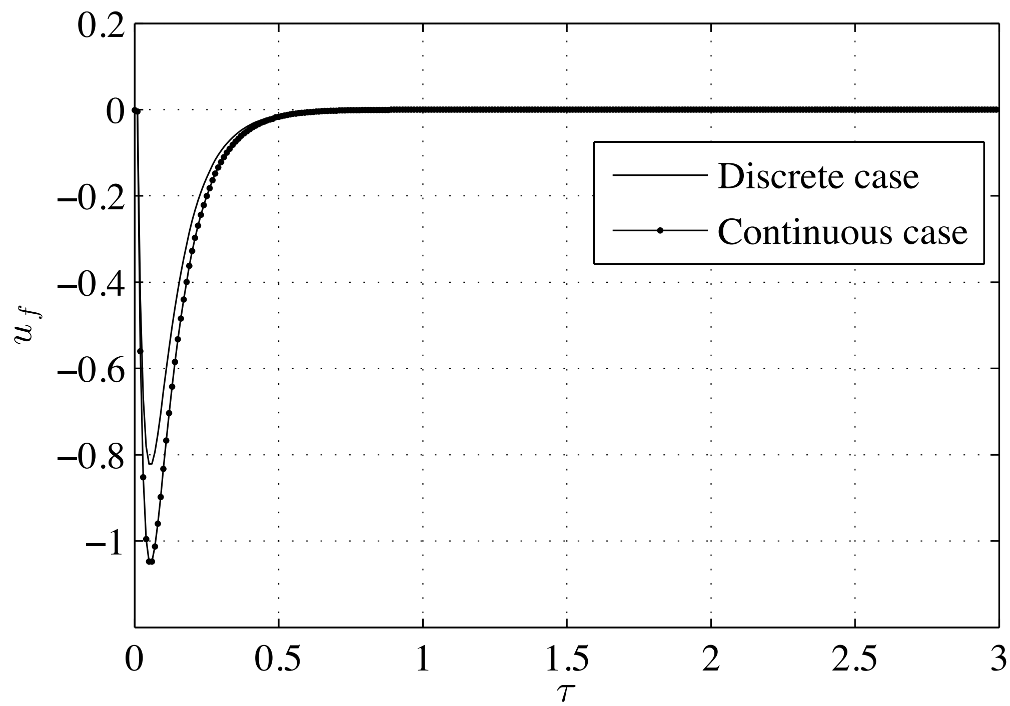


Figure 3.1: Trajectories of boundary input for optimal controller of continuous and discrete time.

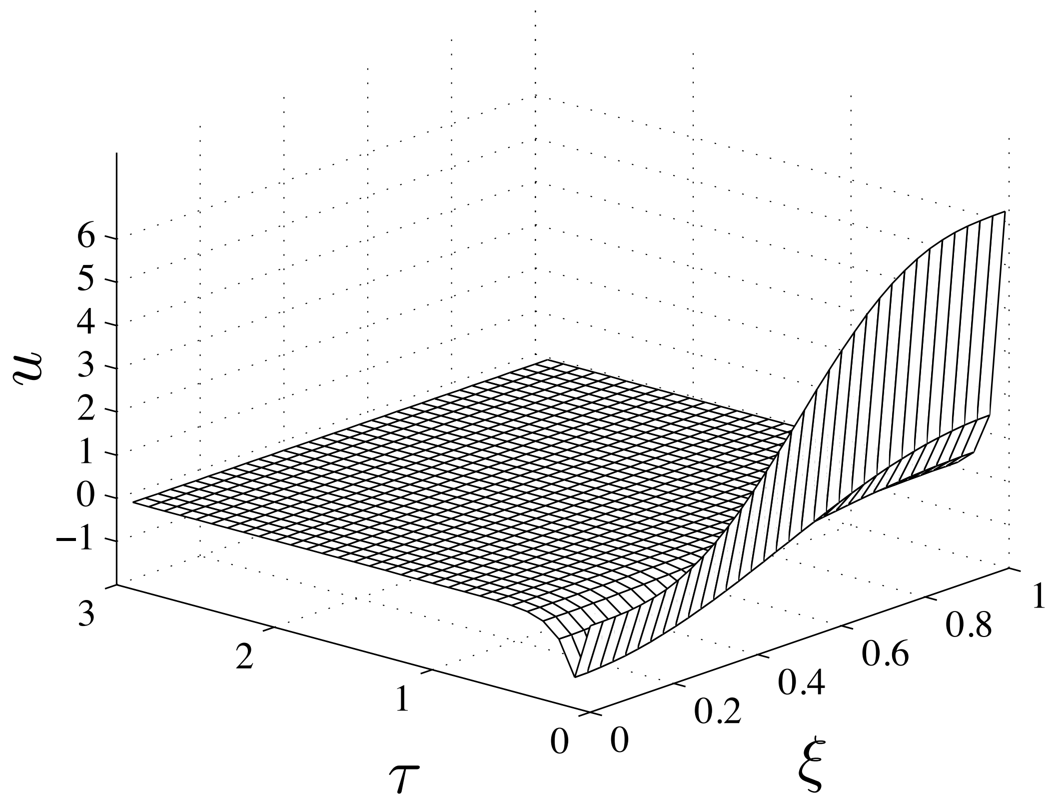


Figure 3.2: State evolution via optimal full-state feedback controller.

Table 3.1: Comparison of the cost function for continuous and discrete cases

Controller	J
Continuous case	71.4650
Discrete case with first two $\mathbf{\Phi}$	54.3307
Discrete case with first three $\mathbf{\Phi}$	49.3975

cost more numerical calculations, see [22].

Solution to ARE and DARE for a Simple Case

Consider the 1D equation below

$$\begin{aligned} \dot{x} &= 2x + u \\ y &= x + u \end{aligned} \tag{3.24}$$

the algebraic Riccati equation is given by

$$PA + A'P + C'C - (PB + C'D)(D'D)^{-1}(D'C + B'P) = 0$$

Solving this equation and knowing that $P \geq 0$, one can see that $P = 0$ is a solution to above ARE.

Solving the discrete case Riccati equation based on the definitions for A_d, B_d, C_d, and D_d will give the following

$$A_d^* \Pi A_d - \Pi + C_d^* C_d - \mathbf{K}^* (B_d^* \Pi B_d + D_d^* D_d)^{-1} \mathbf{K} = 0$$

Here $\mathbf{K} = B_d^* \Pi A_d + D_d^* C_d$.

Finding the discrete coefficients and knowing that for DARE $P \geq 0$, one can see the solution to the DARE would be $P = 0$.

Hence, the solution to ARE is equal to DARE.

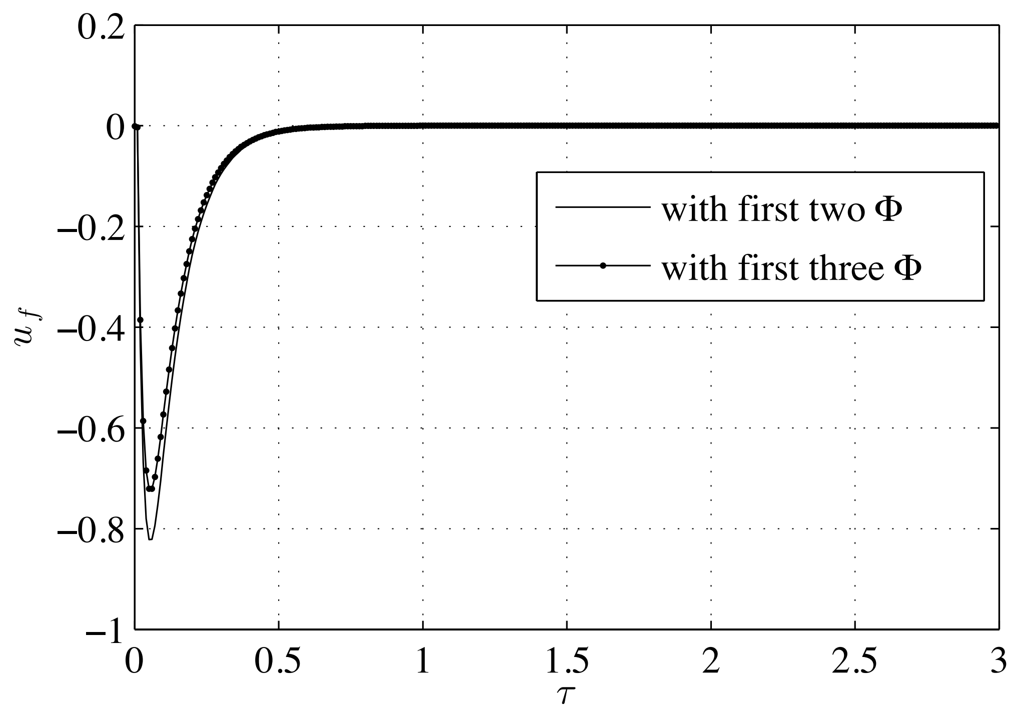


Figure 3.3: Effect of the Π approximation on the trajectories of boundary input.

3.3 Stability Analysis

Theorem 3 *Consider the extended operator $\{A^e(t)\}_{t>0}$ given by Equation 2.34. Then, $\{A^e(t)\}_{t>0}$ is a stable infinitesimal generator of C_0-semigroup on $\mathcal{H}$.*

Proof. Operator $\mathcal{A}$ is a self-adjoint spatial operator. Therefore, $\mathcal{A}$ is the infinitesimal generator of C_0-semigroup T, [26], [10]. As discussed in eigenvalue problem (§2.3), eigenvalues of $\mathcal{A}^e$ consist of eigenvalues of $\mathcal{A}$ and 0. So, operator $\mathcal{A}^e$ has real, countable and distinct eigenvalues. Furthermore, eigenfunctions of $\mathcal{A}^e$ are biorthogonal. Thus, the operator $\mathcal{A}^e$ is a Riesz spectral operator [10]. By [9], Lemma 3.2.2, the operator $\mathcal{A}^e$ is the infinitesimal generator of the C_0-semigroup T^e given by

$$T^e(t) = \begin{bmatrix} I & 0 \\ T_{21}(t) & T \end{bmatrix} \tag{3.25}$$

where

$$T_{21}(t)x = \int_0^t T(s)\mathcal{A}Bx\mathrm{d}s \tag{3.26}$$

■

Theorem 4 *Consider the state linear system $\Sigma(A, B, -)$, where A is a Riesz spectral operator on the Hilbert space $\mathcal{Z}$ with compact resolvent and the representation*

$$Az = \sum_{n=1}^{\infty} \lambda_n \sum_{j=1}^{r_n} \langle z, \psi_{nj} \rangle \phi_{nj} \tag{3.27}$$

for $z \in D(A) = \{z \in \mathcal{Z} | \sum_{n=1}^{\infty} |\lambda_n|^2 \sum_{j=1}^{r_n} |\langle z, \phi_{nj}\rangle|^2 < \infty\}$, where $\{\lambda_n, n \geq 1\}$ are eigenvalues of A with finite multiplicity r_n, and $\{\phi_{nj}, j = 1, \ldots r_n, n \geq 1\}$ are generalized eigenfunctions of A (and A^*). B is a finite rank operator defined by

$$Bu = \sum_{i=1}^{m} b_i u_i, \qquad \textit{where } b_i \in \mathcal{Z} \tag{3.28}$$

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

$$\mathit{rank} \begin{pmatrix} \langle b_1, \psi_{n1} \rangle & \cdots & \langle b_m, \psi_{n1} \rangle \\ \vdots & & \vdots \\ \langle b_1, \psi_{nr_n} \rangle & \cdots & \langle b_m, \psi_{nr_n} \rangle \end{pmatrix} = r_n \tag{3.29}$$

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

Proof. Since $\sigma^+_{\beta-\epsilon}(A)$ comprises at most finitely many eigenvalues, $\mathcal{Z}^+_{\beta-\epsilon}$ is finite dimensional. Therefore, A satisfies the spectrum decomposition assumption at $\beta-\epsilon$ [9] and the corresponding spectral projection on the finite dimensional subspace $\mathcal{Z}^+_{\beta-\epsilon}$ is given by

$$P_{\beta-\epsilon}z = \frac{1}{2\pi j}\int_{\Gamma_{\beta-\epsilon}}(\lambda I - A)^{-1}z\mathrm{d}\lambda = \sum_{\lambda_n\in\sigma^+_{\beta-\epsilon}}\sum_{j=1}^{r_n}\langle z,\psi_{nj}\rangle\phi_{nj} \tag{3.30}$$

Consequently, it can be shown that

$$\mathcal{Z}^+_{\beta-\epsilon} = \underset{\lambda_n\in\sigma^+_{\beta-\epsilon}}{\operatorname{span}}\ \{\phi_{nj}, j=1,\dots,r_n\} \tag{3.31}$$

$$\mathcal{Z}^-_{\beta-\epsilon} = \underset{\lambda_n\in\sigma^-_{\beta-\epsilon}}{\overline{\operatorname{span}}}\ \{\phi_{nj}, j=1,\dots,r_n\} \tag{3.32}$$

$$T^-_{\beta-\epsilon}(t)z = \sum_{\lambda_n\in\sigma^-_{\beta-\epsilon}}\mathrm{e}^{\lambda_n t}\sum_{j=1}^{r_n}\langle z,\psi_{nj}\rangle\phi_{nj} \tag{3.33}$$

$$A^+_{\beta-\epsilon}(t)z = \sum_{\lambda_n\in\sigma^+_{\beta-\epsilon}}\lambda_n\sum_{j=1}^{r_n}\langle z,\psi_{nj}\rangle\phi_{nj} \tag{3.34}$$

$$B^+_{\beta-\epsilon}(t)u = \sum_{\lambda_n\in\sigma^+_{\beta-\epsilon}}\sum_{j=1}^{r_n}\langle Bu,\psi_{nj}\rangle\phi_{nj} \tag{3.35}$$

From this, it is seen that $T^-_{\beta-\epsilon}(t)$ is a C_0-semigroup corresponding to a Riesz spectral operator on $\mathcal{Z}^-_{\beta-\epsilon}$. Hence, it satisfies the spectrum determined growth assumption and it is β-exponentially stable. Now, one shall show that the finite-dimensional system $\Sigma(A^+_{\beta-\epsilon}, B^+_{\beta-\epsilon}, -)$ is controllable. It can be done by proving that the reachability subspace of $\Sigma(A^+_{\beta-\epsilon}, B^+_{\beta-\epsilon}, -)$ is dense in $\mathcal{Z}^+_{\beta-\epsilon}$. From [9] (Definition A.2.29), $\mathcal{R}$ is dense in $\mathcal{Z}^+_{\beta-\epsilon}$ if and only if when for the orthogonal complement of $\mathcal{R}$ we have $\mathcal{R}^\perp = \{0\}$.

Both $\mathcal{R}$ and $\mathcal{R}^\perp$ are given as

$$\begin{aligned}\mathcal{R} := \{z\in\mathcal{Z}^+_{\beta-\epsilon} \mid \exists\ \tau>0 \text{ and } u\in\mathcal{L}_2([0,\tau];U)\\ \text{s.t. } z=\int_0^\tau T^+_{\beta-\epsilon}(\tau-s)B^+_{\beta-\epsilon}u(s)\mathrm{d}s\}\end{aligned} \tag{3.36}$$

$$\mathcal{R}^\perp := \{x\in\mathcal{Z}^+_{\beta-\epsilon} \mid \langle x,y\rangle = 0, \forall\ y\in\mathcal{R}\} \tag{3.37}$$

In order to have $\mathcal{R}^\perp = \{0\}$, there should be no $x\in\mathcal{Z}^+_{\beta-\epsilon}$ that is orthogonal to the reachability subspace $\mathcal{R}$. This means that for every $x\in\mathcal{Z}^+_{\beta-\epsilon}$, there is a u such that $\langle x, \int_0^\tau T^+_{\beta-\epsilon}(\tau-s)B^+_{\beta-\epsilon}u(s)\mathrm{d}s\rangle \neq 0$. As shown in [9], this condition is equivalent to

$$\sum_{\lambda_n\in\sigma^-_{\beta-\epsilon}}\mathrm{e}^{\lambda_n(t-s)}\sum_{j=1}^{r_n}\langle x,\phi_{nj}\rangle\langle Bu,\psi_{nj}\rangle \neq 0 \tag{3.38}$$

Therefore, it can be shown that it is equivalent to say that

$$B_n U_n \neq 0 \tag{3.39}$$

$$B_n = \begin{bmatrix} \langle b_1, \psi_{n1} \rangle & \cdots & \langle b_m, \psi_{n1} \rangle \\ \vdots & & \vdots \\ \langle b_1, \psi_{nr_n} \rangle & \cdots & \langle b_m, \psi_{nr_n} \rangle \end{bmatrix} \tag{3.40}$$

$$U_n = \begin{bmatrix} \langle u_1, \psi_{n1} \rangle & \cdots & \langle u_m, \psi_{n1} \rangle \\ \vdots & & \vdots \\ \langle u_1, \psi_{nr_n} \rangle & \cdots & \langle u_m, \psi_{nr_n} \rangle \end{bmatrix} \tag{3.41}$$

If $\text{rank}(B_n) < r_n$, there exists a $u \neq 0$ such that $B_n U_n = 0$. Thus, the system is uncontrollable if $\text{rank}(B_n) < r_n$. If $\text{rank}(B_n) = r_n$, the only solution for $B_n U_n = 0$ is $u = 0$ and therefore $\mathcal{R}^{\perp} = \{0\}$ and the system is controllable.
By duality, as shown in [15], $\Sigma(A, -, C)$ is β-exponentially detectable, if $\Sigma(A^*, C^*, -)$ is β-exponentially stabilizable. Similarly, the system $\Sigma(A^e, -, C^e)$ is β-exponentially detectable. ■

Remark 5 *Consider the infinite dimensional system $\Sigma(\mathcal{A}^e, B^e, -)$ given by Equation 2.34. As discussed in eigenvalue problem, the eigenvalues of $\mathcal{A}^e$ consist of eigenvalues of $\mathcal{A}$ and 0 with finite multiplicity m. Since $\mathcal{A}$ is Sturm-Liouville operator, the spectrum of $\mathcal{A}$ is finitely bounded (i.e., there exists an ω such that all $\lambda \in \sigma(\mathcal{A}) < \omega$). Therefore, for any arbitrary β, $\sigma^{+}_{\beta-\epsilon}(\mathcal{A}^e)$ comprises finitely many eigenvalues and the first condition of previous theorem holds.*

Chapter 4

Summary and Conclusions

This thesis was concerned with the problem of the infinite dimensional optimal controller design for distributed parameter systems with special emphasis on transport processes (i.e. tubular reactors) that are normally modeled by partial differential equations. It is obvious that the governing transport phenomenon in this system determines the type of the PDE involved in the modeling, which in this case is parabolic PDE. The goal was to develop the required mathematical tools for solution of the optimal control problem for a general class of distributed parameter systems representing a tubular reactor with minimum number of simplifying assumptions in the modeling of the reactor. Besides, it was desired to show the implementation of exact time discretization for designing the optimal controller.

Chapter 2 addressed the problem of the tubular reactors and self-adjoint operators. The mathematical modeling of tubular reactors via parabolic PDEs was shown. The governing PDE was turned into well-posed abstract boundary control problem via exact transformation. Then the eigenvalue problem of the governing parabolic spatial operator was solved and corresponding eigenvalues and eigenfunctions of the self-adjoint operator were found. Then, the proposed time discretization method was brought up and applied to the problem. Discrete system evolution through time was then studied; first, the evolution of the system was inspected under no control input and some prescribed initial condition. After that, system evolution was studied under the effect of constant input. At the end of this chapter, a gain-based full-state feedback controller was designed and the system response to different gain values was studied via numerical simulation. In the last section of this chapter, numerical models for time discretization were discussed. Explicit Euler method was first introduced and its stability condition was shown through theoretical formulation. Then a numerical simulation was run for a general case and the effect of this method over stability was shown. Implicit Euler method was after that treated with the same approach and it was shown that this method does stabilize every system, regardless of their intrinsic stability. There was a numerical simulation of the general case to show these results for this method too. Finally, symplectic Euler method was introduced and its region of stability was shown. Through conformal mapping it was depicted that this scheme does not have any effects on the stability of the system. As a conclusion, a mapping was given to show the stability region and the effect of each scheme on the stability of a system.

In Chapter 3, optimal boundary control of infinite dimensional systems described by a parabolic PDE with was studied. Using an exact transformation, the boundary control problem was transformed into a well-posed infinite dimensional system. It was proven that the resulting system is a Riesz spectral system. Stabilizability of the system was investigated using the spectral properties of the system. The spectrum of the system was required to solve the optimal control problem for Riesz spectral systems and it was solved in Chapter 2. Then, by using the spectral properties of the system, the operator Riccati equation was converted to a set of algebraic equations that could be solved numerically. The LQ problem was first solved for the continuous case and after that the solution for Π was used for discrete case. The performance of the formulated controller was then compared to a LQ controller from continuous case. Simulation results showed that the infinite dimensional controller with exact time discretization leads to better performance in terms boundary input trajectory.

4.1 Directions for Future Work

This thesis took a leap towards building required tools for solution of optimal control problem for a class of distributed parameter systems with special focus on tubular reactors with self-adjoint operators. It was shown that exact time discretization is applicable to this type of PDEs. A number of challenges remain in the development of the infinite dimensional controller for processes modeled by a general form of infinite dimensional systems.

The method proposed in Chapter 2 had a limitation on the structure of the operator $\mathcal{A}$. In order to solve the eigenvalue problem it was assumed that the infinite dimensional operator had a triangular form, which means the coupling of the state variables is one way. Solution of the eigenvalue problem for general form of infinite dimensional operators cannot be performed analytically. For special cases the infinite dimensional operator can be triangularized using a transformation. Exploration of the conditions for existence of such a transformation is the topic that needs to be addressed in future work.

Besides, non-self-adjoint operators can be studied, for which the eigenvalue problem can be of a more complex form. For example, special case of boundary value problems with mixed and oblique derivative boundary conditions can be studied. In that case, complex variables arise in eigenvalue problem. This would be a potential topic to be investigated in future endeavor.

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Appendix A

Calculation of B_d^*

To obtain the adjoint of the operator B_d, one will use the adjoint property from [21]. Therefore, for a spatial operator $\mathcal{F}$ and any arbitrary functions Φ and Ψ in Hilbert space $\mathcal{H}$, there will be

$$\langle \mathcal{F}\Phi, \Psi^* \rangle = \langle \Phi, \mathcal{F}^*\Psi^* \rangle \tag{A.1}$$

where the asterisk denotes the adjoint of each element here.
Now, doing the same procedure for B_d, one will have:

$$\begin{aligned}
\langle B_d\Phi, \Psi^* \rangle = \int_0^1 \Bigg[&- 2\frac{\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
&\times \int_0^1 \cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Phi(x)\mathrm{d}x \\
&+ 2\int_0^\xi \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Phi(x)\mathrm{d}x\Bigg]\Psi^*(\xi)\mathrm{d}\xi
\end{aligned} \tag{A.2}$$

Now, by taking Ψ^* into the integrals, Equation A.2 becomes as

$$\begin{aligned}
\langle B_d\Phi, \Psi^*\rangle = &\int_0^1\int_0^1 \Bigg[-2\frac{\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)+\frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})+\frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
&\times\cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Phi(x)\Psi^*(\xi)\Bigg]\,\mathrm{d}x\,\mathrm{d}\xi \\
&+2\int_0^1\int_0^\xi \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Phi(x)\Psi^*(\xi)\,\mathrm{d}x\,\mathrm{d}\xi \\
= &\int_0^1\int_0^1 \Bigg[-2\frac{\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)+\frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}\xi)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})+\frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
&\times\cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-x)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Phi(x)\Psi^*(\xi)\Bigg]\,\mathrm{d}\xi\,\mathrm{d}x \\
&+2\int_0^1\int_x^1 \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(\xi-x)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Phi(x)\Psi^*(\xi)\,\mathrm{d}\xi\,\mathrm{d}x
\end{aligned} \tag{A.3}$$

Now, by interchanging the roles of x and ξ, one can write

$$
\begin{aligned}
&\langle B_d\Phi, \Psi^*\rangle \\
&= \int_0^1 \int_0^1 \Bigg[-2\frac{\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}x) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}x)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
&\quad \times \cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-\xi)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Phi(\xi)\Psi^*(x)\Bigg]\ \mathrm{d}x\ \mathrm{d}\xi \\
&+ 2\int_0^1\int_\xi^1 \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(x-\xi)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Phi(\xi)\Psi^*(x)\ \mathrm{d}x\ \mathrm{d}\xi \\
&= \int_0^1 \Bigg[-2\frac{\cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-\xi)\big)\big(\gamma\frac{\Delta t}{2}+1\big)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}) + \frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
&\quad \times \int_0^1 \Big[\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}x) + \frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}x)\Big]\Psi^*(x)\ \mathrm{d}x \\
&\quad + 2\int_\xi^1 \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(x-\xi)\big)\big(\gamma\frac{\Delta t}{2}+1\big)\Psi^*(x)\ \mathrm{d}x\ \Bigg]\Phi(\xi)\mathrm{d}\xi \\
&= \langle \Phi, B_d^*\Psi^*\rangle
\end{aligned}
\tag{A.4}
$$

Therefore, it is obvious that the adjoint of the operator B_d is defined as

$$
\begin{aligned}
B_d^*(.) = -2 & \frac{\cosh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(1-\xi)\big)\big(\gamma\frac{\Delta t}{2}+1\big)}{\sqrt{\frac{2}{\Delta t}+\gamma}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma})+\frac{\mathrm{Pe}}{2}\cosh(\sqrt{\frac{2}{\Delta t}+\gamma})} \\
& \times \int_0^1 \Big[\cosh(\sqrt{\frac{2}{\Delta t}+\gamma}x)+\frac{\mathrm{Pe}}{2}\frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh(\sqrt{\frac{2}{\Delta t}+\gamma}x)\Big](.)\mathrm{d}x \\
& + 2\int_\xi^1 \frac{1}{\sqrt{\frac{2}{\Delta t}+\gamma}}\sinh\big(\sqrt{\frac{2}{\Delta t}+\gamma}(x-\xi)\big)\big(\gamma\frac{\Delta t}{2}+1\big)(.)\mathrm{d}x
\end{aligned}
\tag{A.5}
$$