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MASTER EN SCIENCES MATHÉMATIQUES

Dynamical analysis of a nonisothermal axial dispersion reactor

HASTIR, Anthony

Award date:
2018

Awarding institution:
Universite de Namur

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UNIVERSITE DE NAMUR

Faculté des Sciences

Dynamical analysis of a nonisothermal axial dispersion reactor

Mémoire présenté pour l'obtention

du grade académique de master en Sciences mathématiques à finalité approfondie

Anthony HASTIR

Juin 2018

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Promoteur :

Pr. Joseph WINKIN

Encadrant :

François LAMOLINE

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Remerciements

Mes premiers remerciements vont tout naturellement à mon promoteur, Joseph WINKIN, tout d'abord pour avoir accepté d'encadrer ce mémoire. Je le remercie de plus pour ses conseils, pour son suivi, pour la patience dont il a fait preuve et pour toutes les discussions mathématiques constructives que nous avons eues durant la réalisation de ce mémoire. Ce manuscrit n'aurait jamais vu le jour sans lui. Merci également pour son soutien et ses encouragements !

Le seconde personne que je remercie est François LAMOLINE, qui, en plus d'avoir contribué à l'amélioration de ce mémoire, s'est montré à chaque fois disponible et prêt à répondre à mes questions. Merci infiniment.

Je souhaite également remercier Denis DOCHAIN et à nouveau Joseph WINKIN et François LAMOLINE pour leur collaboration lors de la réalisation du papier scientifique lié à ce mémoire.

Merci aussi à Jérémy DEHAYE pour les précieux conseils qu'il m'a apportés.

Je remercie également les différentes personnes qui liront ce mémoire, en particulier les différents membres du jury.

Last but not least, je remercie ma famille et mes proches, en particulier mes parents et mon oncle (Daniel) pour le soutien et l'aide inconditionnels qu'ils m'apportent sans cesse et qui ont été des éléments d'une importance capitale dans la réalisation de ce mémoire. Une attention spéciale à mon papa et mon oncle pour leur relecture méticuleuse de ce manuscrit et un petit clin d'oeil à Alice !

Anthony HASTIR

Résumé

La conception d'une loi de contrôle afin de stabiliser la température et la concentration des composants chimiques lors d'une réaction dans un réacteur tubulaire non isotherme avec dispersion axiale reste encore un défi dans le milieu du génie des procédés. Des étapes préliminaires telles que le caractère bien posé, l'analyse de stabilité et l'analyse des équilibres d'un tel réacteur chimique sont alors cruciales. Dans ce mémoire, ces différentes étapes sont développées pour une réaction du type $A \to B$ où A représente le réactif et B le produit. Ce type de système à paramètres répartis est régi par des équations aux dérivées partielles dites de réaction-convection-diffusion avec un terme non linéaire. Nous montrons d'abord que le système étudié est bien posé au moyen de la théorie des semi-groupes linéaires et non linéaires notamment. Ensuite, la stabilité exponentielle de la partie linéaire est prouvée. L'étape suivante est l'analyse des équilibres qui s'articule autour de deux nombres spécifiques, le nombre de Peclet massique et le nombre de Peclet thermique. Les analyses déjà présentes sont étendues dans le cas où ces deux nombres sont différents. Le résultat principal obtenu est que le réacteur peut exhiber un ou trois équilibres, notamment en fonction du coefficient de diffusion. De plus, des formes analytiques approchées des profils d'équilibre sont calculées explicitement au moyen de la théorie des perturbations. La dernière partie de ce mémoire traite de la stabilité des profils d'équilibre. Un modèle linéarisé autour des différents équilibres est construit et le caractère bien posé de celui-ci est démontré. En ce qui concerne l'étude de stabilité, diverses approches sont mises en oeuvre. Une méthode numérique connue sous le nom de méthode des résidus de Galerkin est notamment développée pour des nombres de Peclet égaux et étendue à des nombres de Peclet différents. Toutes les analyses et les résultats obtenus sont appuyés par des simulations numériques.

Mots-clés : Réacteur tubulaire non isotherme - Semi-groupes positifs - Système non linéaire de dimension infinie - Nombre de Peclet thermique, massique - Stabilité exponentielle - Profils d'équilibre

Abstract

The design of a control law to stabilize the temperature and the concentration of the chemical components during a reaction in a nonisothermal tubular reactor with axial dispersion is still a challenge in process engineering. Preliminary steps like the well-posedness, the stability analysis or the analysis of the equilibrium profiles in such a reactor are important. In this master's thesis, these different steps are developed for a reaction of the form $A \to B$ where A denotes the reactant and B the product. This kind of distributed parameter systems is governed by partial differential equations known as reaction-convection-diffusion with a supplementary nonlinear term. We first show that the system under consideration is well-posed using the theory of linear and nonlinear semigroups, notably. Then, the exponential stability of the linear part is proved. The next step is the analysis of the equilibrium profiles which is based on two specific numbers, the mass Peclet number and the thermal Peclet number. The well defined analysis are extended to the case of two different Peclet numbers. The main result is that the reactor can exhibit one or three equilibrium profiles, especially depending on the diffusion coefficient. Moreover, approximated analytic forms of these equilibria are computed using perturbation theory. The last part of this thesis is dedicated to the stability analysis of the equilibrium profiles. A linearized model around the different equilibria is constructed and the well-posedness of this model is proven. For the stability analysis, different approaches are used. A numerical method known as Galerkin's residuals method is developed for equal Peclet numbers and extended to different Peclet numbers. The analysis and the results are illustrated by numerical simulations.

Keywords : Nonisothermal tubular reactor - Positive semigroups - Infinite-dimensional nonlinear systems - Mass, thermal Peclet number - Exponential stability - Equilibrium profiles

Contents

Introduction

Controlled systems are ubiquitous in real life. A lot of current technologies use such systems daily, see e.g. automation, driving assistant systems, ... They play also an important role in industrial processes and in particular in chemical and biochemical engineering. Many dynamical models describing controlled systems are governed by partial differential equations that exhibit most of the time nonlinear aspects. Moreover, this kind of systems possesses generally unstable equilibria or equilibria that do not have a desired behavior. The design/modeling and the implementation of a robust control law that forces a physical system to have a predetermined behavior is then necessary. Before controlling a dynamical system, preliminary steps are also fundamental and not trivial. These encompass notably the well-posedness (existence and unicity of a solution), the stability and also the equilibrium analysis.

The controlled system under study in this master's thesis is a distributed parameter system, which is a model of a nonisothermal tubular reactor with axial dispersion. This class of systems are dynamical controlled systems for which the state space is infinite-dimensional.

Since 1980, a mathematical theory has been developed to model, analyse and build control laws for distributed parameters systems. This theory is based on the strongly continuous semigroup of bounded linear operators approach for the modeling and the dynamical analysis parts essentially. More recently, this theory focuses on the well-posedness of abstract dynamical models involving unbounded control and observation operators and is a nontrivial extension of the existing theories for finite-dimensional systems, see e.g. (Curtain and Zwart, 1995; Jacob and Zwart, 2012; Callier and Winkin, 1992; Curtain and Pritchard, 1978).

In (Aksikas et al., 2007), the nonisothermal plug flow reactor is studied. For this model and the corresponding axial dispersion reactor, some results were obtained, notably for the existence and the uniqueness of solutions (well-posedness). This comprises the linearized model with axial dispersion (Winkin et al., 2000), the nonlinear plug flow model and the nonlinear reactor with axial dispersion respectively (Laabissi et al., 2001). Therefore, the semigroup approach was used, both in the linear and in the nonlinear cases. In (Laabissi et al., 2005), the exponential stability of the linear operator describing the dynamic is proven. More generally, a stability analysis of chemical reactors similar to the one under considerations in this master's thesis is developed in (Delattre et al., 2003; Drame et al., 2008; Laabissi et al., 2001). The methodology is notably based on the notions of Riesz-Spectral operators and Sturm-Liouville ones. In (Drame et al., 2008), which is dedicated to the asymptotic behavior and to the stability of solutions of a distributed parameters model of a biochemical reactor, a qualitative method was applied for the existence and the multiplicity of equilibrium profiles. This method is based on an analysis of the model when the axial dispersion phenomenon dominates the plug flow, i.e. the diffusion coefficient is dominant on the superficial velocity of the fluid. The stability analysis of the equilibrium profiles of a chemical reactor has

also been envisaged in (McGowin and Perlmutter, 1970) and in (Varma and Aris, 1977) where different techniques are highlighted and especially numerical techniques.

In this master's thesis, the well-posedness, the stability and the equilibrium analysis of a nonisothermal tubular reactor with axial dispersion are studied for an irreversible chemical reaction $A \to B$, where A denotes the reactant and B the product. For the well-posedness and the stability of the linear operator describing the dynamic, some results in the literature are recalled and proven. These results are based mainly on the semigroup approach. Furthermore, this analysis is considered using the port-Hamiltonian formalism, see e.g. (Jacob and Zwart, 2012), for which the results can be more easily deduced once the equations describing the system are written in this formalism. The explorating part of this master's thesis concerns the analysis of the equilibrium profiles, which comprises the existence, the multiplicity and the stability. This analysis focuses on the relation between two physical numbers, the mass and the thermal Peclet numbers. Some results are already present in the literature in the case of two equal Peclet numbers. These results are extended here in the cases of different or close Peclet numbers. The existence and the multiplicity analysis goes along the lives of (Drame et al., 2008). In particular, it is shown that the reactor can exhibit one or three equilibria, depending on the parameters of the system and especially on the diffusion coefficients. Analytical approximated expressions of the equilibria are given both in the cases of equal and different Peclet numbers using perturbation theory. For the stability analysis, a linearized model around an equilibrium is built and it is shown that it is well-posed, using the semigroup approach. A numerical method known as Galerkin's residuals method is studied. In (McGowin and Perlmutter, 1970), this approach is developed in the case of equal Peclet numbers. This method is extended to different or close Peclet numbers. Numerical simulations illustrate the theoretical results.

Contents

This master's thesis is divided into different chapters. A brief description of each of them is provided below.

- **Chapter 1.** This chapter is more an introductive chapter and is dedicated to the presentation of some concepts of chemical engineering. The notions of chemical reaction, reaction rate are provided. An overview of some types of chemical reactors is also presented and a real life tubular reactor is highlighted.
- **Chapter 2.** The nonlinear PDEs describing the dynamic of a nonisothermal tubular reactor with axial dispersion are introduced. A state space representation is provided and the definition of a well-posed system is given. It is shown that the nonlinear PDEs are well-posed using the semigroup approach. The port-Hamiltonian formalism is introduced and it is shown that the linear part of the system under study fits the class of dissipative port-Hamiltonian systems.
- **Chapter 3.** The exponential stability analysis of the linear operator of the dynamic is studied. The notions of Riesz basis, Riesz spectral operator and Sturm-Liouville systems are described. It is proven that the linear operator of the dynamic is a Riesz spectral operator and in this case, the

stability analysis reduces to an eigenvalue problem. In particular, it is shown that this operator is exponentially stable.

- **Chapter 4.** In this chapter, the analysis of the existence and the multiplicity of equilibrium profiles of a nonisothermal axial dispersion tubular reactor is developed. The results supposing two equal Peclet numbers are extended to different or close ones. It is shown that the reactor can exhibit one or three equilibria depending on the parameters of the system, especially on the diffusion coefficient. Some numerical simulations support the theoretical results.

- **Chapter 5.** The stability of the equilibrium profiles is studied. A linearized model around an equilibrium is built and it is shown that it is well-posed. Then, the stability is analysed from an *eigenvalues* point of view. Some theoretical results and also numerical ones are exposed, which are based notably on the Galerkin's residuals method. In particular, for equal Peclet numbers, it is shown that in the case of one equilibrium, the latter is always exponentially stable and in the case of three equilibria, the pattern « exponentially stable – unstable – exponentially stable » is present. However, it is not always the case for different or close Peclet numbers. The more the Peclet numbers are different, the more the central equilibrium becomes exponentially stable. For different or close Peclet numbers, the Galerkin's method is developed and some numerical simulations are highlighted.

Contributions

The main contribution of this master's thesis concerns the existence and the multiplicity of the equilibrium profiles. Theoretical results were highlighted in the cases of equal, different or close Peclet numbers providing necessary and sufficient conditions for the reactor to exhibit equilibrium profiles. These researches and these results were made and obtained in collaboration with François Lamoline, a FRIA researcher of the department of mathematics at the University of Namur, Professor Joseph Winkin, full professor and researcher in the same department and Professor Denis Dochain, full professor and researcher at the ICTEAM, « Institute of Information and Communication Technologies, Electronics and Applied Mathematics », Polytechnic University of Louvain, UCL. This collaboration led to the submission of a scientific paper, as full paper, in the « IEEE Transactions on Automatic Control », see (Hastir et al., 2018).

Chapter 1

Chemical reactors

Contents

This first introductive chapter is dedicated to the presentation of some notions related to chemical engineering. In particular, the roles of chemical reactors and some usages of them in the industry are discussed. Then, the concepts of chemical reaction and reaction rates are exposed. Several types of reactors are introduced with a short description, notably making the distinction between isothermal and nonisothermal reactors. One example of a chemical reactor in real life, the anaerobic digestion pilot reactor of INRA - LBE, Narbonne, is presented.

1.1 General considerations

Basically, a chemical reactor is a device where a chemical reaction occurs. The main objective of working with such systems is to transform inexpensive chemicals into valuable ones. Before entering the reactor and after leaving it, the materials (raw materials at the entrance and products at the output) have to be purified such that the reactor behaves well, notably. These steps are called the *separation processes* (see Figure 1.1) and are the most expensive ones among the successive steps of a chemical process. In that way, improvments in the reactor usually have enormous impact on the two separation processes and the aim of designing a chemical reactor is to ensure that the reaction proceeds with the highest efficiency as possible while producing the desired output at the lowest costs as possible.

The type of chemical reaction we are interested in is the *irreversible reaction*

$$A \to B, \tag{1.1}$$

where A denotes the reactant and B is the product. *Irreversible* means that the reactant can change to the product but the product cannot change back to the reactant. That kind of reaction is the most used example in chemical kinetics, see e.g. combustion reactions. Combustion occurs whenever a fuel burns. During the reaction, fuel may combine with oxygen to produce carbon dioxide and water, see e.g. the

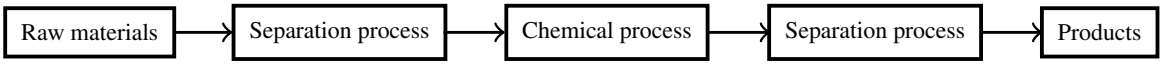

Fig. 1.1 – Chemical process.

combustion of methane

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O.$$

The products (carbon dioxide and water) cannot react (back) to find methane and oxygen again so that the reaction is irreversible.

An important concept in chemical engineering is the reaction rate. This is an empirical expression, denoted by k, that describes the dependence of the rate of transformation (of reactant into products) on the parameters of the system, see (Schmidt, 1998). Generally, the reaction rate depends on the temperature of the reaction and an empirical expression of it is given by Arrhenius Law (see (Schmidt, 1998; Aksikas et al., 2007))

$$k(T) = k_0 e^{-\frac{E}{RT}}, \tag{1.2}$$

where T denotes the temperature, E the activation energy of the reaction, R the gaz constant and k_0 is a kinetic constant. The Arrhenius Law describes the variation of the velocity of a chemical reaction as a function of the temperature. The activation energy plays an important role here. Indeed, if the latter is small (which implies a large reaction rate), then the reaction occurs quickly. However, if that energy is large, then the reaction occurs slowly. Looking at (1.2), a similar reasoning holds with the temperature. A large temperature implies a fast reaction while a small one produces a low reaction.

1.2 Different types of chemical reactors

The classification of the different chemical reactors we present here is not exhaustive but covers a relatively large class of them.

Chemical reactors can either operate in *batch* or in *flow* modes. No mass can be added into or out of a batch reactor after time $t = 0$; for this reason, a batch reactor is sometimes called a closed reactor. On the other hand, flow reactors can be *loaded* during the reaction.

The following distinction concerns only flow reactors. They operate between limits of completely unmixed contents and completely mixed ones, involving different phases : solid, liquid and gas. Reactors for which the medium is homogeneous are called tank reactors (e.g. the CSTR or Continuous Stirred Tank Reactor) and if the medium can be nonhomogeneous, they are said to be tubular reactors, e.g. the PFTR (Plug Flow Tubular Reactor).

The reactors we are interested in are the tubular reactors. One can still make a separation for these reactors, considering on one hand the plug flow tubular reactor wherein the flow is supposed to be laminar, i.e. no turbulances are allowed inside the reactor, which assumes low reaction velocities and which is not realistic in chemical engineering. On the other hand, one introduces the concept of axial mixing which takes into account the fact that the contents of the reactor can move from right to left and vice versa during the reaction process, see e.g. plug flow reactors with axial mixing (or the TRAD : Tubular Reactor with Axial Dispersion). Tubular reactors are sometimes called diffusion-convection-reaction reactors.

The diffusion phenomenon is symbolized by displacement of atoms or molecules from regions with high concentration to regions with low ones. The diffusion occurs in tubular reactors notably because of the axial mixing. Moreover, the convection models the heat transfer through the reactor and is due to the plug flow effect in tubular reactors. Furthermore, the reactors are called adiabatic if no heat exchange occurs between the inside of them and the external environment, and nonadiabatic otherwise.

One can still go a step further distinguishing isothermal reactors from nonisothermal ones. Isothermal reactors are reactors in which the temperature is fixed, specified and does not change during the reaction process. These kind of reactors are relatively idealistic since reactions generate or absorb large amounts of heat (exothermic or endothermic reactions), which produces a lot of variations in the temperature in the reactor. For this reason, one speaks more generally of nonisothermal reactors. For these reactors, we have to consider two conflicting aspects. First, we notice that the temperature inside these reactors has to be sufficiently high to activate the reaction but it cannot blow up or be too high. In this case, the equilibrium limitation can limit the conversion and slow the activation of the reaction down, or simply overheating can happen or thermal runaway can produce pressure buildup and release of chemicals. The reason for considering this kind of reactors and trying to control the temperature inside of them is because it represents the major cause of accidents in chemical plants !

The equations governing the dynamic of a nonisothermal tubular reactor are nonlinear partial differential equations (PDEs) derived from mass and energy balances, based notably on the laws of thermodynamics. The nonlinearities are located in the kinetic terms. On one hand, we usually use the well-known Arrhenius Law for the dependence of these terms on the temperature, see (1.2), and on the other hand, the dependence of the kinetic terms on the reactant concentration can be represented by many mathematical expressions, depending on the reaction we are interested in. For example, one finds the *mass action law* which assume that the kinetic terms depend on the product of the concentration of the reactant and the product, each term raised to a power which depends on the stoechiometric constant, see (Schmidt, 1998). The one under consideration here is a first order dependence. Denoting by C the chemical concentration of the components in the reactor, the kinetic term that is exhibited here is $k_0 C e^{-\frac{E}{RT}}$, see e.g. (Aksikas, 2005). In addition to this nonlinearity, the linear part of the PDEs is called the diffusion-convection-reaction part since it includes these different phenomena. The diffusion (or the axial dispersion) is modelised by a second order spatial derivative operator while the convection is modeled by a first order spatial derivative operator. The complete PDEs with the associated boundary conditions can be found in the first section of Chapter 2.

The classification of the different reactors introduced in this section is depicted in Figure 1.2.

1.3 The anaerobic digestor

This section is dedicated to a brief presentation of a particular tubular reactor namely, the anaerobic reactor. An illustration of such a reactor can be found in Figure 1.3, wherein the reactor of INRA – LBE of Narbonne is presented.

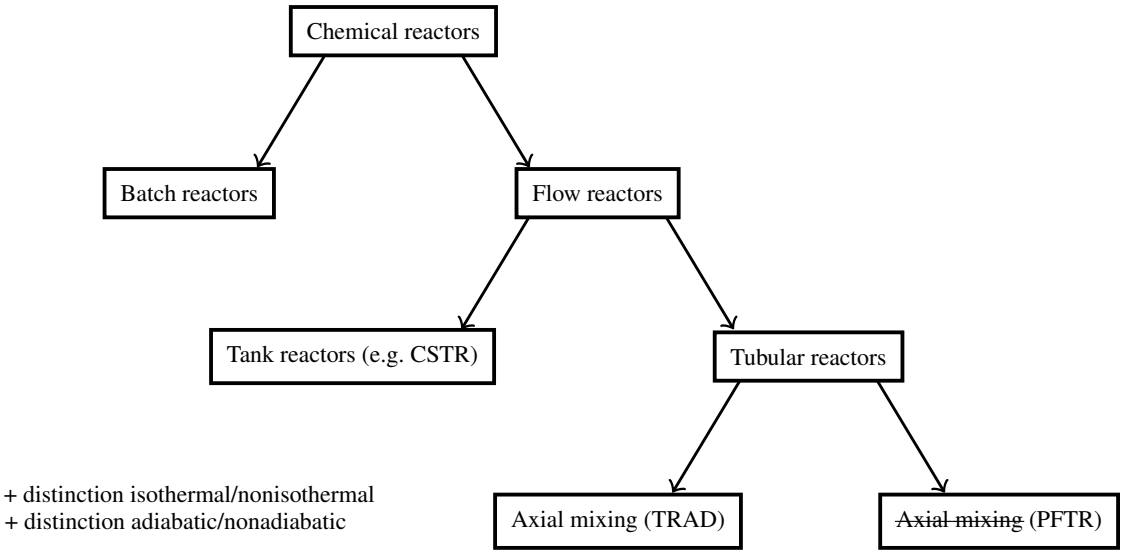

Fig. 1.2 – Classification of the different reactors.

Fig. 1.3 – Anaerobic digestion pilot reactor of INRA - LBE, Narbonne, see (Gouzé and Steyer, 2007).

Anaerobic digestion is a chemical/biochemical process in which biodegradable material is degraded in the absence of oxygen. It occurs naturally in lakes, paddy fields, ... but it is sometimes convenient to

accelerate and maintain the process. Therefore, anaerobic digestion can take place in chemical reactors in which dark waters or sludge are transformed in usable methane (called biogas or biomethane) and substratum. This kind of reactors are sometimes called methanisors since one of the expected output (or product) is the methane.

The anaerobic reactor presented in this section fits the class of chemical reactors that are under study in this master's thesis since the latter is a tubular reactor that can involve axial mixing and behave nonisothermal, see also Figure 1.2, part *Axial mixing (TRAD)*.

Chapter 2

Dynamical analysis of the model

Contents

This chapter is dedicated to the dynamical analysis of a nonisothermal tubular reactor with axial dispersion. It is organized as follows. We first introduce the equations (PDEs) related to the considered model with the associated boundary conditions. Then, we present a dimensional reduction of these equations. The next section is devoted to the well-posedness of both linear and nonlinear parts of the PDEs governing the model. In particular, it is shown that the operators describing the dynamic generate a C_0-semigroup, which is nonlinear. In the last section of this chapter, the port-Hamiltonian formalism is presented and it is shown that the linear part of the PDEs governing the model can be written in this formalism, notably by adding a dissipation term in the classical definition of a linear port-Hamiltonian system. In addition, results concerning notably well-posedness will be presented using this approach.

2.1 Introduction of the model

We are interested in tubular reactors involving a chemical reaction of the form

$$A \rightarrow B$$

where A denotes the reactant and B the product. In the model, the state components are defined as the temperature $(T\,[K])$ and the concentration of reactant $(C\,[mol/l])$. The equations of a nonisothermal tubular reactor are directly deduced from mass and energy balances on a slice of infinitesimal tickness dz during an infinitesimal time dt, as depicted on Figure 2.1. They are given by the following nonlinear PDEs (see (Laabissi et al., 2001))

$$\begin{cases} \frac{\partial T}{\partial t} = -v\frac{\partial T}{\partial z} + \frac{\lambda_{ea}}{\rho C_p}\frac{\partial^2 T}{\partial z^2} - \frac{\Delta H}{\rho C_p}k_0 C e^{-\frac{E}{RT}} + \frac{4h}{\rho C_p d}(T_w - T) \\ \frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial z} + D_{ma}\frac{\partial^2 C}{\partial z^2} - k_0 C e^{-\frac{E}{RT}}. \end{cases} \tag{2.1}$$

Constant	Unit	Description
L	m	Reactor's length
v	$\frac{m}{s}$	Fluid superficial velocity
λ_{ea}	$\frac{kJ}{msK}$	Axial energy dispersion coefficient
D_{ma}	$\frac{m^2}{s}$	Axial mass dispersion coefficient
ΔH	$\frac{kJ}{kg}$	Heat transfer coefficient
ρ	$\frac{kg}{m^3}$	Fluid density
C_p	$\frac{kJ}{kgK}$	Specific heat
k_0	$\frac{1}{s}$	Kinetic constant
E	$\frac{kJ}{kg}$	Activation energy
R	$\frac{kJ}{kgK}$	Gas constant
h	$\frac{kJ}{m^2Ks}$	Wall heat transfer coefficient
d	m	Reactor's diameter
T_w	K	Coolant temperature
T_{in}	K	Input temperature
C_{in}	$\frac{kg}{m^3}$	Input reactant concentration

TABLE 2.1 – System parameters.

where $T(t,z)$ and $C(t,z)$ denote the temperature in the reactor and the concentration of the reactant respectively at time t and position z. Note that t takes values in $[0,+\infty)$ and z in $[0,L]$ where L denotes the length of the reactor. Such equations are usually called convection-diffusion-reaction equations (CDR). The meaning and the units of the parameters are summarized in Table 2.1.

To the PDEs (2.1), we associate specific boundary conditions, known as the Danckwerts'conditions (Danckwerts, 1953), which are given by

$$\begin{aligned}
\frac{\lambda_{ea}}{\rho C_p}\frac{\partial T}{\partial z}(t,0) &= v(T(t,0)-T_{in}),\\
D_{ma}\frac{\partial C}{\partial z}(t,0) &= v(C(t,0)-C_{in}),\\
\frac{\partial T}{\partial z}(t,L) = 0 \text{ and } &\frac{\partial C}{\partial z}(t,L) = 0,
\end{aligned}$$

for all t in $[0,+\infty)$.

2.2 Reduction of the model

The following step is to introduce a state space representation of the model governed by Equations (2.1) and moreover, to write the PDEs (2.1) with an abstract differential equation. This representation has the form

$$\begin{cases} \dot{x}(t) = Ax(t) + N(x(t)), \\ x(0) = x_0 \end{cases} \tag{2.2}$$

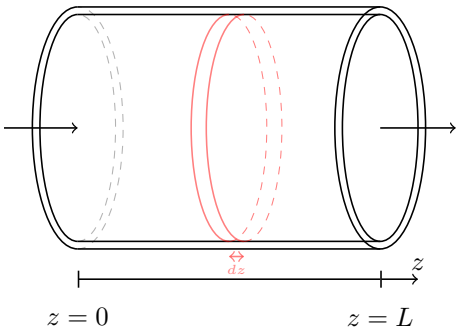

Fig. 2.1 – Profile view of a tubular reactor.

where A is the linear (unbounded) operator associated to PDEs (2.1) and N represents the nonlinear operator associated to the same PDEs [1].

To reach such a representation, we first consider the following change of coordinates

$$\tau = t\frac{v}{L}, \zeta = \frac{z}{L}.$$

In this way, the derivative operators become

$$\frac{\partial}{\partial t} = \frac{v}{L}\frac{\partial}{\partial \tau}, \frac{\partial}{\partial z} = \frac{1}{L}\frac{\partial}{\partial \zeta}, \frac{\partial^2}{\partial z^2} = \frac{1}{L^2}\frac{\partial^2}{\partial \zeta^2}.$$

Applying this change of coordinates [2] to (2.1) yields the following equivalent PDEs

$$\begin{cases} \frac{\partial T}{\partial \tau} = -\frac{\partial T}{\partial \zeta} + \frac{1}{Pe_h}\frac{\partial^2 T}{\partial \zeta^2} - \frac{\Delta HL}{\rho C_p v}k_0 Ce^{-\frac{E}{RT}} - \frac{4hL}{\rho C_p dv}(T - T_w) \\ \frac{\partial C}{\partial \tau} = -\frac{\partial C}{\partial \zeta} + \frac{1}{Pe_m}\frac{\partial^2 C}{\partial \zeta^2} - \frac{k_0 L}{v}Ce^{-\frac{E}{RT}}. \end{cases} \tag{2.3}$$

where Pe_h and Pe_m denote the thermal and the mass Peclet numbers respectively, which are given by

$$Pe_h = \frac{\rho C_p vL}{\lambda_{ea}}, Pe_m = \frac{vL}{D_{ma}}. \tag{2.4}$$

These are dimensionless numbers representing the ratio between the convection transfer and the conduction transfer (thermal Peclet number) or the ratio between the convection transfer and the diffusion transfer (mass Peclet number).

1. Equations (2.2) hold pointwise in t, i.e. hold for each $t \in [0, +\infty)$.
2. One can easily verify that τ and ζ are dimensionless variables defined on $[0, +\infty)$ and $[0, 1]$ respectively.

The corresponding boundary conditions are given by

$$\begin{aligned}
&\frac{\partial T}{\partial \zeta}(\tau,0) = Pe_h\left(T(\tau,0) - T_{in}\right),\\
&\frac{\partial C}{\partial \zeta}(\tau,0) = Pe_m\left(C(\tau,0) - C_{in}\right),\\
&\frac{\partial T}{\partial \zeta}(\tau,1) = 0 \text{ and } \frac{\partial C}{\partial \zeta}(\tau,1) = 0.
\end{aligned} \tag{2.5}$$

Notice that the system (2.3) with the boundary conditions (2.5) is a system of *controlled* PDEs. In fact, these are controlled at the boundary by the input temperature, T_{in}, and by the input reactant concentration, C_{in} respectively. These are also controlled along the spatial domain (distributed control) by the coolant temperature, T_w.

Finally, assuming that T_w, T_{in} and C_{in} are constant, we consider the further change of variables

$$x_1 = \frac{T - T_{in}}{T_{in}},\ x_2 = \frac{C_{in} - C}{C_{in}},\ x_w = \frac{T_w - T_{in}}{T_{in}}. \tag{2.6}$$

From now, we consider T_w and T_{in} equal, which entails that x_w is equal to 0. In this way, (2.3) can be rewritten as

$$\begin{cases}
\frac{\partial x_1}{\partial \tau} = \left[\frac{1}{Pe_h}\frac{\partial^2 x_1}{\partial \zeta^2} - \frac{\partial x_1}{\partial \zeta} - \gamma x_1\right] + \alpha\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}}\\
\frac{\partial x_2}{\partial \tau} = \left[\frac{1}{Pe_m}\frac{\partial^2 x_2}{\partial \zeta^2} - \frac{\partial x_2}{\partial \zeta}\right] + \alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}},
\end{cases} \tag{2.7}$$

where

$$\mu = \frac{E}{RT_{in}},\ \alpha = \frac{k_0 L}{v}e^{-\mu},\ \delta = \frac{-\Delta H}{\rho C_p}\frac{C_{in}}{T_{in}}, \gamma = \frac{4hL}{\rho C_p d v}. \tag{2.8}$$

The associated boundary conditions are given by

$$\begin{aligned}
&\frac{\partial x_1}{\partial \zeta}(\tau,0) = Pe_h x_1(\tau,0), \frac{\partial x_2}{\partial \zeta}(\tau,0) = Pe_m x_2(\tau,0)\\
&\frac{\partial x_1}{\partial \zeta}(\tau,1) = 0, \frac{\partial x_2}{\partial \zeta}(\tau,1) = 0.
\end{aligned}$$

Let us now define the linear (unbounded) operator

$$Ax = \begin{pmatrix} \beta_1\frac{d^2}{d\zeta^2} - \frac{d}{d\zeta} - \gamma I & 0\\ 0 & \beta_2\frac{d^2}{d\zeta^2} - \frac{d}{d\zeta}\end{pmatrix}\begin{pmatrix} x_1\\ x_2\end{pmatrix} \tag{2.9}$$

on the domain $D(A)$ defined as

$$\left\{x \in H | x \text{ a.c.}, \frac{dx}{d\zeta} \in H \text{ a.c.}, \frac{d^2x}{d\zeta^2} \in H, \beta_i\frac{dx_i}{d\zeta}(0) - x_i(0) = 0 = \frac{dx_i}{d\zeta}(1), i = 1,2\right\}, \tag{2.10}$$

in the Hilbert space $H = L^2(0,1) \times L^2(0,1)$ where the notation

$$\beta_1 = \frac{1}{Pe_h}, \beta_2 = \frac{1}{Pe_m}$$

is adopted. Moreover, the nonlinear operator $N : D \to H$ is defined as (see (Laabissi et al., 2001))

$$N(x) = \left(\alpha\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}}, \quad \alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}}\right)^T \tag{2.11}$$

on the domain

$$D := \{x \in H | -1 \leq x_1(\zeta), 0 \leq x_2(\zeta) \leq 1, \text{ for a.e. } \zeta \in [0,1]\}. \tag{2.12}$$

Using these operators, the system (2.7) with the associated boundary conditions and with initial condition can be described by the following abstract differential equation

$$\dot{x}(\tau) = Ax(\tau) + N(x(\tau)), \; x(0) = x_0, \tag{2.13}$$

where the vector x is defined for $\tau \in [0, +\infty)$ by

$$\begin{aligned} x(\tau) : [0,1] &\to \mathbb{R}^2 \\ \zeta \quad &\rightsquigarrow (x(\tau))(\zeta) := (x_1(\tau,\zeta), x_2(\tau,\zeta))^T, \end{aligned}$$

where x_1 and x_2 are the functions defined by (2.6).

2.3 Well-posedness

In this section, we show that the model introduced in the previous section is well-posed, i.e. that (2.13) possesses a unique mild solution on $[0, +\infty)$. By mild solution, we mean the following definition, see (Jacob and Zwart, 2012, Definition 2.2.2.).

Definition 1. *A continuous function $x : [0, +\infty) \to H$ is called a mild solution of (2.13) if x is continuous and satisfies the integrated version of the differential equation (2.13), i.e., if it satisfies*

$$x(t) = x_0 + \int_0^t Ax(s) + N(x(s))\, ds, \quad \textit{for } t \geq 0. \tag{2.14}$$

In order to show that the model is well-posed, we use the semigroup approach. We first show that the operator describing the linear part of the system, A, is the infinitesimal generator of a contraction C_0-semigroup, using the Lumer-Phillips theorem. Then, looking at the nonlinear operator, N, it is shown that $A+N$ is the infinitesimal generator of a nonlinear semigroup. All these considerations provide well-posedness in the sense we defined it.

2.3.1 Linear operator

In this part, we show that the operator A defined by (2.9) and (2.10) is the infinitesimal generator of a C_0-semigroup and moreover, a contraction semigroup. We start by defining the notion of C_0-semigroup,

see (Jacob and Zwart, 2012, Definition 5.1.2.).

Definition 2. *Let H be a Hilbert space. $(T(t))_{t\geq 0}$ is called a C_0-semigroup, or strongly continuous semigroup, if the following conditions hold*

1. *For all $t \geq 0$, $T(t) \in \mathcal{L}(H)$, i.e $T(t)$ is a bounded linear operator on H,*
2. $T(0) = I$,
3. $\forall t, s \geq 0, T(t+s) = T(t)T(s)$,
4. $\forall x_0 \in H, \lim\limits_{t\to 0^+} ||T(t)x_0 - x_0|| = 0$.

Furthermore, the semigroup $(T(t))_{t\geq 0}$ is called a contraction semigroup if the inequality

$$\|T(t)\| \leq 1$$

holds for all $t \geq 0$, see (Jacob and Zwart, 2012, Definition 6.1.1.). We introduce now the notion of infinitesimal generator of a C_0-semigroup, see (Jacob and Zwart, 2012, Definition 5.2.1.).

Definition 3. *Let H be a Hilbert space and $(T(t))_{t\geq 0}$ a C_0-semigroup on H. Operator A with domain $D(A)$ is called the infinitesimal generator of $(T(t))_{t\geq 0}$ if*

$$Ax = \lim_{t\to 0^+} \frac{T(t)x - x}{t}$$

for all $x \in D(A)$. Moreover, $D(A)$ is given by

$$D(A) = \left\{ x \in H, \lim_{t\to 0^+} \frac{T(t)x - x}{t} \text{ exists} \right\}.$$

Ax can be viewed as the time derivative of the C_0-semigroup in a strong sense.

The following theorem, called the Lumer-Phillips Theorem, gives conditions on an operator A to be the infinitesimal generator of a strongly continuous contraction semigroup on a Hilbert space H, see (Jacob and Zwart, 2012, Theorem 6.1.7.).

Theorem 1. *Let A with domain $D(A)$ be an operator on a Hilbert space H. A is the infinitesimal generator of a strongly continuous contraction semigroup $(T(t))_{t\geq 0}$ on H if and only if A is dissipative and $\mathrm{Im}(I - A) = H$, i.e. $I - A$ is onto.*

Before applying this theorem to the operator A defined by (2.9) and (2.10), we introduce some definitions. The first is the dissipativity of a linear operator, see (Jacob and Zwart, 2012, Definition 6.1.4.).

Definition 4. *Let A be a linear operator with domain $D(A)$ on a Hilbert space H. A is dissipative if and only if*

$$\mathfrak{Re}\langle Ax, x\rangle \leq 0,\ x \in D(A) \tag{2.15}$$

where $\langle\cdot,\cdot\rangle$ denotes the inner product on H.

Then, the inner products in the Lebesgue spaces $L^2(0,1)$ and $L^2(0,1)\times L^2(0,1)$ are recalled.

Definition 5. *Let x and y be two elements of the Lebesgue space $L^2(0,1)$. The inner product between x and y, denoted by $\langle x,y\rangle_{L^2(0,1)}$ is defined as*

$$\int_0^1 x(\zeta)\overline{y(\zeta)}d\zeta. \tag{2.16}$$

Definition 6. *Let x and y be two elements of the product Lebesgue space $L^2(0,1)\times L^2(0,1) = H$.*

$$\langle x,y\rangle_{L^2(0,1)\times L^2(0,1)} := \langle x_1,y_1\rangle_{L^2(0,1)} + \langle x_2,y_2\rangle_{L^2(0,1)},$$

where $x = (x_1\ x_2)^T$, $y = (y_1\ y_2)^T$.

The two assumptions of the Lumer-Phillips theorem will be successively verified, beginning by the dissipativity of the operator A.

Proposition 1. *The operator A defined by (2.9) and (2.10) is dissipative.*

Proof. Let x be in $D(A)$. Due to the definition 6, inequality (2.15) becomes :

$$\mathfrak{Re}\langle Ax,x\rangle = \mathfrak{Re}\langle (Ax)_1,x_1\rangle + \mathfrak{Re}\langle (Ax)_2,x_2\rangle \leq 0.$$

One way to prove this inequality is to show that both $\mathfrak{Re}\langle (Ax)_1,x_1\rangle \leq 0$ and $\mathfrak{Re}\langle (Ax)_2,x_2\rangle \leq 0$. We will only prove that $\mathfrak{Re}\langle (Ax)_1,x_1\rangle \leq 0$. The proof for the other component can be found in Appendix A. By (2.9), we have

$$\begin{aligned}
\mathfrak{Re}\langle (Ax)_1,x_1\rangle &= \mathfrak{Re}\left(\int_0^1 (Ax)_1(\zeta)x_1(\zeta)d\zeta\right)\\
&= \mathfrak{Re}\left(\int_0^1 \left(\begin{pmatrix}\beta_1\frac{d^2}{d\zeta^2}-\frac{d}{d\zeta}-\gamma I & 0\\ 0 & \beta_2\frac{d^2}{d\zeta^2}-\frac{d}{d\zeta}\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix}\right)_1(\zeta)x_1(\zeta)d\zeta\right)\\
&= \mathfrak{Re}\left(\int_0^1 \left(\beta_1\frac{d^2x_1}{d\zeta^2}(\zeta)-\frac{dx_1}{d\zeta}(\zeta)-\gamma x_1(\zeta)\right)(x_1(\zeta))d\zeta\right)\\
&= \underbrace{\mathfrak{Re}\left(\int_0^1 \beta_1 x_1(\zeta)\frac{d^2x_1}{d\zeta^2}(\zeta)d\zeta\right)}_{(a)} - \underbrace{\mathfrak{Re}\left(\int_0^1 x_1(\zeta)\frac{dx_1}{d\zeta}(\zeta)d\zeta\right)}_{(b)} - \underbrace{\mathfrak{Re}\left(\int_0^1 \gamma x_1^2(\zeta)d\zeta\right)}_{(c)}.
\end{aligned}$$

The three integrals will be computed separatively, using essentially integration by parts. Note also that the real parts are not mentionned anymore, the quantities being real.

(a) Let $f = x_1$ and $\frac{dg}{d\zeta} = \frac{d^2x_1}{d\zeta^2}$, we have $\frac{df}{d\zeta} = \frac{dx_1}{d\zeta}$ and $g = \frac{dx_1}{d\zeta}$. Using integration by parts like

$$\int f\frac{dg}{d\zeta} = fg - \int \frac{df}{d\zeta}g,$$

yields the following

$$\begin{aligned}
\int_0^1 \beta_1 x_1(\zeta)\frac{d^2x_1}{d\zeta^2}(\zeta)d\zeta &= \left[\beta_1 x_1(\zeta)\frac{dx_1}{d\zeta}(\zeta)\right]_0^1 - \int_0^1 \beta_1\left(\frac{dx_1}{d\zeta}(\zeta)\right)^2 d\zeta \\
&= \beta_1 x_1(1)\frac{dx_1}{d\zeta}(1) - \beta_1 x_1(0)\frac{dx_1}{d\zeta}(0) - \int_0^1 \beta_1\left(\frac{dx_1}{d\zeta}(\zeta)\right)^2 d\zeta \\
&\overset{(2.10)}{=} -\beta_1^2\left(\frac{d^2x_1}{d\zeta^2}(0)\right)^2 - \int_0^1 \beta_1\left(\frac{dx_1}{d\zeta}(\zeta)\right)^2 d\zeta \\
&\overset{not.}{=} -\beta_1^2\left(\frac{dx_1}{d\zeta}(0)\right)^2 - k_1^2.
\end{aligned}$$

(b) Let $f = x_1$, $\frac{dg}{d\zeta} = \frac{dx_1}{d\zeta}$. In this way, $\frac{df}{d\zeta} = \frac{dx_1}{d\zeta}$ and $g = x_1$, which implies that

$$\int_0^1 x_1(\zeta)\frac{dx_1}{d\zeta}(\zeta)d\zeta = \left[x_1^2(\zeta)\right]_0^1 - \int_0^1 \frac{dx_1}{d\zeta}(\zeta)x_1(\zeta)d\zeta.$$

This is also equivalent to

$$\int_0^1 x_1(\zeta)\frac{dx_1}{d\zeta}(\zeta)d\zeta = \frac{\left[x_1^2(\zeta)\right]_0^1}{2}.$$

(c) We introduce the notation

$$\int_0^1 \gamma x_1^2(\zeta)d\zeta = k_2^2.$$

Combining (a), (b) and (c), we have

$$\begin{aligned}
\langle (Ax)_1, x_1\rangle &= -\beta_1^2\left(\frac{dx_1}{d\zeta}(0)\right)^2 - k_1^2 - \frac{\left[x_1^2(\zeta)\right]_0^1}{2} - k_2^2 \\
&= -\beta_1^2\left(\frac{dx_1}{d\zeta}(0)\right)^2 - k_1^2 - \frac{x_1^2(1)}{2} + \frac{x_1^2(0)}{2} - k_2^2 \\
&\overset{(2.10)}{=} -\beta_1^2\left(\frac{dx_1}{d\zeta}(0)\right)^2 - k_1^2 - \frac{x_1^2(1)}{2} + \frac{1}{2}\beta_1^2\left(\frac{dx_1(0)}{d\zeta}\right)^2 - k_2^2 \\
&= -\beta_1^2\frac{1}{2}\left(\frac{dx_1}{d\zeta}(0)\right)^2 - k_1^2 - \frac{x_1^2(1)}{2} - k_2^2 \leq 0.
\end{aligned}$$

The same result holds for $\langle (Ax)_2, x_2\rangle$, see Appendix A. Hence, the operator A is dissipative. ■

Proposition 2. *Considering the operator A defined by (2.9) and (2.10), we have* $Im(I-A)=H$, *where I is the identity operator on* $H=L^2(0,1)\times L^2(0,1)$.

Proof. To get the surjectivity of $I-A$, we will show that $Im(I-A)\subset H$ and $Im(I-A)\supset H$.

We start by the first inclusion, $Im(I-A)\subset H$, which is directly deducted from (2.10).

Considering the second one, $Im(I-A)\supset H$, it is equivalent to the fact that for all $y\in H$ there exists $x\in D(A)$ such that $(I-A)x=y$ holds. Let us consider $y=\begin{pmatrix}y_1 & y_2\end{pmatrix}^T$ in H. In what follows, we will find explicitly a vector $x=\begin{pmatrix}x_1 & x_2\end{pmatrix}^T$ in $D(A)$ which satisfies $(I-A)x=y$. Developing $(I-A)x=y$, we have

$$\begin{aligned}(I-A)x=y &\Leftrightarrow \left(\begin{pmatrix}I & 0\\ 0 & I\end{pmatrix}-\begin{pmatrix}\beta_1\frac{d^2}{d\zeta^2}-\frac{d}{d\zeta}-\gamma I & 0\\ 0 & \beta_2\frac{d^2}{d\zeta^2}-\frac{d}{d\zeta}\end{pmatrix}\right)\begin{pmatrix}x_1\\ x_2\end{pmatrix}=\begin{pmatrix}y_1\\ y_2\end{pmatrix}\\ &\Leftrightarrow \begin{pmatrix}-\beta_1\frac{d^2}{d\zeta^2}+\frac{d}{d\zeta}+(\gamma+1)I & 0\\ 0 & -\beta_2\frac{d^2}{d\zeta^2}+\frac{d}{d\zeta}+I\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}=\begin{pmatrix}y_1\\ y_2\end{pmatrix}\\ &\Leftrightarrow \begin{cases}-\beta_1\frac{d^2x_1}{d\zeta^2}+\frac{dx_1}{d\zeta}+(\gamma+1)x_1=y_1\\ -\beta_2\frac{d^2x_2}{d\zeta^2}+\frac{dx_2}{d\zeta}+x_2=y_2.\end{cases}\end{aligned}$$

Each of the two equations above can be treated separately, because of the fact that they do not depend on each other. Looking at the first one,

$$-\beta_1\frac{d^2x_1}{d\zeta^2}+\frac{dx_1}{d\zeta}+(\gamma+1)x_1=y_1, \tag{2.17}$$

which is a second order ODE, putting $u=\frac{dx_1}{d\zeta}$ and $v=x_1$, we have

$$\begin{cases}\frac{du}{d\zeta}=\frac{1}{\beta_1}u+\frac{\gamma+1}{\beta_1}v-\frac{1}{\beta_1}y_1\\ \frac{dv}{d\zeta}=u.\end{cases}$$

Rewriting previous system in a matrix form yields

$$\frac{d}{d\zeta}\begin{pmatrix}u\\ v\end{pmatrix}=\begin{pmatrix}\frac{1}{\beta_1} & \frac{\gamma+1}{\beta_1}\\ 1 & 0\end{pmatrix}\begin{pmatrix}u\\ v\end{pmatrix}+\begin{pmatrix}-\frac{1}{\beta_1}\\ 0\end{pmatrix}y_1. \tag{2.18}$$

To express analytically the solution of such systems, an analogy is made with systems of the form

$$\begin{cases}\frac{dx}{d\zeta}=Ax+Bu,\\ x(0)=x_0\end{cases} \tag{2.19}$$

where x represents a state vector (whose dimension is n) depending on the spatial variable ζ, A is a n dimensional matrix, B is a vector of length n and u a function depending on ζ. The solution of (2.19) is

given by

$$x(\zeta) = \exp(A\zeta)x_0 + \int_0^{\zeta} \exp(A(\zeta - z))Bu(z)dz,$$

see (Winkin, 2017, Chapter 2, page 45). To use (2.19) in the case of (2.18), we denote A_1 the matrix

$$\begin{pmatrix} \frac{1}{\beta_1} & \frac{\gamma+1}{\beta_1} \\ 1 & 0 \end{pmatrix}$$

and B_1 the vector $\begin{pmatrix} -\frac{1}{\beta_1} & 0 \end{pmatrix}^T$. In this way,

$$\begin{pmatrix} u(\zeta) \\ v(\zeta) \end{pmatrix} = \exp(A_1\,\zeta) \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \int_0^{\zeta} \exp(A_1\,(\zeta - z))B_1 y_1(z)dz. \tag{2.20}$$

Note that the state vector x from (2.19) is $\begin{pmatrix} u & v \end{pmatrix}^T$ in our particular case. We still have to put the boundary conditions, given by (2.10), in the solution. The condition on the state and its first order derivative for $\zeta = 0$ is expressed as

$$\beta_1 u_0 = v_0. \tag{2.21}$$

In order to use the other boundary condition, we first evaluate (2.20) in $\zeta = 1$, which gives

$$\begin{pmatrix} u(1) \\ v(1) \end{pmatrix} = \exp(A_1) \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \int_0^{1} \exp(A_1(1 - z))B_1 y_1(z)dz. \tag{2.22}$$

For a sake of readability, we denote by $w_1 = \begin{pmatrix} w_{11} & w_{12} \end{pmatrix}^T$ the vector

$$\int_0^{1} \exp(A_1(1 - z))B_1 y_1(z)dz.$$

Furthermore, the matrix $\exp(A_1)$ is noted

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}.$$

With the introduced notations, (2.22) becomes

$$\begin{pmatrix} u(1) \\ v(1) \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \begin{pmatrix} w_{11} \\ w_{12} \end{pmatrix}.$$

Using the boundary condition for $\zeta = 1$, we have

$$0 = a_{11}u_0 + a_{12}v_0 + w_{11}. \tag{2.23}$$

Keeping together equations (2.21) and (2.23), we have a system of two equations with two unknowns in

the variables u_0 et v_0, which is given by

$$\begin{cases} \beta_1 u_0 - v_0 = 0, \\ a_{11}u_0 + a_{12}v_0 + w_{11} = 0 \end{cases}$$

and whose solution is

$$\begin{cases} u_0 = -\frac{w_{11}}{a_{11}+a_{12}\beta_1}, \\ v_0 = -\frac{\beta_1 w_{11}}{a_{11}+a_{12}\beta_1}. \end{cases}$$

We are only interested in the second component of $\begin{pmatrix} u & v \end{pmatrix}^T$, the latter representing the first component of the state $x = \begin{pmatrix} x_1 & x_2 \end{pmatrix}^T$. With all the above, we have

$$v(\zeta) = x_1(\zeta) = -M_{\zeta 21}\frac{w_{11}}{a_{11}+a_{12}\beta_1} - M_{\zeta 22}\frac{\beta_1 w_{11}}{a_{11}+a_{12}\beta_1} + \mathcal{W}(\zeta)_{12} \tag{2.24}$$

where

$$\exp(A_1\zeta) = \begin{pmatrix} M_{\zeta 11} & M_{\zeta 12} \\ M_{\zeta 21} & M_{\zeta 22} \end{pmatrix}$$

and

$$\int_0^\zeta \exp(A_1(\zeta - z))B_1 y_1(z)dz = \begin{pmatrix} \mathcal{W}(\zeta)_{11} \\ \mathcal{W}(\zeta)_{12} \end{pmatrix}.$$

We now take a look at the equation

$$-\beta_2\frac{d^2x_2}{d\zeta^2} + \frac{dx_2}{d\zeta} + x_2 = y_2.$$

We will hold a similar reasoning to the previous one used for (2.17). Therefore, let $u = \frac{dx_2}{d\zeta}$ and $v = x_2$. The ODE takes the form of the following system

$$\frac{d}{d\zeta}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \frac{1}{\beta_2} & \frac{1}{\beta_2} \\ 1 & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} -\frac{1}{\beta_2} \\ 0 \end{pmatrix} y_2.$$

Denoting by A_2 the matrix

$$\begin{pmatrix} \frac{1}{\beta_2} & \frac{1}{\beta_2} \\ 1 & 0 \end{pmatrix}$$

and B_2 the vector $\begin{pmatrix} -\frac{1}{\beta_2} & 0 \end{pmatrix}^T$, we have

$$\begin{pmatrix} u(\zeta) \\ v(\zeta) \end{pmatrix} = \exp(A_2\zeta)\begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \int_0^\zeta \exp(A_2(\zeta - z))B_2 y_2(z)dz,$$

where (Winkin, 2017, Chapter 2, page 45) is used again. To find $\begin{pmatrix} u_0 & v_0 \end{pmatrix}^T$, (2.10) is used. For the boundary condition in $\zeta = 0$, we have

$$\beta_2 u_0 = v_0. \tag{2.25}$$

Developing the other condition, for $\zeta = 1$, one gets

$$\begin{pmatrix} u(1) \\ v(1) \end{pmatrix} = \exp(A_2) \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \int_0^1 \exp(A_2(1-z))B_2 y_2(z)dz.$$

We denote by $\exp(A_2)$ the matrix

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

and by $w_2 = \begin{pmatrix} w_{21} & w_{22} \end{pmatrix}^T$ the vector

$$\int_0^1 \exp(A_2(1-z))B_2 y_2(z)dz.$$

In this way, we have the following

$$\begin{pmatrix} u(1) \\ v(1) \end{pmatrix} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \begin{pmatrix} w_{21} \\ w_{22} \end{pmatrix}.$$

By exploiting the fact that $u(1) = 0$, we obtain

$$0 = b_{11}u_0 + b_{12}v_0 + w_{21}. \tag{2.26}$$

By bringing together equations (2.25) and (2.26), we have the system

$$\begin{cases} \beta_2 u_0 - v_0 = 0, \\ b_{11}u_0 + b_{12}v_0 + w_{21} = 0, \end{cases}$$

whose solution is given by

$$\begin{cases} u_0 = -\frac{w_{21}}{b_{11}+b_{12}\beta_2}, \\ v_0 = -\frac{\beta_2 w_{21}}{b_{11}+b_{12}\beta_2}. \end{cases}$$

By gathering all the elements, there holds

$$v(\zeta) = x_2(\zeta) = -N_{\zeta 21}\frac{w_{21}}{b_{11}+b_{12}\beta_2} - N_{\zeta 22}\frac{\beta_2 w_{21}}{b_{11}+b_{12}\beta_2} + \mathcal{W}(\zeta)_{22} \tag{2.27}$$

where

$$\exp(A_2\zeta) = \begin{pmatrix} N_{\zeta 11} & N_{\zeta 12} \\ N_{\zeta 21} & N_{\zeta 22} \end{pmatrix}$$

and

$$\int_0^\zeta \exp(A_2(\zeta - z))B_2 y_2(z)dz = \begin{pmatrix} \mathcal{W}(\zeta)_{21} \\ \mathcal{W}(\zeta)_{22} \end{pmatrix}.$$

Using (2.24) and (2.27), the whole state trajectory $x = \begin{pmatrix} x_1 & x_2 \end{pmatrix}^T$ is given by

$$x(\zeta) = \begin{pmatrix} x_1(\zeta) \\ x_2(\zeta) \end{pmatrix} = \begin{pmatrix} -M_{\zeta_{21}} \frac{w_{11}}{a_{11}+a_{12}\beta_1} - M_{\zeta_{22}} \frac{\beta_1 w_{11}}{a_{11}+a_{12}\beta_1} + \mathcal{W}(\zeta)_{12} \\ -N_{\zeta_{21}} \frac{w_{21}}{b_{11}+b_{12}\beta_2} - N_{\zeta_{22}} \frac{\beta_2 w_{21}}{b_{11}+b_{12}\beta_2} + \mathcal{W}(\zeta)_{22} \end{pmatrix}.$$

Thus, the vector x has been found in an explicit way. Moreover, this vector is in $D(A)$. We conclude that $H \subset \mathrm{Im}(I-A)$.

So, the relation $\mathrm{Im}(I-A) = H$ holds. ■

Keeping Propositions 1 and 2 in mind, the following result is stated.

Proposition 3. *The operator A defined by (2.9) and (2.10) is the infinitesimal generator of a contraction semigroup on $D(A)$.*

Proof. Lumer-Phillips theorem is used in order to prove this proposition, see (Jacob and Zwart, 2012, Theorem 6.1.7.). The result follows directly by Propositions 1 and 2. ■

2.3.2 Nonlinear operator

In this subsection, we will analyze the nonlinear operator (2.11), which is given by

$$N(x) = \begin{pmatrix} \alpha\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}} & \alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}} \end{pmatrix}^T$$

for $x = (x_1\ x_2)^T$ in the domain

$$D := \{x \in H | -1 \leq x_1(\zeta), 0 \leq x_2(\zeta) \leq 1, \text{ for a.e. } \zeta \in [0,1]\}.$$

The aim is to prove that the sum of the linear operator A defined by (2.9) and (2.10) and the nonlinear one is the infinitesimal generator of a nonlinear semigroup on D. Therefore, we will use a theorem described and proved in (Laabissi et al., 2001). In order to understand this theorem, the following definition is presented.

Definition 7. *Let D be a subset of the Hilbert space $H = L^2(0,1) \times L^2(0,1)$. For each $y \in H$, the distance between the vector y and the subset D, noted $d(y;D)$ is defined as*

$$d(y;D) = \inf_{x \in D} d(x,y)$$

where $d(x,y)$ is the distance induced by the norm in H, i.e. $d(x,y) = \|x-y\|_{L^2(0,1)\times L^2(0,1)}$.

Denoting by $(T(t))_{t\geq 0}$ the linear semigroup generated by operator A, the following result is introduced.

Theorem 2. *Let*

- *D be $T(t)-$invariant, i.e $T(t)D \subset D$ for each $t \geq 0$*
- *For each x in D,*
$$\lim_{h\to 0^+} \frac{1}{h} d\left(x+hN(x);D\right) = 0$$
- *N is a continuous function on D and there exists $l_N \in [0,+\infty)$ such that $(N - l_N I)$ is dissipative on D.*

Then, equation (2.2) possesses a « mild solution » $x(t,x_0)$ on $[0,+\infty)$ for each x_0 in D. Furthermore if $S(t)$ is defined on D for each $t \neq 0$ and for each $x_0 \in D$ by $S(t)x_0 = x(t,x_0)$, it is a nonlinear semigroup on D whose $A+N$ is the infinitesimal generator.

The proof of this theorem is not recalled. However, we note that it provides us the well-posedness of the model under considerations, which is quite an important step in the dynamical analysis. In this way, problems like asymptotic stability, exponential stability, ... can be considered. Before we start with these kinds of questions, we introduce in the next section the *port-Hamiltonian formalism*, which provides easier results to study the well-posedness or the stability of a system and which is interesting from a physical point of view.

2.4 port-Hamiltonian formalism

In this section, the general class of port-Hamiltonian systems is first introduced. The well-posedness for this class of systems is recalled. Then, port-Hamiltonian systems with dissipation are addressed by showing that the system under study fits this class.

2.4.1 First order port-Hamiltonian systems

The equation (PDE) describing a first order port-Hamiltonian system is

$$\frac{\partial x}{\partial t}(\zeta,t) = P_1 \frac{\partial}{\partial \zeta}\left(\mathcal{H}(\zeta)x(\zeta,t)\right) + P_0 \mathcal{H}(\zeta)x(\zeta,t) \tag{2.28}$$

where $P_1 \in \mathbb{R}^{n\times n}$ is invertible and symmetric, i.e. $P_1^T = P_1$, $P_0 \in \mathbb{R}^{n\times n}$ is skew-symmetric, i.e. $P_0^T = -P_0$ and $\mathcal{H} \in L^\infty\left([a,b];\mathbb{R}^{n\times n}\right)$ is symmetric and satisfies $mI \leq \mathcal{H}(\zeta) \leq MI$ for a.e. $\zeta \in [a,b]$, for some $m,M > 0$, see also (Jacob and Zwart, 2012, Definition 7.2.1.). The Hilbert space $\mathcal{X} = L^2\left([a,b];\mathbb{R}^n\right)$ is equipped with the inner product

$$\langle f,g\rangle_{\mathcal{X}} = \int_a^b g(\zeta)^* \mathcal{H}(\zeta) f(\zeta) d\zeta. \tag{2.29}$$

The corresponding Hamiltonian to (2.28), or equivalently the energy, $E : [0,\infty) \to \mathbb{R}$, is given by

$$E(t) = \frac{1}{2}\langle x,x\rangle_{\mathcal{X}}, \tag{2.30}$$

see (Jacob and Zwart, 2012, Definition 7.2.1.). To the PDE (2.28), we associate some controlled and homogeneous boundary conditions, formulated in term of the boundary effort, noted e_∂ and the boundary flow, noted f_∂, given by

$$u(t) = W_{B,1}\begin{bmatrix} f_\partial \\ e_\partial \end{bmatrix}, \; 0 = W_{B,2}\begin{bmatrix} f_\partial \\ e_\partial \end{bmatrix} \tag{2.31}$$

where $e_\partial = \frac{1}{\sqrt{2}}\left(\mathcal{H}x(b) + (\mathcal{H}x)(a)\right)$ and $f_\partial = \frac{1}{\sqrt{2}}\left(P_1\mathcal{H}x(b) - P_1(\mathcal{H}x)(a)\right)$, see (Jacob and Zwart, 2012, Section 7.2) and where $W_B = \begin{bmatrix} W_{B,1} \\ W_{B,2} \end{bmatrix} \in \mathbb{R}^{n\times 2n}$. We write the homogeneous (uncontrolled) PDE (2.28) as an abstract ODE, which is given by

$$\frac{dx}{dt}(t) = P_1\frac{d}{d\zeta}\left(\mathcal{H}x(t)\right) + P_0\left(\mathcal{H}x(t)\right) \tag{2.32}$$

and which holds pointwise in t. Hence, we can define the operator

$$Ax := P_1\frac{d}{d\zeta}\left(\mathcal{H}x\right) + P_0\left(\mathcal{H}x\right) \tag{2.33}$$

on the domain

$$D(A) = \left\{ x \in \mathcal{X} \,|\, \mathcal{H}x \in H^1\left([a,b];\mathbb{R}^n\right), \begin{bmatrix} f_\partial \\ e_\partial \end{bmatrix} \in \mathrm{Ker}\left(W_B\right) \right\} \tag{2.34}$$

where $H^1\left([a,b];\mathbb{R}^n\right)$ denotes the Sobolev space defined by

$$H^1\left([a,b];\mathbb{R}^n\right) = \left\{ f \in L^2\left([a,b];\mathbb{R}^n\right) | f \text{ a.c.}, \frac{df}{d\zeta} \in L^2\left([a,b];\mathbb{R}^n\right) \right\}. \tag{2.35}$$

2.4.2 Well-posedness

This subsection is dedicated to the presentation of a theorem from (Jacob and Zwart, 2012, Theorem 7.2.4.) which provides conditions so that the operator A defined by (2.33) and (2.34) is the generator of a contraction semigroup on $\mathcal{X}$. In this way, one has the following result,

Theorem 3. *Consider operator A defined by (2.33) and (2.34) associated to (2.28). Moreover, the matrix W_B introduced in the previous section is an $n \times 2n$ matrix of rank n. Then the following statements are equivalent.*

- *A is the infinitesimal generator of a contraction semigroup on $\mathcal{X}$.*
- *$\mathfrak{Re}\left\langle Ax, x\right\rangle_{\mathcal{X}} \leq 0$ for every $x \in D(A)$.*
- *$W_B\Sigma W_B^* \geq 0$. where $\Sigma = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \in \mathbb{R}^{2n\times 2n}$.*

Notice that by the last condition, the generation of a contraction semigroup is reduced to the product of three matrices, which is quite easy to compute. It is precisly that condition that we will use in order to

prove that the linear part of the model under study generates a contraction semigroup. We shall introduce now the dissipative port-Hamiltonian systems which are essential in our case, in order to model the diffusion part of our PDEs.

2.4.3 Dissipative port-Hamiltonian systems

Considering the general PDE describing a first order port-Hamiltonian system, see (2.28), the addition of a dissipation term results in the PDE

$$\frac{\partial x}{\partial t}(\zeta,t) = (A - \mathcal{G}_R S \mathcal{G}_R^\star)(\mathcal{H}x)(\zeta,t), \tag{2.36}$$

where the operator A is defined by (2.33) and (2.34) and where

$$\mathcal{G}_R f = G_1 \frac{\partial f}{\partial \zeta} + G_0 f, \mathcal{G}_R^\star x = -G_1^T \frac{\partial x}{\partial \zeta} + G_0^T x, \tag{2.37}$$

see (Zwart and Jacob, 2009, Section 7.2). The operator $\mathcal{G}_R^\star$ is known as the formal adjoint operator of $\mathcal{G}_R$. Moreover, we assume that $G_0, G_1 \in \mathbb{R}^{n\times r}$, $S \in L^\infty([a,b];\mathbb{R}^{r\times r})$ is symmetric and satisfies $m_1 I \leq S(\zeta) \leq M_1 I$ for some constants $m_1, M_1 > 0$.

2.4.4 The nonisothermal tubular reactor as a dissipative port-Hamiltonian system

In a first time, we just recall the linear part of the system we study, which is a system of uncoupled second order PDEs. The diffusion part (second order derivative of the state) is then modeled as a dissipation term, see (Zwart and Jacob, 2009, Chapter 7). An extended model will be constructed to retrieve the form of a first order port-Hamiltonian system, see (2.28). Notice that the time variable is denoted by t.

Considering only the linear part of (2.3) with the associated boundary conditions, it yields

$$\begin{cases} \frac{\partial T}{\partial t} = \frac{1}{Pe_h}\frac{\partial^2 T}{\partial \zeta^2} - \frac{\partial T}{\partial \zeta} - \gamma T \\ \frac{\partial C}{\partial t} = \frac{1}{Pe_m}\frac{\partial^2 C}{\partial \zeta^2} - \frac{\partial C}{\partial \zeta} \\ \frac{\partial T}{\partial \zeta}(t,0) = Pe_h\left(T(t,0) - T_{in}\right), \frac{\partial C}{\partial \zeta}(t,0) = Pe_m\left(C(t,0) - C_{in}\right) \\ \frac{\partial T}{\partial \zeta}(t,1) = 0 = \frac{\partial C}{\partial \zeta}(t,1) = 0. \end{cases} \tag{2.38}$$

Due to the fact that the PDEs are uncoupled, we will distinguish the variables T and C to show that this system fits the dissipative port-Hamiltonian formalism. We shall separetaly work on

$$\begin{cases} \frac{\partial T}{\partial t} = \frac{1}{Pe_h}\frac{\partial^2 T}{\partial \zeta^2} - \frac{\partial T}{\partial \zeta} - \gamma T \\ \frac{1}{Pe_h}\frac{\partial T}{\partial \zeta}(t,0) = T(t,0) - T_{in} \\ \frac{\partial T}{\partial \zeta}(t,1) = 0 \end{cases} \quad \text{and} \quad \begin{cases} \frac{\partial C}{\partial t} = \frac{1}{Pe_m}\frac{\partial^2 C}{\partial \zeta^2} - \frac{\partial C}{\partial \zeta} \\ \frac{1}{Pe_m}\frac{\partial C}{\partial \zeta}(t,0) = C(t,0) - C_{in} \\ \frac{\partial C}{\partial \zeta}(t,1) = 0. \end{cases} \tag{2.39}$$

- **First system without dissipation**
  By posing $x(t,\zeta) = T(t,\zeta), P_1 = -1, P_0 = 0, \mathcal{H}(\zeta) = 1$, the first system of (2.39) without the second order derivative term and without the term $-\gamma T$ has exactly the same form as (2.28) and

describes a first order port-Hamiltonian system, i.e.

$$\frac{\partial T}{\partial t} = -\frac{\partial T}{\partial \zeta} \tag{2.40}$$

describes a first order port-Hamiltonian system.

- **First system with dissipation**

The remaining term, $\frac{1}{Pe_h}\frac{\partial^2 T}{\partial \zeta^2} - \gamma T$, is modeled as a dissipative term, i.e.

$$-\mathcal{G}_R S \mathcal{G}_R^\star = \frac{1}{Pe_h}\frac{d^2}{d\zeta^2} - \gamma I. \tag{2.41}$$

By posing $S = \begin{bmatrix} \frac{1}{Pe_h} & 0 \\ 0 & \gamma \end{bmatrix}, G_0 = \begin{bmatrix} 0 & 1 \end{bmatrix}, G_1 = \begin{bmatrix} 1 & 0 \end{bmatrix}$, one has $\mathcal{G}_R = \begin{bmatrix} \frac{d}{d\zeta} & I \end{bmatrix}$ and $\mathcal{G}_R^\star = \begin{bmatrix} -\frac{d}{d\zeta} \\ I \end{bmatrix}$. Hence, equation (2.41) is satisfied and

$$\frac{\partial x}{\partial t}(t,\zeta) = \left(\mathcal{J}_1 - \mathcal{G}_R S \mathcal{G}_R^\star\right)(\mathcal{H}x)(t,\zeta) \tag{2.42}$$

where operator $\mathcal{J}_1$ is defined by $\mathcal{J}_1 x = -\frac{\partial x}{\partial \zeta}$. To prove that the operator $\mathcal{J}_1 - \mathcal{G}_R S \mathcal{G}_R^\star$ is the infinitesimal generator of a contraction semigroup, one has to rewrite the dissipative port-Hamiltonian system (2.42) as an extended port-Hamiltonian system. By (Zwart and Jacob, 2009, Lemma 7.2.6.), the operator $\mathcal{J}_1 - \mathcal{G}_R S \mathcal{G}_R^\star$ can be seen as the mapping $\mathcal{J}_e$ together with the closure relation $e_p = S f_p$ where $\mathcal{J}_e$ is defined by

$$\mathcal{J}_e \begin{pmatrix} e_1 \\ e_p \end{pmatrix} = \begin{pmatrix} P_1 & G_1 \\ G_1^T & 0 \end{pmatrix} \frac{\partial}{\partial \zeta} \begin{pmatrix} e_1 \\ e_p \end{pmatrix} + \begin{pmatrix} P_0 & G_0 \\ -G_0^T & 0 \end{pmatrix} \begin{pmatrix} e_1 \\ e_p \end{pmatrix} \tag{2.43}$$

where e_1 can be seen as the initial variables and e_p as the extended variables. From equation (2.43), we define new matrices $P_{1,\text{ext}}$ and $P_{0,\text{ext}}$ by

$$\begin{pmatrix} P_1 & G_1 \\ G_1^T & 0 \end{pmatrix} \text{ and } \begin{pmatrix} P_0 & G_0 \\ -G_0^T & 0 \end{pmatrix} \tag{2.44}$$

respectively. We can observe that equation (2.43) fits exactly equation (2.28) and also the related assumptions. In this way, by (Zwart and Jacob, 2009, page 111), one can define the extended Hilbert space $\mathcal{X}_{\text{ext}} = L^2([0,1];\mathbb{R}^{n+r})$ where $n = 1$ and $r = 2$ in this case. By using the closure relation $e_p = S f_p$ and the mapping $\mathcal{J}_e$ defined by (2.43), the extended variable, noted x_p, is $S\left(G_1^T \frac{\partial}{\partial \zeta} e_1 - G_0^T e_1\right)$, or equivalently $\begin{bmatrix} \frac{1}{Pe_h}\frac{\partial T}{\partial \zeta} \\ -\gamma T \end{bmatrix}$. By (Zwart and Jacob, 2009, page 111), we equip the space $\mathcal{X}_{\text{ext}}$ with the inner product

$$\left\langle \begin{pmatrix} x \\ x_p \end{pmatrix}, \begin{pmatrix} z \\ z_p \end{pmatrix} \right\rangle_{\mathcal{X}_{\text{ext}}} = \int_0^1 x(\zeta)^T \mathcal{H}(\zeta) z(\zeta) d\zeta + \int_0^1 x_p(\zeta)^T z_p(\zeta) d\zeta. \tag{2.45}$$

The associated extended boundary effort and boundary flow are given by

$$\begin{pmatrix} f_{\partial,\mathcal{H}x,x_p} \\ e_{\partial,\mathcal{H}x,x_p} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} P_{1,\text{ext}} & -P_{1,\text{ext}} \\ I_{n+r} & I_{n+r} \end{pmatrix} \begin{pmatrix} (\mathcal{H}x)(1) \\ x_p(1) \\ (\mathcal{H}x)(0) \\ x_p(0) \end{pmatrix}. \tag{2.46}$$

Using all the matrices introduced before, the extended boundary flow and effort are given by

$$\begin{aligned} \begin{pmatrix} f_{\partial,\mathcal{H}x,x_p} \\ e_{\partial,\mathcal{H}x,x_p} \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1 & 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} T(1) \\ \frac{1}{Pe_h}\frac{dT}{d\zeta}(1) \\ -\gamma T(1) \\ T(0) \\ \frac{1}{Pe_h}\frac{dT}{d\zeta}(0) \\ -\gamma T(0) \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} -(T(1)-T(0)) + \frac{1}{Pe_h}\left(\frac{dT}{d\zeta}(1) - \frac{dT}{d\zeta}(0)\right) \\ T(1)-T(0) \\ 0 \\ T(1)+T(0) \\ \frac{1}{Pe_h}\left(\frac{dT}{d\zeta}(1) + \frac{dT}{d\zeta}(0)\right) \\ -\gamma(T(1)+T(0)) \end{pmatrix}. \end{aligned} \tag{2.47}$$

It remains to compute the matrix W_B satisfying

$$\begin{bmatrix} u(t) \\ 0 \\ 0 \end{bmatrix} = W_B \begin{bmatrix} f_{\partial,\mathcal{H}x,x_p} \\ e_{\partial,\mathcal{H}x,x_p} \end{bmatrix}, \tag{2.48}$$

where $f_{\partial,\mathcal{H}x,x_p}$ and $e_{\partial,\mathcal{H}x,x_p}$ are expressed by (2.47) and where the boundary control $u(t)$ is given by $-T_{in}(t)$. In this way, the matrix W_B is given by

$$W_B = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 0 & \gamma & -1 & 1 & 0 \\ 1 & 1 & -\gamma & 0 & 1 & 0 \\ 0 & 0 & 1 & \gamma & 0 & 1 \end{bmatrix}. \tag{2.49}$$

We have now all the elements to write the first system of (2.39) as an extended dissipative port-Hamiltonian system. Therefore, let us define the operator A_{ext} by

$$A_{\text{ext}} \begin{pmatrix} x \\ x_p \end{pmatrix} = P_{1,\text{ext}} \frac{\partial}{\partial \zeta} \begin{pmatrix} (\mathcal{H}x) \\ x_p \end{pmatrix} + P_{0,\text{ext}} \begin{pmatrix} (\mathcal{H}x) \\ x_p \end{pmatrix} \tag{2.50}$$

on the domain

$$D(A_{\text{ext}}) = \left\{ \begin{pmatrix} x \\ x_p \end{pmatrix} \in \mathcal{X}_{\text{ext}} | \begin{pmatrix} \mathcal{H}x \\ x \end{pmatrix} \in H^1\left([0,1];\mathbb{R}^3\right), W_B \begin{bmatrix} f_{\partial,\mathcal{H}x,x_p} \\ e_{\partial,\mathcal{H}x,x_p} \end{bmatrix} = \begin{bmatrix} u(t) \\ 0 \\ 0 \end{bmatrix} \right\} \tag{2.51}$$

such that

$$\frac{\partial}{\partial t} \begin{pmatrix} x \\ x_p \end{pmatrix} = A_{\text{ext}} \begin{pmatrix} x \\ x_p \end{pmatrix}. \tag{2.52}$$

The last step consists in showing that the operator A_{ext} is the infinitesimal generator of a contraction semigroup on $D(A_{\text{ext}})$. Therefore, we recall a theorem which provides a condition similar as in Theorem 3, see (Zwart and Jacob, 2009, Theorem 7.2.8.).

Theorem 4. *The operator A_{ext} defined by (2.50) and (2.51) generates a contraction semigroup on $\mathcal{X}_{ext}$ if and only if $W_B \Sigma W_B^T \geq 0$.*

Computing the matrix $W_B \Sigma W_B^T$, one finds

$$W_B \Sigma W_B^T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

which is a positive definite matrix. Hence, operator A_{ext} generates a contraction semigroup on $\mathcal{X}_{\text{ext}}$.

All the process will not be repeated for the second system of (2.39) but is quite similar. In fact, it can be proven in a same way that the second system of (2.39) fits the extended dissipative port-Hamiltonian formalism. In this case, it can also be shown that the extended operator A_{ext} for the second system of (2.39) generates a contraction semigroup on the extended Hilbert space $L^2\left([0,1];\mathbb{R}^2\right)$ using Theorem 4.

In conclusion, one can remark that checking the generation of a contraction semigroup is quite easier with the port-Hamiltonian formalism than by using Lumer-Phillips theorem. However, showing that the model fits the port-Hamiltonian formalism, and moreover the dissipative port-Hamiltonian formalism, is not necessarily obvious.

Chapter 3

Stability analysis

Contents

An important part of this chapter is dedicated to the analysis of the stability of the semigroup whose infinitesimal generator is the operator A defined by (2.9) and (2.10), and especially the exponential stability. In this way, the notion of Sturm-Liouville and Riesz-spectral operators will be introduced. In particular, it is shown that the opposite of the linear operator A is a Sturm-Liouville operator and in this case, by (Delattre et al., 2003), it is a Riesz-Spectral operator. Thus, the exponential stability can be addressed by an eigenvalue problem. In our case, it is shown that the linear operator A is exponentially stable. The eigenvalues and the eigenvectors of this operator will be computed explicitly and the resolvent equations are presented. After the stability analysis, we will take a look at the resolvent operator of the operator A and also at the corresponding resolvent set. An explicit form of the resolvent operator will be given from a Riesz-Spectral point a view. For the *classical* expression, the reader is referred to the Appendix B.

3.1 Exponential stability

We start this section by defining the concept of exponential stability of a semigroup, see (Jacob and Zwart, 2012, Definition 8.1.1).

Definition 8. *The semigroup $(T(t))_{t\geq 0}$ on the Hilbert space H is said to be exponentially stable if there exist positive constants M and α such that*

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

Notice that this definition is not the only one. There exist also some others characterizations of the exponential stability we do not recall here. As said in the introduction of this chapter, the concept of Riesz-Spectral operators is used in order to prove exponential stability. We need therefore two concepts : *Riesz-Spectral basis* and *Riesz-Spectral operator*, see (Curtain and Zwart, 1995, Definition 2.3.1.) and (Curtain and Zwart, 1995, Definition 2.3.4.) respectively.

Definition 9. *A set of vectors $\{\phi_n, n \geq 1\}$ in a Hilbert space H forms a Riesz basis if*

- $\overline{span}_{n\geq 1}\{\phi_n\} = H$
- *There exist positive constants m and M such that for an arbitrary N in $\mathbb{N}$ and for arbitrary scalars $\alpha_n, n = 1, \ldots, N$ one has*

$$m\sum_{n=1}^{N}|\alpha_n|^2 \leq \left\|\sum_{n=1}^{N}\alpha_n\phi_n\right\|^2 \leq M\sum_{n=1}^{N}|\alpha_n|^2.$$

Definition 10. *Let A be a closed, linear operator on a Hilbert space H. Let $\{\lambda_n, n \geq 1\}$ be the set of eigenvalues of A. Suppose that the corresponding eigenvectors $\{\phi_n, n \geq 1\}$ form a Riesz basis in H. If the closure of $\{\lambda_n, n \geq 1\}$ is disconnected, i.e for all a, b in $\overline{\{\lambda_n, n \geq 1\}}$, $[a,b]$ is not included in $\overline{\{\lambda_n, n \geq 1\}}$, then A is called a Riesz-Spectral operator.*

The following step consists of showing that A is a Riesz-Spectral operator. We will use therefore (Delattre et al., 2003, Lemma 1), which states that if the opposite of an operator is a Sturm-Liouville operator with appropriate boundary conditions, then it is a Riesz-Spectral operator. In order to apply this result, we decompose the operator A as

$$A = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} \tag{3.1}$$

where A_1 et A_2 are operators defined respectively by $\beta_1 \frac{d^2}{d\zeta^2} - \frac{d}{d\zeta} - \gamma I$ and $\beta_2 \frac{d^2}{d\zeta^2} - \frac{d}{d\zeta}$ on

$$D(A_1) = \left\{ x \in L^2(0,1) | x \text{ a.c.}, \frac{dx}{d\zeta} \in L^2(0,1) \text{ a.c.}, \frac{d^2x}{d\zeta^2} \in L^2(0,1), \beta_1 \frac{dx}{d\zeta}(0) = x(0), \frac{dx}{d\zeta}(1) = 0 \right\} \tag{3.2}$$

and

$$D(A_2) = \left\{ x \in L^2(0,1) | x \text{ a.c.}, \frac{dx}{d\zeta} \in L^2(0,1) \text{ a.c.}, \frac{d^2x}{d\zeta^2} \in L^2(0,1), \beta_2 \frac{dx}{d\zeta}(0) = x(0), \frac{dx}{d\zeta}(1) = 0 \right\}. \tag{3.3}$$

Theorem 5. *The opposites of operators A_1 and A_2 are Sturm-Liouville operators.*

Proof. By (Delattre et al., 2003), operator A_1 is a Sturm-Liouville operator if

$$\forall x \in D(A_1), -A_1 x = \frac{1}{\rho(\zeta)} \left(\frac{d}{d\zeta} \left(-p(\zeta) \frac{dx}{d\zeta}(\zeta) \right) + q(\zeta) x(\zeta) \right), \tag{3.4}$$

where $p, dp/d\zeta, q$ and ρ are real continuous functions such that $\rho > 0$ and $p > 0$. Considering

$$\rho(\zeta) = \exp\left(-\frac{1}{\beta_1} \zeta \right), p(\zeta) = \beta_1 \rho(\zeta), q(\zeta) = \gamma \rho(\zeta),$$

we find that (3.4) is satisfied. A similar argument can be formulated for the operator A_2 taking

$$\rho(\zeta) = \exp\left(-\frac{1}{\beta_2} \zeta \right), p(\zeta) = \beta_2 \rho(\zeta), q(\zeta) = 0.$$

■

To apply (Delattre et al., 2003, Lemma 1), we still have to verify that the domains of A_1 and A_2 are in the form

$$\left\{ x \in L^2(a,b), x \text{ a.c.}, \frac{dx}{dz} \text{ a.c.}, \frac{d^2x}{d\zeta^2} \in L^2(a,b), \alpha_a \frac{dx}{d\zeta}(a) + \beta_a x(a) = 0, \alpha_b \frac{dx}{d\zeta}(b) + \beta_b x(b) = 0 \right\},$$

where a and b are real numbers such that $(\alpha_a, \beta_a) \neq (0,0)$ and $(\alpha_b, \beta_b) \neq (0,0)$. This form is respected since $D(A_1)$ and $D(A_2)$ are given by (3.2) and (3.3) respectively. Hence, operators A_1 and A_2 are Riesz-Spectral operators. Because of the diagonal form of operator A whose diagonal elements are operators A_1 and A_2, it is also a Riesz-Spectral operator. In this particular case, it has a lot of interesting properties, notably properties on its eigenvalues, which will completely caracterize the exponential stability of the semigroup $(T(t))_{t\geq 0}$. Let first remark that by (Curtain and Zwart, 1995, Theorem 2.3.5.), the growth bound of $(T(t))_{t\geq 0}$ is given by

$$\omega_0 = \inf_{t>0}\left(\frac{1}{t}\log\left(\|T(t)\|\right)\right) = \sup_{n\geq 1}\mathfrak{Re}(\lambda_n) \tag{3.5}$$

since A is a Riesz-Spectral operator. Notice that $\{\lambda_n, n \geq 1\}$ represents the set of eigenvalues of the operator A. Note also that all the following results concern operators A_1 and A_2 and will be automatically reported on A because of the diagonality of it. The main interest of relation (3.5) is explained by introducing the following definition, see (Jacob and Zwart, 2012, Theorem 5.1.5., point e.).

Definition 11. *Let $(T(t))_{t\geq 0}$ be a semigroup. For all $\omega > \omega_0$, where ω_0 represents the growth bound of $(T(t))_{t\geq 0}$, there exists M_ω such that for all $t \geq 0$,*

$$||T(t)|| \leq M_\omega e^{\omega t}. \tag{3.6}$$

First notice that relation (3.6) is valid for every $\omega > \omega_0$. If $\omega_0 < 0$, it is always possible to find $\varepsilon > 0$ sufficiently small such that $\omega_0 + \varepsilon < 0$. In particular, for each $\omega \in]\omega_0, \omega_0 + \varepsilon[$, (3.6) is satisfied. By choosing $\tilde{\omega} \in]\omega_0, \omega_0 + \varepsilon[$, $\tilde{\omega} < 0$ and

$$\|T(t)\| \leq M_{\tilde{\omega}} e^{\tilde{\omega} t}, \text{ for all } t \geq 0 \tag{3.7}$$

hold. By Definition 8, $(T(t))_{t\geq 0}$ will be exponentially stable. In order to use this argument, it remains to prove that the growth bound of the semigroup is negative, or equivalently that $\sup_{n\geq 1}\mathfrak{Re}(\lambda_n) < 0$. To do so, one has first to compute the eigenvalues of operator A, i.e. the eigenvalues of operators A_1 and A_2 due to the diagonality of A. By denoting $\sigma(A)$ the set of eigenvalues of A,

$$\sigma(A) = \sigma(A_1) \cup \sigma(A_2) \tag{3.8}$$

holds. Looking at operator A_1 and taking $x_n \in D(A_1)$, one finds the eigenvalues equation

$$A_1 x_n = \lambda_{1,n} x_n,$$

which can be written as

$$\beta_1 \frac{d^2 x_n}{d\zeta^2} - \frac{dx_n}{d\zeta} - \gamma x_n = \lambda_{1,n} x_n. \tag{3.9}$$

By finding the eigenvalues and the eigenvectors of A_1, we mean solving the ODE (3.9) with the corresponding boundary conditions given by $D(A_1)$. By (Dehaye and Winkin, 2016), the eigenvalues $\{\lambda_{1,n}\}_{n\geq 1}$

are expressed as

$$\lambda_{1,n} = -\frac{s_{1,n}^2 + 1}{4\beta_1} - \gamma$$

where $s_{1,n}, n \geq 1$ are solutions of the resolvent equation

$$\tan\left(\frac{s}{2\beta_1}\right) = \frac{2s}{s^2 - 1}, s \in [0, +\infty)\,. \tag{3.10}$$

It is obvious that for $n \geq 1$,

$$\lambda_{1,n} \leq -\left(\frac{1}{4\beta_1} + \gamma\right) < 0 \tag{3.11}$$

holds. In such a way, we have

$$\sup_{n\geq 1} \lambda_{1,n} < 0.$$

It remains to prove the same result for operator A_2. By (Dehaye and Winkin, 2016), one has

$$\lambda_{2,n} = -\frac{s_{2,n}^2 + 1}{4\beta_2} \tag{3.12}$$

where $s_{2,n}, n \geq 1$ satisfy the following resolvent equation

$$\tan\left(\frac{s}{2\beta_2}\right) = \frac{2s}{s^2 - 1}, s \in [0, +\infty)\,. \tag{3.13}$$

Moreover, these eigenvalues verify

$$\lambda_{2,n} \leq -\frac{1}{4\beta_2} < 0. \tag{3.14}$$

Hence,

$$\sup_{n\geq 1} \lambda_{2,n} < 0.$$

It follows by these considerations that the supremum of the set of the eigenvalues of operator A is also negative. Thus, the semigroup $(T(t))_{t\geq 0}$ is exponentially stable.

As an indication, some solutions of the resolvent equation (3.10) are depicted in Figure 3.1. To compute them, the function `fzero` was used with the software MATLAB. The initial point given to this function is the root of the left-hand side of (3.10), namely $2n\beta_1\pi$.

3.2 Resolvent operator

This section is devoted to the introduction of the resolvent set and the resolvent operator related to operator A. In order to present these two notions, we will use the fact that the operator A is a Riesz-Spectral operator. We first recall the definition of the resolvent set of an operator and the resolvent operator associated to one element of the resolvent set, see (Jacob and Zwart, 2012, Section 5.2.).

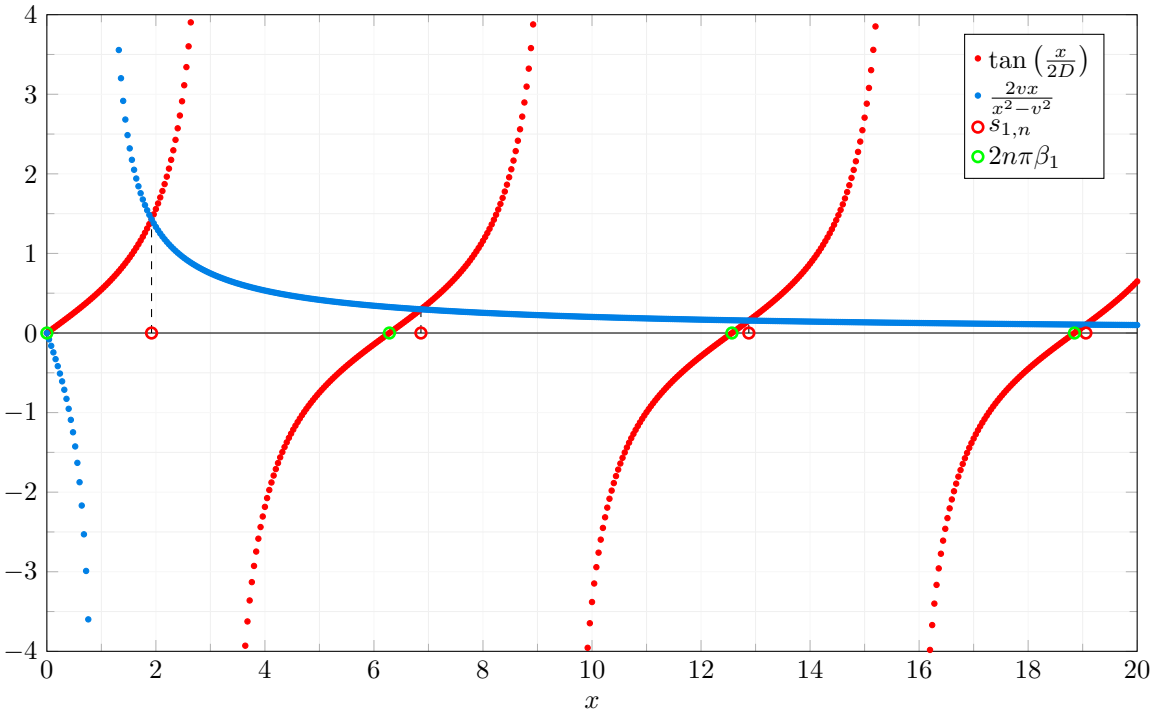

Fig. 3.1 – Solutions of the resolvent equation (3.10) with $\beta_1 = 1$ and $\gamma = 1$.

Definition 12. *The resolvent set of an operator A, noted $\rho(A)$, is defined by*

$$\rho(A) := \left\{ \lambda \in \mathbb{C} \,|\, (\lambda I - A)^{-1} \text{ exists and is bounded} \right\}. \tag{3.15}$$

Taking λ in $\rho(A)$, the operator $(\lambda I - A)^{-1}$ is called the resolvent operator. In the case of a Riesz-Spectral operator, the resolvent set and the resolvent operator have a particular form, provided by the following theorem, see (Curtain and Zwart, 1995, Theorem 2.3.5.).

Theorem 6. *Let A be a Riesz-Spectral operator, $(\lambda_n)_{n\geq 1}$ the set of its eigenvalues, $(\phi_n)_{n\geq 1}$ the corresponding eigenvectors and $(\psi_n)_{n\geq 1}$ the set of the eigenvectors of the adjoint operator*[a] *$A^\star$, where, for all $m,n \geq 1, \langle \phi_n, \psi_m \rangle = \delta_{nm}$. We have*

- $\rho(A) = \{\lambda \in \mathbb{C} | \inf_{n\geq 1} |\lambda - \lambda_n| > 0\}$
- *For λ in $\rho(A)$,*

$$(\lambda I - A)^{-1} = \sum_{n=1}^{+\infty} \frac{1}{\lambda - \lambda_n} \langle \cdot, \psi_n \rangle \phi_n. \tag{3.16}$$

a. The adjoint operator of A, noted $A^\star$ is defined for $x \in D(A)$ and $y \in D(A^\star)$ by $\langle Ax, y \rangle = \langle x, A^\star y \rangle$.

In order to use this result, we will take decomposition (3.1) into account, i.e. we will work on operators A_1 and A_2 separately. Notice that the resolvent operator of A will be a diagonal operator whose diagonal elements are the resolvent operators of A_1 and A_2 respectively. We start by operator A_1, results being

similar for operator A_2. By (Dehaye, 2015, Section 4.1.3.), the eigenvectors of A_1 and of $A_1^\star$ are given for $n \in \mathbb{N}_0$ and for each $\zeta \in [0,1]$ by

$$\phi_{1,n}(\zeta) = K_{1,n} e^{\frac{1}{2\beta_1}\zeta} \left(\cos\left(\frac{s_{1,n}}{2\beta_1}\zeta\right) + \frac{1}{s_{1,n}} \sin\left(\frac{s_{1,n}}{2\beta_1}\zeta\right) \right)$$

and

$$\psi_{1,n}(\zeta) = K_{1,n} e^{-\frac{1}{2\beta_1}\zeta} \left(\cos\left(\frac{s_{1,n}}{2\beta_1}\zeta\right) + \frac{1}{s_{1,n}} \sin\left(\frac{s_{1,n}}{2\beta_1}\zeta\right) \right)$$

respectively. Note that $s_{1,n}, n \geq 1$ are solutions of equation (3.10). Thanks to Theorem 6, the resolvent set of A_1 is given by

$$\rho(A_1) = \left\{ \lambda \in \mathbb{C} | \inf_{n\geq 1} |\lambda - \lambda_{1,n}| > 0 \right\}$$

where $(\lambda_{1,n})_{n\geq 1}$ are the eigenvalues of A_1, given by (3.11). In a similar way, the eigenvectors of A_2 and of $A_2^\star$ are given by

$$\phi_{2,n}(\zeta) = K_{2,n} e^{\frac{1}{2\beta_2}\zeta} \left(\cos\left(\frac{s_{2,n}}{2\beta_2}\zeta\right) + \frac{1}{s_{2,n}} \sin\left(\frac{s_{2,n}}{2\beta_2}\zeta\right) \right)$$

and

$$\psi_{2,n}(\zeta) = K_{2,n} e^{-\frac{1}{2\beta_2}\zeta} \left(\cos\left(\frac{s_{2,n}}{2\beta_2}\zeta\right) + \frac{1}{s_{2,n}} \sin\left(\frac{s_{2,n}}{2\beta_2}\zeta\right) \right)$$

respectively, see (Dehaye, 2015, Section 4.1.3.). The coefficients $s_{2,n}, n \geq 1$ are solutions of equation (3.13). Moreover, the resolvent set of A_2 is given by

$$\rho(A_2) = \left\{ \lambda \in \mathbb{C} | \inf_{n\geq 1} |\lambda - \lambda_{2,n}| > 0 \right\}$$

where $(\lambda_{2,n})_{n\geq 1}$ are the eigenvalues of A_2, given by (3.12). Due to the diagonality of operator A, it is quite natural to define the resolvent set of A, noted $\rho(A)$, by

$$\rho(A) = \rho(A_1) \cap \rho(A_2). \tag{3.17}$$

This definition allows the existence of the resolvent operators of A_1 and A_2 once λ is choosen in $\rho(A)$. Hence, for $\lambda \in \rho(A)$ defined by (3.17),

$$(\lambda I - A)^{-1} = \begin{pmatrix} (\lambda I - A_1)^{-1} & 0 \\ 0 & (\lambda I - A_2)^{-1} \end{pmatrix}.$$

By using Theorem 6,

$$(\lambda I - A)^{-1} = \begin{pmatrix} \sum_{n=1}^{+\infty} \frac{1}{\lambda - \lambda_{1,n}} \langle \cdot, \psi_{1,n} \rangle \phi_{1,n} & 0 \\ 0 & \sum_{n=1}^{+\infty} \frac{1}{\lambda - \lambda_{2,n}} \langle \cdot, \psi_{2,n} \rangle \phi_{2,n} \end{pmatrix},$$

where $\lambda \in \rho(A)$. As an indication and by will of diversity, the integral form of the resolvent operator of the operator A is given in Appendix B.

Chapter 4

Analysis of the existence and the multiplicity of equilibrium profiles

Contents

In this chapter, the existence and the multiplicity of equilibrium profiles are investigated in three different cases depending on the link between the Peclet numbers. As in (Dochain, 2016), we consider adiabatic reactors, i.e. we assume that there is no energy exchange with the environment ($h = 0$, or equivalently $\gamma = 0$). The main idea is to use perturbation theory, see (Hoppensteadt, 2013, Regular Perturbation Theorem). Firstly, we consider the case $Pe_h = Pe_m \overset{\text{not.}}{=} Pe$ for which the analysis of (Dochain, 2016, Section 3) is revised and consolidated. The two other cases are $Pe_h \neq Pe_m$ and $Pe_h = Pe_m + \eta$, where η is a small parameter. To do so, we write equations (2.7) at the equilibrium, which read as follows

$$\begin{cases} \frac{1}{Pe_h}\frac{d^2x_1}{dz^2} - \frac{dx_1}{dz} + \alpha\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = 0 \\ \frac{1}{Pe_m}\frac{d^2x_2}{dz^2} - \frac{dx_2}{dz} + \alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = 0 \\ \\ \frac{dx_1}{dz}(0) - Pe_h x_1(0) = 0 = \frac{dx_1}{dz}(1) \\ \frac{dx_2}{dz}(0) - Pe_m x_2(0) = 0 = \frac{dx_2}{dz}(1), \end{cases} \tag{4.1}$$

where the spatial variable is denoted by z.

4.1 Case 1 : $Pe_h = Pe_m \overset{\text{not.}}{=} \frac{v}{D}$

Considering the change of variables

$$y_1 = x_1, \qquad y_2 = x_1 - \delta x_2,$$

it follows from the second equation and the last boundary conditions of (4.1) that $y_2 \equiv 0$ (formally, y_2 corresponds to a reaction invariant), see (Dochain et al., 1992) and (Gavalas, 1968). Moreover, by using the functions u and w defined by

$$u(z) = y_1(1-z), \qquad w(z) = \frac{dy_1}{dz}(1-z), \tag{4.2}$$

the first equation of (4.1) with the associated boundary conditions take the form

$$\begin{cases} \frac{du}{dz} = -w, \\ \frac{dw}{dz} = -\frac{1}{D}\left(vw - g(u)\right), \\ \\ u(0) = a, w(0) = 0, w(1) = \frac{v}{D}u(1), \end{cases} \tag{4.3}$$

where a is a real parameter and g is the nonlinear function defined by $g(-1)=0$ and, for $x\in(-1,\infty)$, by

$$g(x)=v\alpha\,(\delta-x)\,e^{\frac{\mu x}{1+x}}.$$

Interested readers are referred to Appendix C.1 for calculation details.

Lemma 1. *For some values of the parameters μ and δ, there exist D^* large enough, $v_1^*>0$ and $v_2^*>0$ such that for all $D\geq D^*$, the set of equations (4.3) has either*

- *at least three solutions, if v belongs to $(\min\{v_1^*,v_2^*\},\max\{v_1^*,v_2^*\})$, or*
- *at least one solution, otherwise.*

Remark 1. *We are not interested in finding a solution to (4.3) but in finding a function $v(a,D)$ such that the final condition $w(1)=\frac{v}{D}u(1)$ is satisfied. Thus, if there are $a_1\neq a_2$ and $D>0$ such that $v(a_1,D)=v(a_2,D)$, the equations (4.3) have at least two solutions. To reach this goal, we use pertubation theory (Hoppensteadt, 2013), which consists of disturbing the equations with a small parameter ε. Then, if a solution can be found to the disturbed equations with $\varepsilon=0$, perturbation theory guarantees that the system has a solution for small ε, under a few assumptions, especially continuity conditions.*

Proof. Let us introduce the following notations :

$$\varepsilon=\frac{1}{D},\qquad u_\varepsilon=u,\qquad w_\varepsilon=\frac{1}{\varepsilon}w, \tag{4.4}$$

where D satisfies $D\geq D^*$ for D^* sufficiently large such that ε is small enough. Equations (4.3) can be rewritten as

$$\begin{cases}\frac{du_\varepsilon}{dz}=-\varepsilon w_\varepsilon\\ \frac{dw_\varepsilon}{dz}=-\left(v\varepsilon w_\varepsilon-g(u_\varepsilon)\right)\\ \\ u_\varepsilon(0)=a, w_\varepsilon(0)=0, w_\varepsilon(1)=vu_\varepsilon(1),\end{cases} \tag{4.5}$$

where v is now interpreted as a function of a and ε, denoted by $v(a,\varepsilon)$. These equations have the trivial solution

$$u_\varepsilon(z)=a,\qquad w_\varepsilon(z)=g(a)z$$

for $\varepsilon=0$, provided that using the boundary conditions,

$$g(a)=v(a,0)a.$$

The function v is then given for $\varepsilon=0$ by

$$v(a,0)=\frac{g(a)}{a}=\frac{k_0L\,(\delta-a)\,e^{\frac{-\mu}{1+a}}}{a} \tag{4.6}$$

and its first order derivative is given by

$$k_0 L e^{\frac{-\mu}{1+a}} \left[\frac{-(\mu+\delta)a^2 + \delta(\mu-2)a - \delta}{a^2(1+a)^2} \right].$$

The second order derivative of $v(a,0)$ is equal to

$$\frac{k_0 L e^{\frac{-\mu}{1+a}}}{a^3(1+a)^4}[(2\delta+2\mu)a^4 + (2\mu-\mu^2-4\delta\mu+8\delta)a^3 + (12\delta+\delta\mu^2-6\delta\mu)a^2 + (8\delta-2\delta\mu)a + 2\delta].$$

The stationary points of $v(a,0)$ are thus characterized by the following equation :

$$-(\mu+\delta)a^2 + \delta(\mu-2)a - \delta = 0. \tag{4.7}$$

The discriminant of (4.7) is given by

$$\rho = \mu\delta(\mu\delta - 4\delta - 4) \tag{4.8}$$

and is first considered to be positive. The roots of (4.7) are then given by

$$a_1^* = \frac{\delta(\mu-2)}{2(\mu+\delta)} - \frac{1}{2(\mu+\delta)}\sqrt{\mu\delta(\mu\delta-4\delta-4)} \text{ and } a_2^* = \frac{\delta(\mu-2)}{2(\mu+\delta)} + \frac{1}{2(\mu+\delta)}\sqrt{\mu\delta(\mu\delta-4\delta-4)}.$$

Note also that the function $v(a,0)$ has two singularities in -1 and 0 (Observe that -1 is actually a removable singularity). So, we have to find an interval in which a_1^* and a_2^* are both located and which does not contain any singularity. Combining this constraint with the assumption that ρ is positive, one gets that the only possibility is $a_1^* > 0$ and $a_2^* > 0$. In this case, μ and δ must satisfy either

$$\delta > 0, \quad \mu > 4, \quad \delta(\mu-4) > 4 \quad \text{or} \quad \delta < -2, \quad \mu > 2, \quad \mu+\delta < 0, \quad \delta(\mu-4) < 4.$$

Let us denote $v(a_1^*,0)$ and $v(a_2^*,0)$ by v_1^* and v_2^*, respectively. On one hand, for $\delta > 0, \mu > 4$ and $\delta(\mu-4) > 4$, the point (a_1^*, v_1^*) corresponds to a minimum of $v(a,0)$ and (a_2^*, v_2^*) to a maximum. On the other hand, for $\delta < -2, \mu > 2, \mu+\delta < 0$ and $\delta(\mu-4) < 4$, we get the opposite. Considering both cases, it follows that, if one takes any value v^* in the interval $(\min\{v_1^*, v_2^*\}, \max\{v_1^*, v_2^*\})$, we are sure that there are at least three values of a such that $v(a,0) = v^*$. Otherwise, we are only sure that there exists at least one value of a at which v^* is reached by $v(a,0)$. The only assumption that remains to be checked is

$$\lim_{\varepsilon \to 0} v(a,\varepsilon) = v(a,0).$$

From (Hirsch et al., 2004, Theorem 17.3, p. 192), the functions u_ε and w_ε are both continuous with respect to ε. Observe also that the last boundary condition in (4.5) is equivalent to

$$v(a,\varepsilon) = \frac{w_\varepsilon(1)}{u_\varepsilon(1)}.$$

So $v(a,\varepsilon)$ is continuous with respect to ε, and thus specifically in 0. We shall now develop the cases

where ρ is either negative or equal to 0. When ρ is negative, the first order derivative of v has no real root. So, the function v has no extremum. A chosen value of v can be reached by at most one value of a (on any interval where v is continuous). When ρ is zero, the first order derivative of v has one root, namely

$$a^* = \frac{\delta(\mu-2)}{2(\mu+\delta)}.$$

In addition, il follows from (4.8) that

$$\delta = \frac{4}{\mu-4},$$

which yields

$$a^* = \frac{2}{\mu-2}. \tag{4.9}$$

Moreover, the polynomial factor in the second order derivative of v can be written as

$$\frac{2(\mu-2)^2}{\mu-4}a^4 + \frac{(2-\mu)\left(\mu^2-4\mu+16\right)}{\mu-4}a^3 + \frac{4\mu^2-24\mu+48}{\mu-4}a^2 - 8a + \frac{8}{\mu-4}.$$

See Appendix C.1 for further details. Using (4.9), this polynomial can be factorized as

$$\left[\frac{2(\mu-2)^2}{\mu-4}a^3 + \frac{(2-\mu)\left(\mu^2-4\mu+12\right)}{\mu-4}a^2 + \frac{2\mu^2-16\mu+24}{\mu-4}a + \frac{-4\mu+8}{\mu-4}\right](a-a^*).$$

This means that a^* is also a root of the second order derivative of v. The point $(a^*, v(a^*,0))$ is neither a minimum nor a maximum, but a saddle point of $v(a,0)$. By choosing a value of v denoted by v^*, one can find at most one point in the domain of v at which the value v^* is reached by $v(a,0)$ (on any interval where v is continuous). ■

An illustration of Lemma 1 and its proof can be found in Figure 4.2 for $\rho > 0$ and in Figure 4.1 for $\rho = 0$.

We present now a corollary of Lemma 1 that provides approximated solutions to equations (4.5). Moreover, with these solutions, one can also find solutions of equations (4.1) for equal Peclet numbers using the appropriate change of variables. The method used is based on perturbation theory (Hoppensteadt, 2013).

Corollary 1. *Taking into account the existence of equilibrium profiles under the conditions of Lemma 1, approximated solutions of equations (4.5) are given by*

$$u_\varepsilon(z) = a - \frac{\varepsilon g(a)}{2}z^2,\ w_\varepsilon(z) = g(a)z - \frac{\varepsilon v_\varepsilon g(a)}{2}z^2,$$

that correspond to the approximated form v_ε of function v given by

$$\frac{g(a)}{a} = \frac{k_0 L(\delta-a)e^{\frac{-\mu}{1+a}}}{a}.$$

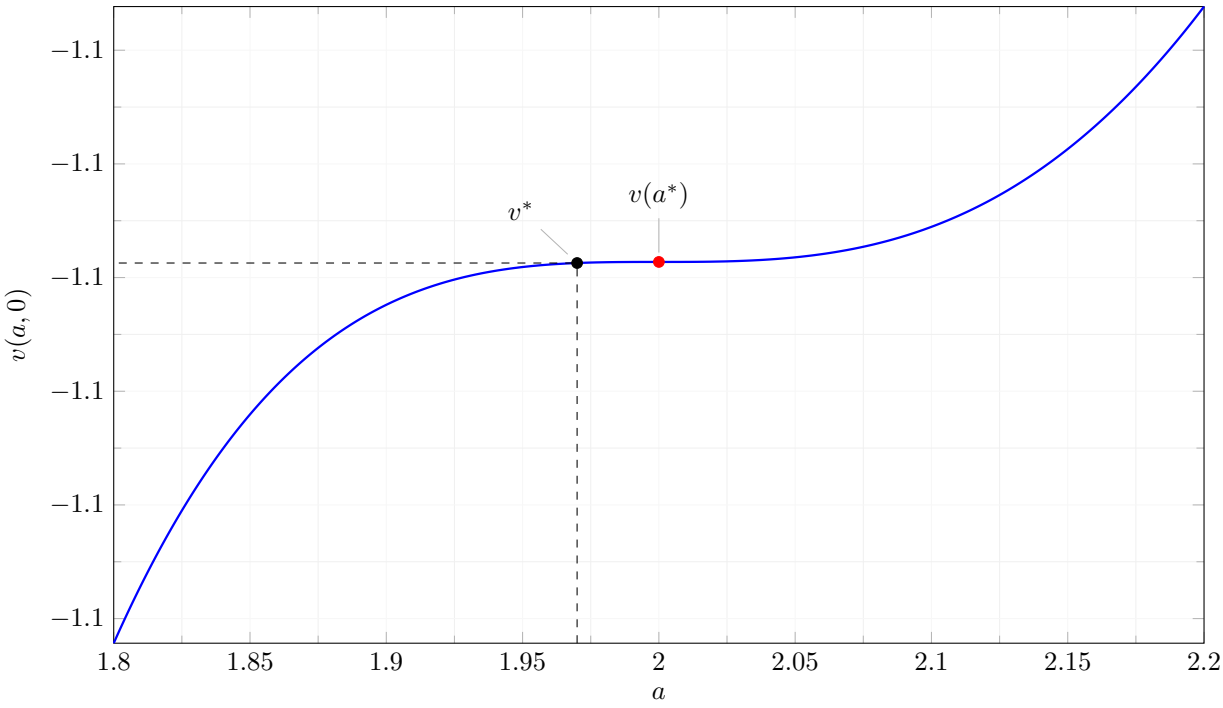

Fig. 4.1 – Illustration of Lemma 1 with $\mu = 3$ and $\delta = -4$ ($\rho = 0$).

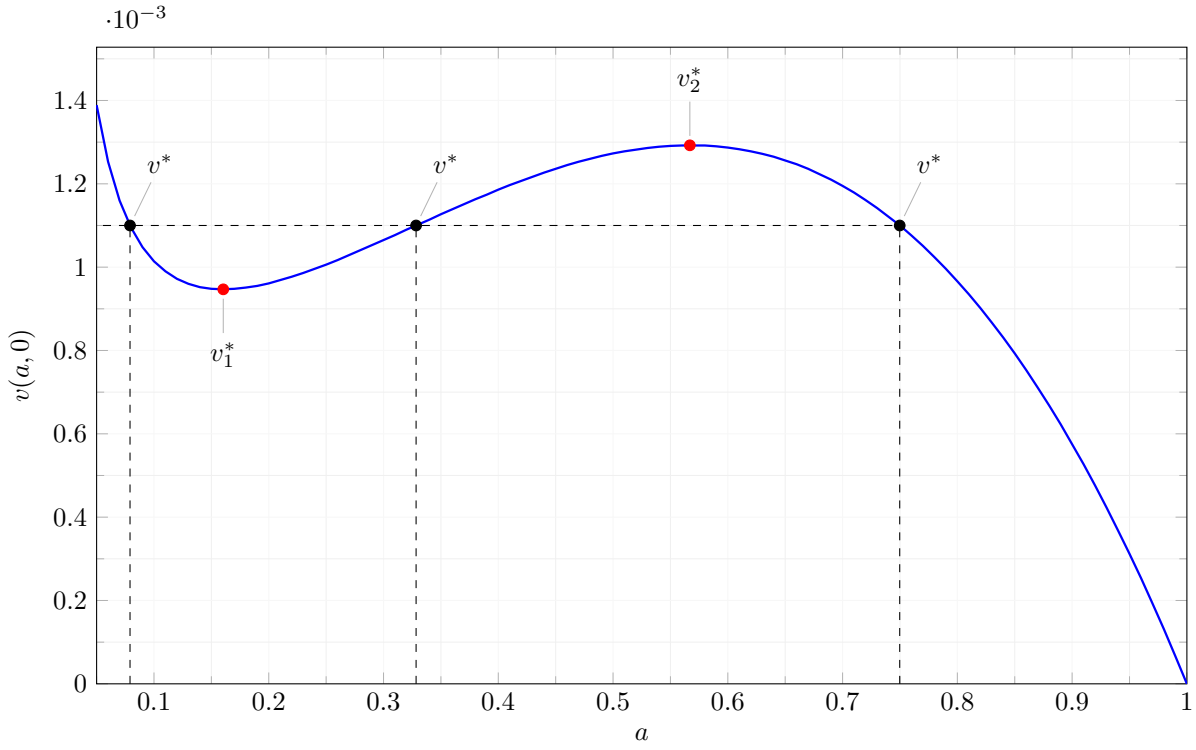

Fig. 4.2 – Illustration of Lemma 1 with $\mu = 10$ and $\delta = 1$ ($\rho > 0$).

Proof. Perturbation theory guarantees that the solutions u_ε and w_ε have the form

$$u_\varepsilon(z) = u_0(z) + u_1(z)\varepsilon + \mathcal{O}(\varepsilon^2) \tag{4.10}$$

$$w_\varepsilon(z) = w_0(z) + w_1(z)\varepsilon + \mathcal{O}(\varepsilon^2). \tag{4.11}$$

Using the same decomposition for function v_ε (also depending on ε), one finds

$$v_\varepsilon = v_0 + v_1\varepsilon + \mathcal{O}(\varepsilon^2). \tag{4.12}$$

Note that all the terms including ε^2 or higher order of ε are considered to be negligible. By plugging (4.10) and (4.11) in equations (4.5), one gets

$$\begin{cases} \frac{du_0}{dz} + \frac{du_1}{dz}\varepsilon = -\varepsilon\,(w_0 + w_1\varepsilon) \\ \frac{dw_0}{dz} + \frac{dw_1}{dz}\varepsilon = -v_\varepsilon w_0\varepsilon - v_\varepsilon w_1\varepsilon^2 + g\,(u_0 + u_1\varepsilon) \\ \\ u_0(0) + u_1(0)\varepsilon = a, w_0(0) + w_1(0)\varepsilon = 0. \end{cases} \tag{4.13}$$

By identification, and by using the approximation $g\,(u_0 + u_1\varepsilon) \approx g\,(u_0)$ for small ε, we have

$$\begin{cases} \frac{du_0}{dz} = 0 \\ \frac{du_1}{dz} = -w_0 \\ \frac{dw_0}{dz} = g(u_0) \\ \frac{dw_1}{dz} = -v_\varepsilon w_0 \\ \\ u_0(0) = a, u_1(0) = 0, w_0(0) = 0, w_1(0) = 0. \end{cases} \tag{4.14}$$

A simple integration yields the desired forms for u_ε and w_ε. The last step is to find the form of v to reach the boundary condition $w_\varepsilon(1) = v_\varepsilon u_\varepsilon(1)$. Knowing the form of functions u_ε and w_ε and using the decomposition of v_ε, provided by (4.12), one has the relation

$$g(a) - \frac{v_0 g(a)}{2}\varepsilon - \frac{v_1 g(a)}{2}\varepsilon^2 = (v_0 + v_1\varepsilon)\left(a - \frac{g(a)}{2}\varepsilon\right).$$

By identification, the function v_ε is given by $\frac{g(a)}{a}$. ■

To estimate the form of solutions of equations (4.1), one has to consider Corollary 1, and relations (4.2) and (4.4). This leads to

$$\begin{aligned} x_1(z) &\simeq a - \frac{g(a)}{2D}\,(1-z)^2, \\ x_2(z) &\simeq \frac{a}{\delta} - \frac{g(a)}{2\delta D}\,(1-z)^2, \end{aligned} \tag{4.15}$$

which are approximated solutions to equilibrium equations for equal Peclet numbers.

The equality assumption between Pe_h and Pe_m appears to be too restrictive. Indeed, the equality entails the following condition :

$$D_{ma} = \frac{\lambda_{ea}}{\rho C_p},$$

which seems to be physically unrealistic and leads us to consider the case $Pe_h \neq Pe_m$ in the next section.

4.2 Case 2 : $Pe_h \neq Pe_m$

The methodology that is followed for this case is quite similar to the one used in the previous section. However, the analysis and the computation are more involved in view of the fact that there are two interconnected sets of equilibrium equations of type (4.3) with an auxiliary function g of two variables : see (4.17) below. Considering that Pe_h and Pe_m are different, a change of variables is no more possible. In the following, the notations D_1 for λ_{ea} and D_2 for D_{ma}, respectively, will be used. We introduce also the notation $k_p := \rho C_p$. Defining the function g for (x_1, x_2) in $\mathbb{R}^2$ such that $-1 < x_1$ and $0 \leq x_2 \leq 1$, by

$$g(x_1,x_2) = v\alpha\,(1-x_2)\,e^{\frac{\mu x_1}{1+x_1}} = k_0 L\,(1-x_2)\,e^{\frac{-\mu}{1+x_1}},$$

and $g(-1,x_2) = 0$, the equilibrium equations become

$$\begin{cases} D_1 \frac{d^2x_1}{dz^2} - vk_p \frac{dx_1}{dz} + k_p \delta g(x_1,x_2) = 0 \\ D_2 \frac{d^2x_2}{dz^2} - v\frac{dx_2}{dz} + g(x_1,x_2) = 0 \\ \\ D_1 \frac{dx_1}{dz}(0) - vk_p x_1(0) = 0 = \frac{dx_1}{dz}(1) \\ D_2 \frac{dx_2}{dz}(0) - vx_2(0) = 0 = \frac{dx_2}{dz}(1). \end{cases} \tag{4.16}$$

We use now the functions

$$u_1(z) = x_1(1-z), \qquad w_1(z) = \frac{dx_1}{dz}(1-z),$$

and

$$u_2(z) = x_2(1-z), \qquad w_2(z) = \frac{dx_2}{dz}(1-z)$$

to rewrite (4.16) as a system of four first order differential equations. Taking the boundary conditions into account, we find

$$\begin{cases} \frac{du_1}{dz} = -w_1 \\ \frac{dw_1}{dz} = -\frac{k_p}{D_1}\,(vw_1 - \delta g(u_1,u_2)) \\ \frac{du_2}{dz} = -w_2 \\ \frac{dw_2}{dz} = -\frac{1}{D_2}\,(vw_2 - g(u_1,u_2)) \\ \\ u_1(0) = a_1, w_1(0) = 0, w_1(1) = \frac{vk_p}{D_1} u_1(1) \\ u_2(0) = a_2, w_2(0) = 0, w_2(1) = \frac{v}{D_2} u_2(1). \end{cases} \tag{4.17}$$

Once again we have to find $v(a_1,a_2,D_1,D_2)$ s.t. $w_1(1)=\frac{vk_p}{D_1}u_1(1)$ and $w_2(1)=\frac{v}{D_2}u_2(1)$ hold. A similar argument as for the one-dimensional case is developed. If there are $(a_1,a_2)\neq(a_3,a_4)$, $D_1>0$ and $D_2>0$ such that

$$v(a_1,a_2,D_1,D_2)=v(a_3,a_4,D_1,D_2),$$

then the system (4.17) has at least two solutions. In order to find the function v, perturbation theory is applied to (4.17). To do so, we introduce

$$\varepsilon_1=\frac{1}{D_1},\qquad u_{\varepsilon_1}=u_1,\qquad w_{\varepsilon_1}=\frac{1}{\varepsilon_1}w_1$$

and

$$\varepsilon_2=\frac{1}{D_2},\qquad u_{\varepsilon_2}=u_2,\qquad w_{\varepsilon_2}=\frac{1}{\varepsilon_2}w_2,$$

where D_1 and D_2 verify $D_1\geq D_1^*$ and $D_2\geq D_2^*$ respectively with D_1^* and D_2^* sufficiently large such that ε_1 and ε_2 are small enough. Thus, the system (4.17) takes the form

$$\begin{cases}\frac{du_{\varepsilon_1}}{dz}=-\varepsilon_1 w_{\varepsilon_1},\\ \frac{dw_{\varepsilon_1}}{dz}=-\left(k_p v\varepsilon_1 w_{\varepsilon_1}-k_p\delta g(u_{\varepsilon_1},u_{\varepsilon_2})\right),\\ \frac{du_{\varepsilon_2}}{dz}=-\varepsilon_2 w_{\varepsilon_2},\\ \frac{dw_{\varepsilon_2}}{dz}=-\left(v\varepsilon_2 w_{\varepsilon_2}-g(u_{\varepsilon_1},u_{\varepsilon_2})\right),\\ \\ u_{\varepsilon_1}(0)=a_1, w_{\varepsilon_1}(0)=0, w_{\varepsilon_1}(1)=vk_p u_{\varepsilon_1}(1),\\ u_{\varepsilon_2}(0)=a_2, w_{\varepsilon_2}(0)=0, w_{\varepsilon_2}(1)=vu_{\varepsilon_2}(1),\end{cases}\tag{4.18}$$

whose solution with $\varepsilon_1=\varepsilon_2=0$ is given by

$$u_{\varepsilon_1}(z)=a_1,\qquad w_{\varepsilon_1}(z)=k_p\delta g(a_1,a_2)z$$

and

$$u_{\varepsilon_2}(z)=a_2,\qquad w_{\varepsilon_2}(z)=g(a_1,a_2)z.$$

Taking the difference of the boundary conditions for $z=1$, it follows that

$$v\,(a_1,a_2,0,0)=(1-\delta)\,k_0L\frac{(1-a_2)\,e^{\frac{-\mu}{1+a_1}}}{a_2-a_1},\tag{4.19}$$

which is a necessary form for the function v. The reader is referred to Appendix C.2 for further calculation details. The continuity assumption described by

$$\lim_{\varepsilon_1,\varepsilon_2\to 0}v(a_1,a_2,\varepsilon_1,\varepsilon_2)=v(a_1,a_2,0,0)$$

holds since

$$v=\frac{w_{\varepsilon_1}(1)}{k_p u_{\varepsilon_1}(1)}\text{ and }v=\frac{w_{\varepsilon_2}(1)}{u_{\varepsilon_2}(1)}\tag{4.20}$$

are both continuous with respect to ε_1 and ε_2. This is a consequence of the theorem of dependence of the solutions of differential equations on parameters (see (Hirsch et al., 2004, 17.3, p. 192)). Keeping in mind that our study of equilibrium is qualitative, we first give the gradient of function v :

$$\overrightarrow{\nabla} v(a_1,a_2,0,0) = (1-\delta)\,k_0 L e^{\frac{-\mu}{1+a_1}} \begin{pmatrix} \frac{(1-a_2)\left((1+a_1)^2+\mu(a_2-a_1)\right)}{(a_2-a_1)^2(1+a_1)^2} \\ \frac{a_1-1}{(a_2-a_1)^2} \end{pmatrix}. \tag{4.21}$$

Observe also that the entries of the Hessian matrix of function v, denoted by $\nabla^2 v(a_1,a_2,0,0) \overset{\text{not.}}{=} \mathscr{H}(a_1,a_2)$, are given by

$$\begin{aligned}
\mathscr{H}_{11}(a_1,a_2) &= \frac{1-a_2}{a_2-a_1}(1-\delta)\,k_0 L e^{\frac{-\mu}{1+a_1}}\,\tilde{\mathscr{H}}_{11}, \\
\mathscr{H}_{12}(a_1,a_2) &= \mathscr{H}_{21}(a_1,a_2) = (1-\delta)\,k_0 L e^{\frac{-\mu}{1+a_1}}\,\tilde{\mathscr{H}}_{12}, \\
\mathscr{H}_{22}(a_1,a_2) &= \frac{-2(a_1-1)}{(a_2-a_1)^3}(1-\delta)\,k_0 L e^{\frac{-\mu}{1+a_1}},
\end{aligned}$$

where

$$\tilde{\mathscr{H}}_{12} = \frac{1}{(a_2-a_1)^2} + \frac{2(a_1-1)}{(a_2-a_1)^3} + \frac{\mu(a_1-1)}{(a_2-a_1)^2(1+a_1)^2}$$

and

$$\tilde{\mathscr{H}}_{11} = \frac{2}{(a_2-a_1)^2} + \frac{2\mu}{(a_2-a_1)(1+a_1)^2} - \frac{2\mu}{(1+a_1)^3} + \frac{\mu^2}{(1+a_1)^4}.$$

Setting (4.21) to 0, we find that the only possibility is

$$(a_1,a_2) = \left(1, \frac{\mu-4}{\mu}\right) := (a_1^*, a_2^*). \tag{4.22}$$

Plugging (4.22) in $\mathscr{H}$, we obtain that

$$\mathscr{H}\left(1,\frac{\mu-4}{\mu}\right) = k_0 L(1-\delta)\,e^{\frac{-\mu}{2}} \begin{pmatrix} -\frac{\mu^2}{16}+\frac{\mu}{16} & \frac{\mu^2}{16} \\ \frac{\mu^2}{16} & 0 \end{pmatrix}.$$

Therefore, the point (a_1^*, a_2^*) is a saddle point.

Observe that we are dealing with equilibrium curves and no more discrete set of points. A level v^* of function v satisfies equation

$$v^* = (1-\delta)\,k_0 L \frac{1-a_2}{a_2-a_1} e^{\frac{-\mu}{1+a_1}}.$$

The set of equilibrium points for a level v^* of function v is given by

$$\mathscr{C}_{v^*} = \left\{ (a_1,a_2) \in \mathbb{R}^2 : a_1 \neq a_2, a_2 = \frac{(1-\delta)\,k_0 L e^{\frac{-\mu}{1+a_1}} + a_1 v^*}{v^* + (1-\delta)\,k_0 L e^{\frac{-\mu}{1+a_1}}} \right\}. \tag{4.23}$$

We now present a preliminary result related to the existence of equilibrium profiles in this case. To expand this analysis, we focus on a specific direction, namely, an affine direction of the form $a_2 = \alpha a_1 + \beta$ with $\alpha, \beta \in \mathbb{R}$.

Lemma 2. *For some values of the parameters μ and δ, taking an affine direction of the form $a_2 = \alpha a_1 + \beta$ with $\alpha, \beta \in \mathbb{R}$, there exist D_1^* and D_2^* sufficiently large, $v_1^* > 0, v_2^* > 0$ such that for $D_1 \geq D_1^*, D_2 \geq D_2^*$ the system (4.17) has either*

- *at least three solutions if v belongs to $(\min\{v_1^*, v_2^*\}, \max\{v_1^*, v_2^*\})$, or*
- *at least one solution otherwise.*

Proof. Function v (see (4.19)) in the direction $a_2 = \alpha a_1 + \beta$ becomes

$$v(a_1, \alpha a_1 + \beta, 0, 0) = \frac{(1-\delta) k_0 L (1 - \beta - \alpha a_1) e^{\frac{-\mu}{1+a_1}}}{(\alpha - 1) a_1 + \beta} \tag{4.24}$$

and its first order derivative is given by

$$\begin{aligned} &\frac{(1-\delta) k_0 L e^{\frac{-\mu}{1+a_1}}}{((\alpha-1)a_1+\beta)^2 (1+a_1)^2} (-(\alpha\mu(\alpha-1)+(\alpha-1)+\beta) a_1^2 \\ &\quad +(\alpha(-2+\mu-2\beta\mu)+(-1+\beta)(-2+\mu)) a_1 \\ &+(-\alpha-(-1+\beta)(1+\beta\mu))). \end{aligned}$$

The discriminant of the polynomial factor in this first order derivative has the form

$$-(-1+\alpha+\beta)\mu\left[-4+4(\alpha-\beta)^2+\mu-(\alpha+\beta)\mu\right]$$

and is considered to be positive here. In this case, the first order derivative of v has two real roots, which are denoted a_{11}^* and a_{12}^*. Furthermore, let us denote

$$v_1^* = v(a_{11}^*, \alpha a_{11}^* + \beta, 0, 0) \text{ and } v_2^* = v(a_{12}^*, \alpha a_{12}^* + \beta, 0, 0).$$

Applying the same method as in the proof of Lemma 1, the result follows. ■

Lemma 2 is illustrated in Figure 4.3, where a zoom on the first extremum of the function is provided for the sake of readability.

Remark 2. *Note that Lemma 2 provides necessary conditions for the existence of equilibrium profiles. To have necessary and sufficient conditions, one has to adapt the form of function v. By considering equations (4.20) for $\varepsilon_1 = \varepsilon_2 = 0$, one finds that a_2 has to be equal to $\frac{1}{\delta} a_1$. This implies that the affine direction is described by $\alpha a_1 + \beta$ with $\alpha = \frac{1}{\delta}$ and $\beta = 0$.*

Taking Remark 2 into account, a theorem is now stated which gives necessary and sufficient conditions for the multiplicity of equilibrium profiles for distinct Peclet numbers.

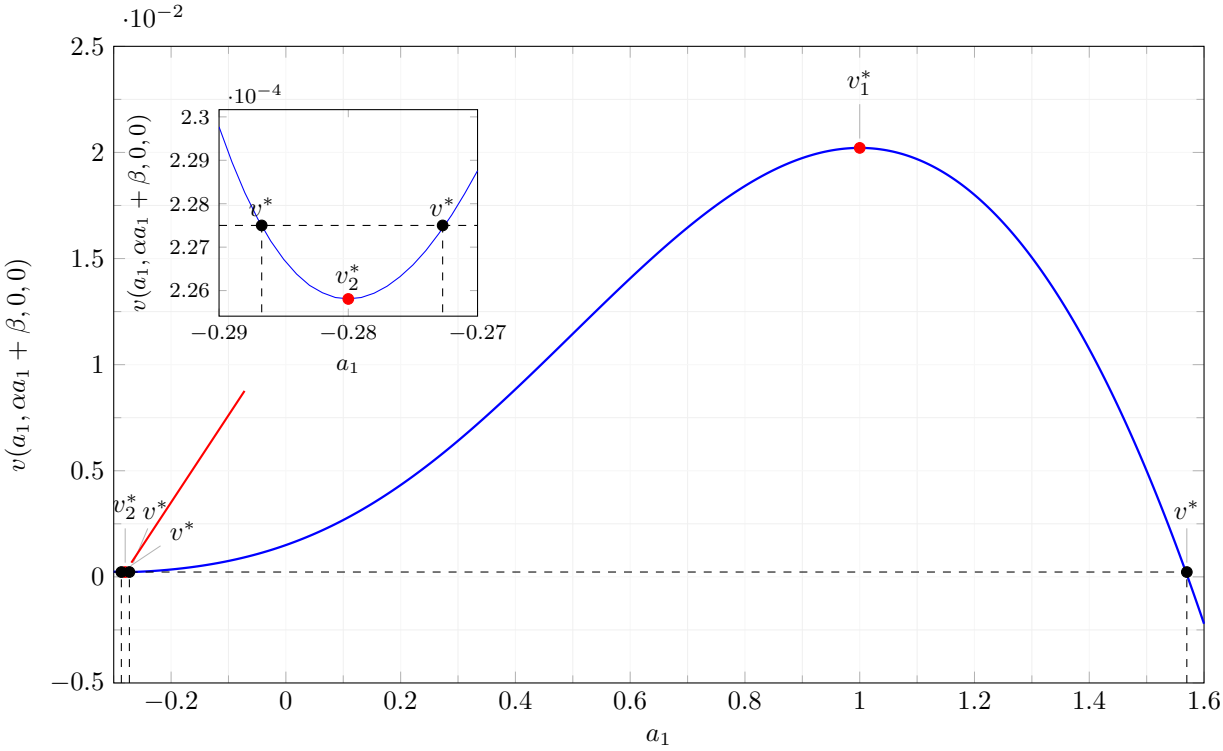

Fig. 4.3 – Illustration of Lemma 2 with $\mu = 10, \delta = 4, \alpha = 0.7$ and $\beta = -0.1$.

Theorem 7. *For some values of the parameters μ and δ, there exist D_1^* and D_2^* sufficiently large, $v_1^* > 0, v_2^* > 0$ such that for $D_1 \geq D_1^*, D_2 \geq D_2^*$ the system (4.17) has either*

- *at least three solutions if v belongs to $(\min\{v_1^*, v_2^*\}, \max\{v_1^*, v_2^*\})$, or*
- *at least one solution otherwise.*

Proof. Based on Remark 2, the function v has to be restricted in the direction $a_2 = \alpha a_1 + \beta$ with $\alpha = \frac{1}{\delta}$ and $\beta = 0$. By injecting $\alpha = \frac{1}{\delta}$ and $\beta = 0$ in (4.24), this leads to

$$\begin{aligned} v\left(a_1, \frac{1}{\delta}a_1, 0, 0\right) &= \frac{(1-\delta)\, k_0 L \left(1 - 0 - \frac{1}{\delta}a_1\right) e^{\frac{-\mu}{1+a_1}}}{\left(\frac{1}{\delta} - 1\right) a_1 + 0} \\ &= \frac{(1-\delta)\, k_0 L \left(\frac{\delta - a_1}{\delta}\right) e^{\frac{-\mu}{1+a_1}}}{\left(\frac{1-\delta}{\delta}\right) a_1} \\ &= \frac{k_0 L (\delta - a_1)\, e^{\frac{-\mu}{1+a_1}}}{a_1}. \end{aligned}$$

The conclusion follows by Lemma 2 and by noting that function v has the same expression as in Lemma 1 (see equation (4.6)). ■

Similarly as in Case 1, approximated solutions of equations (4.18) are given in the following corollary.

Corollary 2. *Taking into account the existence of equilibrium profiles under the conditions of Theorem 7, approximated solutions of equations (4.18) are given by*

$$u_{\varepsilon_1}(z) = a_1 - \frac{\varepsilon_1 k_p \delta g\left(a_1, \frac{1}{\delta}a_1\right)}{2} z^2,\ w_{\varepsilon_1}(z) = k_p \delta g\left(a_1, \frac{1}{\delta}a_1\right) z - \frac{\varepsilon_1 k_p^2 v_{\varepsilon_1,\varepsilon_2} \delta g\left(a_1, \frac{1}{\delta}a_1\right)}{2} z^2,$$

$$u_{\varepsilon_2}(z) = \frac{1}{\delta}a_1 - \frac{\varepsilon_2 g\left(a_1, \frac{1}{\delta}a_1\right)}{2} z^2,\ w_{\varepsilon_2}(z) = g\left(a_1, \frac{1}{\delta}a_1\right) z - \frac{\varepsilon_2 v_{\varepsilon_1,\varepsilon_2} g\left(a_1, \frac{1}{\delta}a_1\right)}{2} z^2,$$

that correspond to the approximated form $v_{\varepsilon_1,\varepsilon_2}$ of function v given by

$$\frac{k_0 L(\delta - a_1)\, e^{\frac{-\mu}{1+a_1}}}{a_1}.$$

Proof. The method used to find these approximated functions is exactly the same as the one used in the case of equal Peclet numbers. Just note for example that $u_{\varepsilon_1}(z)$ is developed as $u_{0_1}(z) + u_{1_1}(z)\varepsilon_1$ and also that $g\left(u_{0_1} + u_{1_1}\varepsilon_1, u_{0_2} + u_{1_2}\varepsilon_2\right)$ is approximated by $g\left(u_{0_1}, u_{0_2}\right)$ for $\varepsilon_1, \varepsilon_2$ small enough. ■

As in Case 1, approximated solutions of equilibrium equations (4.16) are obtained by applying Corollary 2. These are expressed as

$$x_1(z) \simeq a_1 - \frac{k_p \delta g\left(a_1, \frac{1}{\delta}a_1\right)}{2D_1}(1-z)^2,\ x_2(z) \simeq \frac{a_1}{\delta} - \frac{g\left(a_1, \frac{1}{\delta}a_1\right)}{2D_2}(1-z)^2. \tag{4.25}$$

The last case considered is $Pe_h = Pe_m + \eta$ with η small enough.

4.3 Case 3 : $Pe_h = Pe_m + \eta$

The approach used here is similar to the one used for $Pe_h \neq Pe_m$. Writing the equations (4.1) again with $Pe_m + \eta$ and Pe_m, we get

$$\begin{cases} \frac{d^2x_1}{dz^2} - (Pe_m + \eta)\frac{dx_1}{dz} + (Pe_m + \eta)\alpha\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = 0 \\ \frac{d^2x_2}{dz^2} - Pe_m\frac{dx_2}{dz} + Pe_m\alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = 0 \\ \\ \frac{dx_1}{dz}(0) - (Pe_m + \eta)x_1(0) = \frac{dx_1}{dz}(1) = 0 \\ \frac{dx_2}{dz}(0) - Pe_m x_2(0) = \frac{dx_2}{dz}(1) = 0. \end{cases}$$

Since $Pe_m = \frac{vL}{D}$, the equilibrium equations are given by

$$\begin{cases} D\frac{d^2x_1}{dz^2} - (v + \eta D)\frac{dx_1}{dz} + (v + \eta D)\alpha\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = 0 \\ D\frac{d^2x_2}{dz^2} - v\frac{dx_2}{dz} + v\alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = 0 \\ \\ D\frac{dx_1}{dz}(0) - (v + \eta D)x_1(0) = \frac{dx_1}{dz}(1) = 0 \\ D\frac{dx_2}{dz}(0) - vx_2(0) = \frac{dx_2}{dz}(1) = 0. \end{cases}$$

Let us introduce the coefficient k_η, that verifies $v+\eta D = vk_\eta$, i.e. $k_\eta = 1+\frac{1}{Pe_m}$. Then, the equilibrium equations take the form

$$\begin{cases} D\frac{d^2x_1}{dz^2} - vk_\eta \frac{dx_1}{dz} + k_\eta \delta g(x_1,x_2) = 0 \\ D\frac{d^2x_2}{dz^2} - v\frac{dx_2}{dz} + g(x_1,x_2) = 0 \\ \\ D\frac{dx_1}{dz}(0) - vk_\eta x_1(0) = \frac{dx_1}{dz}(1) = 0 \\ D\frac{dx_2}{dz}(0) - vx_2(0) = \frac{dx_2}{dz}(1) = 0 \end{cases} \tag{4.26}$$

where the function g is defined as

$$g(x_1,x_2) = v\alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}}$$

for $-1 < x_1$ and $0 \leq x_2 \leq 1$ and $g(-1,x_2) = 0$. Observe that equations (4.26) have the same form as the equations (4.16). Hence, the analysis is the same as in Section 4.2. Note also that if one lets $\eta \to 0$, then one recovers the case $Pe_m = Pe_h$.

Chapter 5

Stability of the equilibrium profiles

Contents

In this chapter, an analysis of the exponential stability of the equilibrium profiles is performed. We first construct a linearized model of the nominal one around a specific equilibrium profile. Then, we study the well-posedness of this linearized model. After this step, three cases are taken into account, especially based on the relation between the Peclet numbers, as for the analysis of the existence of equilibrium profiles. In this way, some changes of variables are introduced to put the linearized model in some form in order to show notably that the stability analysis is reduced to an eigenvalue problem. Some numerical simulations support the theoretical results.

5.1 Construction of a linearized model around an equilibrium profile

In order to write a linearized model around an equilibrium denoted by $(x_1^\star, x_2^\star)$, we consider PDEs (2.3) with the associated boundary conditions and we define the variables

$$\begin{cases} \xi_1(t,z) = x_1(t,z) - x_1^\star(z), \\ \xi_2(t,z) = x_2(t,z) - x_2^\star(z), \end{cases} \tag{5.1}$$

for $t \in [0,+\infty)$ and $z \in [0,1]$, being the time and the spatial variables respectively. Note that these variables represent the perturbations about the equilibrium $(x_1^\star, x_2^\star)$. For the sake of simplicity, we denote by g the function defined for (x_1,x_2) in $\mathbb{R}^2$ such that $-1 < x_1$ and $0 \leq x_2 \leq 1$ by

$$g(x_1,x_2) = \alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = \frac{k_0 L}{v}(1-x_2)e^{\frac{-\mu}{1+x_1}}.$$

Looking at the time derivative of the first variable of (5.1) and taking PDEs (2.7) into account, we have

$$\begin{aligned} \frac{\partial \xi_1}{\partial t} = \frac{\partial x_1}{\partial t} &= \frac{1}{Pe_h}\frac{\partial^2 x_1}{\partial z^2} - \frac{\partial x_1}{\partial z} - \gamma x_1 + \delta g(x_1,x_2) \\ &= \frac{1}{Pe_h}\frac{\partial^2 (\xi_1 + x_1^\star)}{\partial z^2} - \frac{\partial (\xi_1 + x_1^\star)}{\partial z} - \gamma(\xi_1 + x_1^\star) + \delta g(\xi_1 + x_1^\star, \xi_2 + x_2^\star) \end{aligned}$$

$$= \frac{1}{Pe_h}\frac{\partial^2 \xi_1}{\partial z^2} - \frac{\partial \xi_1}{\partial z} - \gamma \xi_1 + \frac{1}{Pe_h}\frac{d^2 x_1^\star}{dz^2} - \frac{dx_1^\star}{dz} - \gamma x_1^\star + \delta g\left(\xi_1 + x_1^\star, \xi_2 + x_1^\star\right).$$

Notice that the different parameters are available in Table 2.1 and in equations (2.4) and (2.8). To linearize the model, we have to approximate the function g by its first order approximation around the equilibrium $(x_1^\star, x_2^\star)$, which is given by

$$g\left(\xi_1 + x_1^\star, \xi_2 + x_2^\star\right) \simeq g\left(x_1^\star, x_2^\star\right) + \frac{\partial g}{\partial x_1}\left(x_1^\star, x_2^\star\right)\xi_1 + \frac{\partial g}{\partial x_2}\left(x_1^\star, x_2^\star\right)\xi_2. \tag{5.2}$$

By plugging (5.2) into the time derivative of ξ_1 and denoting the functions $\frac{\partial g}{\partial x_1}\left(x_1^\star, x_2^\star\right)$ and $\frac{\partial g}{\partial x_2}\left(x_1^\star, x_2^\star\right)$ by $g_{x_1}^\star(z)$ and $g_{x_2}^\star(z)$ respectively, it follows that

$$\begin{aligned}\frac{\partial \xi_1}{\partial t} &= \frac{1}{Pe_h}\frac{\partial^2 \xi_1}{\partial z^2} - \frac{\partial \xi_1}{\partial z} - \gamma \xi_1 + \delta g_{x_1}^\star(z)\xi_1 + \delta g_{x_2}^\star(z)\xi_2 + \left(\frac{1}{Pe_h}\frac{d^2 x_1^\star}{dz^2} - \frac{dx_1^\star}{dz} - \gamma x_1^\star + \delta g\left(x_1^\star, x_2^\star\right)\right) \\ &= \frac{1}{Pe_h}\frac{\partial^2 \xi_1}{\partial z^2} - \frac{\partial \xi_1}{\partial z} - \gamma \xi_1 + \delta g_{x_1}^\star(z)\xi_1 + \delta g_{x_2}^\star(z)\xi_2,\end{aligned}$$

where the last equality is deduced from the equilibrium equations (4.1). Similarly, we have

$$\frac{\partial \xi_2}{\partial z} = \frac{1}{Pe_m}\frac{\partial^2 \xi_2}{\partial z^2} - \frac{\partial \xi_2}{\partial z} + g_{x_1}^\star(z)\xi_1 + g_{x_2}^\star(z)\xi_2. \tag{5.3}$$

The associated boundary conditions are expressed as

$$\begin{aligned}\frac{\partial \xi_1}{\partial z}(t,0) = \frac{\partial x_1}{\partial z}(t,0) - \frac{dx_1^\star}{dz}(0) &= Pe_h x_1(t,0) - Pe_h x_1^\star(0) \\ &= Pe_h\left(x_1(t,0) - x_1^\star(0)\right) \\ &= Pe_h \xi_1(t,0),\end{aligned}$$

and

$$\frac{\partial \xi_2}{\partial z}(t,0) = Pe_m \xi_2(t,0),\ \frac{\partial \xi_1}{\partial z}(t,1) = 0,\ \frac{\partial \xi_2}{\partial z}(t,1) = 0.$$

So, the whole linearized model around the equilibrium $(x_1^\star, x_2^\star)$ is given by

$$\begin{cases} \frac{\partial \xi_1}{\partial t} = \frac{1}{Pe_h}\frac{\partial^2 \xi_1}{\partial z^2} - \frac{\partial \xi_1}{\partial z} - \gamma \xi_1 + \delta g_{x_1}^\star(z)\xi_1 + \delta g_{x_2}^\star(z)\xi_2 \\ \frac{\partial \xi_2}{\partial z} = \frac{1}{Pe_m}\frac{\partial^2 \xi_2}{\partial z^2} - \frac{\partial \xi_2}{\partial z} + g_{x_1}^\star(z)\xi_1 + g_{x_2}^\star(z)\xi_2 \\ \frac{\partial \xi_1}{\partial z}(t,0) = Pe_h \xi_1(t,0),\ \frac{\partial \xi_2}{\partial z}(t,0) = Pe_m \xi_2(t,0) \\ \frac{\partial \xi_1}{\partial z}(t,1) = 0,\ \frac{\partial \xi_2}{\partial z}(t,1) = 0. \end{cases} \tag{5.4}$$

5.2 Well-posedness of the linearized model

Before analyzing the stability of the equilibrium profiles, i.e. the stability of the linearized model constructed in the previous section, we have to show that this linearized model is well-posed, i.e. that the linear

(unbounded) operator describing the dynamic is the infinitisimal genarator of a C_0-semigroup. Looking at equations (5.4), this linear operator is given by

$$\begin{pmatrix} \frac{1}{Pe_h}\frac{d^2}{dz^2} - \frac{d}{dz} - \gamma I + \delta g^\star_{x_1}(z) I & \delta g^\star_{x_2}(z) I \\ g^\star_{x_1}(z) & \frac{1}{Pe_m}\frac{d^2}{dz^2} - \frac{d}{dz} + g^\star_{x_2}(z) I \end{pmatrix} \overset{\text{not.}}{=} \hat{A} \tag{5.5}$$

on the domain $D\left(\hat{A}\right) = D(A)$ where A is the operator defined by (2.9) and (2.10). The operator $\hat{A}$ can be decomposed as

$$\hat{A} = \begin{pmatrix} \frac{1}{Pe_h}\frac{d^2}{dz^2} - \frac{d}{dz} - \gamma I & 0 \\ 0 & \frac{1}{Pe_m}\frac{d^2}{dz^2} - \frac{d}{dz} \end{pmatrix} + \begin{pmatrix} \delta g^\star_{x_1}(z) I & \delta g^\star_{x_2}(z) I \\ g^\star_{x_1}(z) I & g^\star_{x_2}(z) I \end{pmatrix} = A + \begin{pmatrix} \delta g^\star_{x_1}(z) I & \delta g^\star_{x_2}(z) I \\ g^\star_{x_1}(z) I & g^\star_{x_2}(z) I \end{pmatrix}. \tag{5.6}$$

In order to show that $\hat{A}$ is the infinitesimal generator of a C_0-semigroup, we present the following result from (Engel and Nagel, 2006, Bounded perturbation theorem) which provides conditions on the operator B such that $A+B$ is the infinitesimal generator of a C_0-semigroup whenever so is A.

Theorem 8. *Let operator A with domain $D(A)$ be the infinitesimal generator of a strongly continuous semigroup $(T(t))_{t\geq 0}$ on a Banach space H satisfying*

$$\|T(t)\| \leq Me^{\omega t} \quad \textit{for all} \quad t \geq 0$$

and some $\omega \in \mathbb{R}, M \geq 1$. If $B \in \mathcal{L}(H)$, then $C := A+B$ with $D(C) := D(A)$ generates a strongly continuous semigroup $(S(t))_{t\geq 0}$ satisfying

$$\|S(t)\| \leq Me^{(\omega + M\|B\|)t} \quad \textit{for all} \quad t \geq 0.$$

We know from Chapter 2 that the operator A defined by (2.9) and (2.10) generates a C_0-semigroup. In order to apply Theorem 8, we still have to show that the operator

$$\begin{pmatrix} \delta g^\star_{x_1}(z) I & \delta g^\star_{x_2}(z) I \\ g^\star_{x_1}(z) I & g^\star_{x_2}(z) I \end{pmatrix} := \tilde{A} \tag{5.7}$$

is linear and bounded from H to H, which will lead to the fact that $A+\tilde{A}$ generates a C_0-semigroup [1], i.e. that the linearized model around the equilibrium is well-posed. In order to perform this step, we decompose $\tilde{A}$ as $\tilde{A}_1 + \tilde{A}_2$ where

$$\tilde{A}_1 := \begin{pmatrix} \delta g^\star_{x_1}(z) I & 0 \\ 0 & g^\star_{x_2}(z) I \end{pmatrix} \tag{5.8}$$

and

$$\tilde{A}_2 := \begin{pmatrix} 0 & \delta g^\star_{x_2}(z) I \\ g^\star_{x_1}(z) I & 0 \end{pmatrix}. \tag{5.9}$$

1. Note that the domain of $\tilde{A}$ is H since it is a matrix whose elements are multiplicative functions depending on the spatial variable.

The operator $\hat{A}$ is now expressed as $A+\tilde{A}_1+\tilde{A}_2$. We will successively apply twice Theorem 8, first on the pair of operators $\left(A,\tilde{A}_1\right)$ and then on $\left(A+\tilde{A}_1,\tilde{A}_2\right)$. To do so, first notice the explicit forms of functions $g^\star_{x_1}(z)$ and $g^\star_{x_2}(z)$, which are given by

$$\frac{k_0 L}{v}\frac{\mu\left(1-x_2^\star(z)\right)}{\left(1+x_1^\star(z)\right)^2}e^{\frac{-\mu}{1+x_1^\star(z)}} \tag{5.10}$$

and

$$-\frac{k_0 L}{v}e^{\frac{-\mu}{1+x_1^\star(z)}} \tag{5.11}$$

respectively. Note also that $x_1^\star(z)$ and $x_2^\star(z)$ satisfy

$$-1\leq x_1^\star(z) \text{ and } 0\leq x_2^\star(z)\leq 1 \tag{5.12}$$

for a.e. $z\in[0,1]$. This is basically due to the fact that the operator A is the infinitesimal generator of a C_0-semigroup on D, which is given by (2.12).

Proposition 4. *The operators $\tilde{A}_1$ and $\tilde{A}_2$ defined by (5.9) with $D\left(\tilde{A}_1\right)=D\left(\tilde{A}_2\right)=H$ are linear and bounded on H, i.e. are in $\mathcal{L}(H)$.*

Proof. The linearity of these two operators can be easily shown. For the boundedness, we will show it only for operator $\tilde{A}_1$. Similar arguments can be used for operator $\tilde{A}_2$. We have to show that there exists some constant $c>0$ such that for every $\xi=\begin{pmatrix}\xi_1 & \xi_2\end{pmatrix}^T\in H$,

$$\|\tilde{A}_1\xi\|\leq c\|\xi\|$$

holds. Taking $\xi\in H$, a straightforward computation of $\|\tilde{A}_1\xi\|^2$ gives

$$\begin{aligned}\left\|\tilde{A}_1\xi\right\|^2&=\left\|\left(\tilde{A}_1\xi\right)_1\right\|^2+\left\|\left(\tilde{A}_1\xi\right)_2\right\|^2\\&=\left\|\delta\frac{k_0L}{v}\left(1-x_2^\star\right)e^{\frac{-\mu}{1+x_1^\star}}\frac{\mu}{\left(1+x_1^\star\right)^2}\xi_1\right\|^2+\left\|-\frac{k_0L}{v}e^{\frac{-\mu}{1+x_1^\star}}\xi_2\right\|^2,\end{aligned}$$

where the norm on H is given in Definition 6. The dependence on the spatial variable of the equilibrium profile has been omitted for the sake of readability. Using relations (5.12) combined with the definition of the norm in $L^2(0,1)$, we have

$$\begin{aligned}\left\|\tilde{A}_1\xi\right\|^2&\leq\frac{\delta^2k_0^2L^2\mu^2}{v^2}\left\|\frac{1}{\left(1+x_1^\star\right)^2}\xi_1\right\|^2+\frac{k_0^2L^2}{v^2}\|\xi_2\|^2\\&\leq\frac{\delta^2k_0^2L^2\mu^2\kappa}{v^2}\|\xi_1\|^2+\frac{k_0^2L^2}{v^2}\|\xi_2\|^2,\end{aligned}$$

where

$$\kappa=\left\|\frac{1}{\left(1+x_1^\star\right)^2}\right\|_\infty,$$

which is constant and finite since $1+x_1^\star$ has no root [2] in $[0,1]$. In this way,

$$\begin{aligned}\left\|\tilde{A}_1\xi\right\|^2 &\leq \max\left\{\frac{\delta^2 k_0^2 L^2 \mu^2 \kappa}{\nu^2}, \frac{k_0^2 L^2}{\nu^2}\right\}\left(\|\xi_1\|^2+\|\xi_2\|^2\right)\\ &= \max\left\{\frac{\delta^2 k_0^2 L^2 \mu^2 \kappa}{\nu^2}, \frac{k_0^2 L^2}{\nu^2}\right\}\|\xi\|^2.\end{aligned}$$

This last inequality provides us with an estimate of $\left\|\tilde{A}_1\right\|$:

$$\left\|\tilde{A}_1\right\| \leq \sqrt{\max\left\{\frac{\delta^2 k_0^2 L^2 \mu^2 \kappa}{\nu^2}, \frac{k_0^2 L^2}{\nu^2}\right\}}.$$

Hence, operator $\tilde{A}_1$ is bounded from H to H. ■

Remark 3. *In the proof of Proposition 4, we used the infinity-norm $\|\cdot\|_\infty$. The space $L^\infty(a,b)$ is defined as the Lebesgue space of complex-valued essentially bounded functions on $[a,b]$, i.e. for a.e. elements of $[a,b]$. Taking $f \in L^\infty(a,b)$, the associated norm, $\|f\|_\infty$ is defined as*

$$\sup_{z\in[a,b]}\operatorname{ess}|f(z)| = \inf\{C \in [0,+\infty) : |f(z)| \leq C \text{ a.e.on } [a,b]\}.$$

Theorem 9. *The operator $\hat{A}$ with domain $D\left(\hat{A}\right) = D(A)$ is the infinitesimal generator of a C_0- semigroup on $D\left(\hat{A}\right)$.*

Proof. The result follows directly by using Theorem 8 successively on $(A,\tilde{A}_1)$ and $(A+\tilde{A}_1,\tilde{A}_2)$ and by taking Proposition 4 into account. ■

5.3 Transformation on the linearized system

This subsection is devoted to the computation of a change of variables on (5.4) in order to express it in a certain form to be able to justify the choice of the method adopted to analyze the stability of the equilibrium profiles in the next sections. This change of variables was proposed in (Varma and Aris, 1977, Section 2.5.2.). Note also that in the following considerations, we suppose the reactor to be adiabatic, which implies that $\gamma = 0$. The proposed change of variables is

$$\begin{cases}\xi_1(t,z) = e^{\frac{Pe_h}{2}}\hat{\xi}_1(t,z)\\ \xi_2(t,z) = e^{\frac{Pe_m}{2}}\hat{\xi}_2(t,z).\end{cases} \tag{5.13}$$

Putting this change of variables in equations (5.4), a straightforward computation yields the new system

2. This is a conjecture. The opposite could not be found in numerical simulations but a proof is still expected.

$$\begin{cases} \frac{\partial \hat{\xi}_1}{\partial t} = \frac{1}{Pe_h}\frac{\partial^2 \hat{\xi}_1}{\partial z^2} - \frac{Pe_h}{4}\hat{\xi}_1 + \delta G_1(z)\hat{\xi}_1 + \delta \hat{G}_2(z)\hat{\xi}_2 \\ \frac{\partial \hat{\xi}_2}{\partial t} = \frac{1}{Pe_m}\frac{\partial^2 \hat{\xi}_2}{\partial z^2} - \frac{Pe_m}{4}\hat{\xi}_2 + \hat{G}_1(z)\hat{\xi}_1 + G_2(z)\hat{\xi}_2 \\ \frac{\partial \hat{\xi}_1}{\partial z}(0) = \frac{Pe_h}{2}\hat{\xi}_1(0),\ \frac{\partial \hat{\xi}_2}{\partial z}(0) = \frac{Pe_m}{2}\hat{\xi}_2(0) \\ \frac{\partial \hat{\xi}_1}{\partial z}(1) = -\frac{Pe_h}{2}\hat{\xi}_1(1),\ \frac{\partial \hat{\xi}_2}{\partial z}(1) = -\frac{Pe_m}{2}\hat{\xi}_2(1), \end{cases} \tag{5.14}$$

where

$$G_1(z) = g_{x_1}\left(x_1^\star, x_2^\star\right),\ G_2(z) = g_{x_2}\left(x_1^\star, x_2^\star\right) \tag{5.15}$$

and

$$\hat{G}_1(z) = G_1(z)e^{\frac{Pe_h - Pe_m}{2}z},\ \hat{G}_2(z) = G_2(z)e^{\frac{Pe_m - Pe_h}{2}z}. \tag{5.16}$$

As pointed out in (Varma and Aris, 1977, Section 2.5.2.), equations (5.14) form a pair of coupled parabolic PDEs with corresponding boundary conditions.

5.4 Case 1 : $Pe_h = Pe_m \overset{\text{not.}}{=} Pe$

In this subsection, the stability of the equilibrium profiles for equal Peclet numbers will be investigated with different tools. Due to the equality between Pe_h and Pe_m, we will first simplify the analysis by reducing the system (5.14). Then, we will present a theorem first introduced in (Amundson, 1965) and then taken up in (Varma and Aris, 1977, Section 2.5.2.1.). This theorem provides necessary and sufficient conditions for an equilibrium to be stable or unstable. Finally, a numerical method for the detection of stability or instability of an equilibrium will be considered. All these concepts are illustrated by some numerical simulations.
First notice that in this case, the identites

$$\hat{G}_1(z) = G_1(z),\ \hat{G}_2(z) = G_2(z)$$

hold for all $z \in [0,1]$. In order to simplify equations (5.14), we introduce the following change of variables, see (Varma and Aris, 1977, Section 2.5.2.)

$$\xi(t,z) = \xi_1(t,z) - \delta\xi_2(t,z). \tag{5.17}$$

In this way, an equivalent system to (5.14) is

$$\begin{cases} \frac{\partial \xi}{\partial t} = \frac{1}{Pe}\frac{\partial^2 \xi}{\partial z^2} - \frac{Pe}{4}\xi \\ \frac{\partial \hat{\xi}_1}{\partial t} = \frac{1}{Pe}\frac{\partial^2 \hat{\xi}_1}{\partial z^2} - G_2(z)\xi - \left(\frac{Pe}{4} - G_2(z) - \delta G_1(z)\right)\hat{\xi}_1 \\ \frac{\partial \xi}{\partial z}(0) = \frac{Pe}{2}\xi(0),\ \frac{\partial \hat{\xi}_1}{\partial z}(0) = \frac{Pe}{2}\hat{\xi}_1(0) \\ \frac{\partial \xi}{\partial z}(1) = -\frac{Pe}{2}\xi(1),\ \frac{\partial \hat{\xi}_1}{\partial z}(1) = -\frac{Pe}{2}\hat{\xi}_1(1). \end{cases} \tag{5.18}$$

The advantage is that the system of PDEs is now uncoupled. The first equation of this system with the

associated boundary and initial conditions is a second order parabolic PDE whose solution is given by

$$\xi(t,z) = \sum_{n=1}^{+\infty} \psi_n K_n \phi_n(z)\, e^{-\left(\beta_n^2 + \frac{Pe}{4}\right)t}, \tag{5.19}$$

where

$$\phi_n(z) = \beta_n\sqrt{Pe}\cos\left(\beta_n\sqrt{Pe}\,z\right) + \frac{Pe}{2}\sin\left(\beta_n\sqrt{Pe}\,z\right),\ \psi_n = \int_0^1 f(z)\phi_n(z)dz,$$

see also (Varma and Aris, 1977, Section 2.5.2.1.). Notice that the coefficients K_n are given by

$$K_n = \left(\int_0^1 \phi_n^2(z)dz\right)^{-\frac{1}{2}} = \left[\frac{2}{\beta_n^2 Pe + Pe + \frac{Pe^2}{4}}\right]^{\frac{1}{2}} \tag{5.20}$$

and that $f(z)$ is the initial condition, i.e. $\xi(0,z) = f(z)$. Note also that the coefficients β_n are solutions of the resolvent equation

$$\tan\left(\beta\sqrt{Pe}\right) = \frac{4\beta\sqrt{Pe}}{4\beta^2 - Pe}. \tag{5.21}$$

It is obvious from equation (5.19) that $\xi(t,z)$ tends exponentially fast to 0 when t tends to $+\infty$. Hence, this term does not influence the exponential stability of the equilibrium profiles. In this way, stability is based on the PDE with boundary conditions

$$\begin{cases} \frac{\partial\hat{\xi}_1}{\partial t} = \frac{1}{Pe}\frac{\partial^2\hat{\xi}_1}{\partial z^2} - \left(\frac{Pe}{4} - G_2(z) - \delta G_1(z)\right)\hat{\xi}_1 \\ \frac{\partial\hat{\xi}_1}{\partial z}(0) = \frac{Pe}{2}\hat{\xi}_1(0),\ \frac{\partial\hat{\xi}_1}{\partial z}(1) = -\frac{Pe}{2}\hat{\xi}_1(1), \end{cases} \tag{5.22}$$

which can be rewritten as

$$\begin{cases} \frac{\partial\hat{\xi}_1}{\partial t} = -\left(\frac{\partial}{\partial z}\left(-\frac{1}{Pe}\frac{\partial\hat{\xi}_1}{\partial z}\right) + q(z)\hat{\xi}_1\right) \\ \frac{\partial\hat{\xi}_1}{\partial z}(0) - \frac{Pe}{2}\hat{\xi}_1(0) = 0,\ \frac{\partial\hat{\xi}_1}{\partial z}(1) + \frac{Pe}{2}\hat{\xi}_1(1) = 0 \end{cases} \tag{5.23}$$

where $q(z) = \frac{Pe}{4} - G_2(z) - \delta G_1(z)$. According to (Delattre et al., 2003, Definition 2), equations (5.23) describe a Sturm-Liouville system. Hence, the stability analysis can be adressed by solving an eigenvalue problem. In view of equations (5.23), this eigenvalue problem is expressed as

$$\begin{cases} \frac{1}{Pe}\frac{d^2\phi_n}{dz^2} - q(z)\phi_n = -\lambda_n\phi_n \\ \frac{d\phi_n}{dz}(0) = \frac{Pe}{2}\phi_n(0),\ \frac{d\phi_n}{dz}(1) = -\frac{Pe}{2}\phi_n(1), \end{cases} \tag{5.24}$$

where $\{\lambda_n\}_{n\in\mathbb{N}}$ represents the set of eigenvalues and $\{\phi_n(z)\}_{n\in\mathbb{N}}$ are the corresponding eigenvectors of operator $\frac{1}{Pe}\frac{d^2}{dz^2} - q(z)I$. Due to the parabolicity of PDE (5.23), the function $\hat{\xi}_1$ has the form

$$\hat{\xi}_1(t,z) = \sum_{n=1}^{+\infty} \alpha_n(t)\phi_n(z) \tag{5.25}$$

where $\alpha_n(t)$ is $e^{-\lambda_n t}$ up to a multiplicative constant and $\phi_n(z)$ is the eigenvector introduced in (5.19). So, the objective is now to estimate the least eigenvalue of (5.23) denoted by λ_1. If λ_1 is positive, it is obvious

from (5.25) that the system (5.23) is exponentially stable. Otherwise, it is unstable. Therefore, we refer to a theorem introduced in (Amundson, 1965) and recalled in (Varma and Aris, 1977, Section 2.5.2.1.).

Theorem 10. *Consider the function q defined for $z \in [0,1]$ by $q(z) = \frac{Pe}{4} - G_2(z) - \delta G_1(z)$ where the functions G_1 and G_2 are given in (5.15). If $p(z)$ is the solution of the system*

$$\begin{cases} \frac{1}{Pe}\frac{d^2p}{dz^2} - qp = 0 \\ p(0) = 1,\ \frac{dp}{dz}(0) = \frac{Pe}{2}, \end{cases} \tag{5.26}$$

then necessary and sufficient conditions for the least eigenvalue of (5.24) to be positive are

- $p(z) > 0$ *for all* $z \in [0,1]$
- $\frac{dp}{dz}(1) + \frac{Pe}{2}p(1) \geq 0$.

Hence, the exponential stability is reduced to the computation of the solution of ODE (5.26). We shall now present the proof of this theorem, first introduced in (Amundson, 1965). The main idea is the following : if the solution of equations (5.26) cuts the axis $[0,1]$, then there is a negative eigenvalue for equations (5.24) and the system is unstable. If it does not cut that axis at any point, the quotient $\frac{\frac{dp}{dz}(1)}{p(1)}$ can be computed. If it is less than $-\frac{Pe}{2}$, there is a negative eigenvalue and the system is unstable.

There is no loss of generality in assuming that the solution of (5.23) has value 1 for $z = 0$ and the derivative of that solution has the value $\frac{Pe}{2}$ for $z = 0$ since any multiple of a solution of (5.24) is also a solution of (5.24). Hence, the boundary condition

$$\frac{d\phi_n}{dz}(0) = \frac{Pe}{2}\phi_n(0)$$

makes sense. Before starting the proof, consider the two systems

$$\begin{cases} \frac{d^2u}{dz^2} - G_1(z)u = 0 \\ u(0) = 1, u'(0) = \frac{Pe}{2} \end{cases} \tag{5.27}$$

and

$$\begin{cases} \frac{d^2v}{dz^2} - G_2(z)v = 0 \\ v(0) = 1, v'(0) = \frac{Pe}{2} \end{cases} \tag{5.28}$$

whose solutions are $u(z)$ and $v(z)$ respectively. Suppose also that $G_1(z)$ and $G_2(z)$ are real continuous functions. Moreover, one introduces two lemmas, see (Amundson, 1965), that will not be proven but necessary to prove Theorem 10.

Lemma 3. *Consider the two systems (5.27) and (5.28). If $G_1(z) \geq G_2(z)$ on $[0,1]$ and $G_1(z) \neq G_2(z)$ on any finite subinterval, then if $u(z)$ has m zeroes on $a < z \leq b$, contained in $[0,1]$, $v(z)$ has also at least m zeroes in the same interval and the $i-th$ zero of $v(z)$ is less than the $i-th$ of $u(z)$.*

Lemma 4. *Assume the same hypothesis as in Lemma 3 on the functions $G_1(z)$ and $G_2(z)$. Consider $a < c \leq b$ an interval contained in $[0,1]$ and suppose c is not a zero of $u(z)$ or $v(z)$. Then, by Lemma 3, $v(z)$ has at least as many zeroes as $u(z)$ in (a,c). Moreover, if c is such that $u(z)$ and $v(z)$ have the same number of zeroes in $a < z < c$, then*

$$\frac{u'(c)}{u(c)} > \frac{v'(c)}{v(c)}. \tag{5.29}$$

Proof of Theorem 10. Consider the systems (5.27) and (5.28). Let $G_2(z)$ be $q(z)$ of Theorem 10 and denote by $v(z)$ the solution of (5.28) with $G_2(z)$. Moreover, consider $G_1(z)$ being $q(z) - \rho$ where the function q is the same as before and ρ is a negative real constant. The solution of (5.27) with $G_1(z)$ is denoted by $u(z)$. Obviously, one has that $G_1(z) > G_2(z)$.

Suppose also that $v(z)$ has at least one zero in $[0,1]$ and that ρ is an arbitrary parameter that is not fixed. In this way, let us start by considering $\rho = 0$ in $G_1(z)$. More ρ decreases (hence, $G_1(z)$ increases), more the curve of $u(z)$ will have fewer and fewer oscillations between positive and negative values, according to Lemma 3. For sufficiently large negative values of ρ, one can even imagine that $u(z)$ will remain strictly positive on $[0,1]$. Fix now $\rho_1 < 0$ such that for $\rho = \rho_1$, $u(1) = 0$ and for $\rho < \rho_1$, $u(z) > 0$ for each $z \in [0,1]$. Let $\varepsilon > 0$; one defines

$$\begin{cases} \overline{G}_1(z) := q(z) - \rho, \ \rho < \rho_1 - \varepsilon \\ \overline{G}_2(z) := q(z) - (\rho_1 - \varepsilon). \end{cases} \tag{5.30}$$

In this way, $\overline{G}_1(z) > \overline{G}_2(z)$. We denote by $U(z)$ the solution of (5.27) with $\overline{G}_1(z)$ and by $V(z)$ the solution of (5.28) with $\overline{G}_2(z)$. By the assumptions and by construction, $V(z)$ has no zeroes in $[0,1]$ and by Lemma 3, so is $U(z)$. By Lemma 4, the relation

$$\frac{U'(1)}{U(1)} > \frac{V'(1)}{V(1)} \tag{5.31}$$

holds. By letting ε tend to 0, the quantity $\frac{V'(1)}{V(1)}$ tends to $-\infty$ because $\overline{G}_2(z)$ tends to $q(z) - \rho_1$ and by assumption, $V(1) = 0$ in this case. Furthermore, for small values of ε, the function V is strictly positive, so the only way to go to zero for $z = 1$ is that V decreases. Hence, $V'(1)$ is negative.

We will now choose ε sufficiently small such that

$$\frac{V'(1)}{V(1)} < -a^* < -\frac{Pe}{2}, \tag{5.32}$$

where a^* is a strictly positive and real constant. As ρ starts at $\rho_1 - \varepsilon$ and further decreases, $\frac{U'(1)}{U(1)}$ varies continuously from $-a^*$ to a positive value [3] and must pass through $-\frac{Pe}{2}$ because of the boundary

3. Since ρ decreases, the function V shows less and less oscillations to remain stricly positive. Consequently, during the process, the only zero of U (for $z = 1$) becomes « less and less » a zero and the slope of U for $z = 1$ becomes less and less negative and even positive.

condition

$$\frac{d\phi_n}{dz}(1) = -\frac{Pe}{2}\phi_n(1).$$

When the quantity $\frac{U'(1)}{U(1)}$ is equal to $-\frac{Pe}{2}$, the value of ρ is negative. At that moment, there is a negative eigenvalue for equations [4] (5.24). Remember that we started by assuming that the solution of (5.26) possesses at least one zero in $[0,1]$. In that case, we showed that, by construction, at least one eigenvalue of (5.24) was negative, which provides instability.

The next step consists of assuming that the solution of (5.26) does not vanish on $[0,1]$. In this case, if that solution, denoted by $v(z)$, satisfies

$$\frac{v'(1)}{v(1)} < -\frac{Pe}{2}, \tag{5.33}$$

then there is a negative eigenvalue. To prove this, consider again $G_2(z) = q(z)$ and $G_1(z) = q(z) - \rho$ ($\rho \leq 0$) whose solutions are $v(z)$ and $u(z)$ respectively. Since by assumption $v(z)$ does not vanish on $[0,1]$ and since $G_1(z) > G_2(z)$, the inequality

$$\frac{u'(1)}{u(1)} \geq \frac{v'(1)}{v(1)} \tag{5.34}$$

holds by Lemma 4. As ρ starts at 0 and becomes $-\infty$, $\frac{u'(1)}{u(1)}$ increases continuously varying from $\frac{v'(1)}{v(1)} < -\frac{Pe}{2}$ to a positive number when ρ is very large and negative. Holding a same reasoning as before, there must be a negative eigenvalue for which

$$\frac{u'(1)}{u(1)} = -\frac{Pe}{2}.$$

Hence, the system is unstable. The only possibility to get stability is that both the solution of (5.24), denoted by $u(z)$, does not vanish on $[0,1]$ and $\frac{u'(1)}{u(1)} \geq -\frac{Pe}{2}$. ■

To go further in the analysis of the stability of an equilibrium profile in a nonisothermal axial dispersion tubular reactor, we present a numerical method introduced in (McGowin and Perlmutter, 1970), known as *Galerkin's method* or *Weighted Residuals method*. The leading idea of this method is to work in a finite-dimensional framework by making approximation estimates of the solution of (5.23). To construct this method, we first consider again the PDE (5.18) in which we estimate the solution $\hat{\xi}_1$ by a trial one, which is given by

$$\tilde{\xi}_1(t,z) = \sum_{n=1}^{m} \alpha_n(t)\phi_n(z), \tag{5.35}$$

i.e. we take the exact solution (5.25) in which we troncate the serie expansion by a finite sum. The more m tends to $+\infty$, the more $\tilde{\xi}_1$ provides a good approximation of $\hat{\xi}_1$. Note that the trial solution (5.35) satisfies the boundary conditions of (5.18). The aim of the method is to rewrite (5.22) as a system

$$\dot{x} = \mathbb{A}x \tag{5.36}$$

4. Notice that the eigenvalues are $\{\lambda_n\}_{n\in\mathbb{N}}$. Hence, a « negative » eigenvalue is symbolized by a positive value of $-\lambda_n$ (for a given n), which means that the system is unstable.

where $\mathbb{A}$ is a finite dimensional matrix in $\mathbb{R}^{m\times m}$ and where the $i-$th element of vector x is $\alpha_i(t)$. Once the matrix $\mathbb{A}$ is built, there is only to look at its eigenvalues which caracterize the modes of the dynamical system (5.36). Hence, the equilibrium profile is exponentially stable if the biggest real part of these eigenvalues is strictly negative and unstable otherwise. In order to obtain the system (5.36), we define the *error residuals* that results from the approximation (5.35) and which is given by

$$\begin{aligned}\Gamma_{\xi_1}(z) &= \frac{\partial\tilde{\xi}_1}{\partial t} - \frac{1}{Pe}\frac{\partial^2\tilde{\xi}_1}{\partial z^2} + q(z)\tilde{\xi}_1 \\ &= \sum_{n=1}^{m}\frac{d\alpha_n}{dt}(t)\phi_n(z) - \frac{1}{Pe}\sum_{n=1}^{m}\alpha_n(t)\frac{d^2\phi_n}{dz^2}(z) + q(z)\sum_{n=1}^{m}\alpha_n(t)\phi_n(z).\end{aligned}$$

The Galerkin's method, see (McGowin and Perlmutter, 1970), makes these residuals orthogonal to the eigenfunctions $\{\phi_n(z)\}_{n=1}^m$, i.e. $\langle\Gamma_{\xi_1},\phi_n\rangle_{L^2(0,1)} = 0$ for $n = 1,\dots,m$. Developping this relation, we have

$$\int_0^1 \Gamma_{\xi_1}(z)\phi_n(z)dz = 0,\ n = 1,\dots,m. \tag{5.37}$$

Expliciting the orthogonality for the $i-$th eigenvector, it yields the following

$$\begin{aligned}&\int_0^1\left[\sum_{n=1}^{m}\frac{d\alpha_n}{dt}(t)\phi_n(z)\right]\phi_i(z)dz - \frac{1}{Pe}\int_0^1\left[\sum_{n=1}^{m}\alpha_n(t)\frac{d^2\phi_n}{dz^2}(z)\right]\phi_i(z)dz \\ &\qquad + \int_0^1\left[q(z)\sum_{n=1}^{m}\alpha_n(t)\phi_n(z)\right]\phi_i(z)dz = 0 \\ \Leftrightarrow &\sum_{n=1}^{m}\frac{d\alpha_n}{dt}(t)\int_0^1\phi_n(z)\phi_i(z)dz = \frac{1}{Pe}\sum_{n=1}^{m}\alpha_n(t)\int_0^1\frac{d^2\phi_n}{dz^2}(z)\phi_i(z)dz - \sum_{n=1}^{m}\alpha_n(t)\int_0^1 q(z)\phi_n(z)\phi_i(z)dz.\end{aligned} \tag{5.38}$$

The following step consists of using the orthogonality of the eigenfunctions $\phi_n(z)$, i.e.

$$\int_0^1\phi_n(z)\phi_i(z)dz = C_n\delta_{ni} \tag{5.39}$$

and the fact that

$$\frac{d^2\phi_n}{dz}(z) = -\beta_n^2 Pe\,\phi_n(z). \tag{5.40}$$

Plugging (5.39) and (5.40) in (5.38), we have that

$$\begin{aligned}&\int_0^1\Gamma_{\xi_1}(z)\phi_i(z)dz = 0 \\ \Leftrightarrow &\sum_{n=1}^{m}\frac{d\alpha_n}{dz}(t)C_n\delta_{ni} = \frac{1}{Pe}\sum_{n=1}^{m}-\beta_n^2 Pe\,\alpha_n(t)C_n\delta_{ni} - \sum_{n=1}^{m}F(i,n)\alpha_n(t) \\ \Leftrightarrow &\frac{d\alpha_i}{dt}(t) = -\beta_i^2\alpha_i(t) - \frac{1}{C_i}\sum_{n=1}^{m}F(i,n)\alpha_n(t),\end{aligned}$$

where

$$F(i,j) = \int_0^1 q(z)\phi_i(z)\phi_j(z)dz.$$

Defining $x_i = \alpha_i(t)$ and $\mathbb{A}_{ij} = -\beta_i^2\delta_{ij} - \frac{1}{C_i}F(i,j)$ for $i,j = 1,\dots,m$, (5.36) is reached. This numerical method is summarized as an algorithm, see Algorithm 1.

Algorithm 1: Galerkin's method applied to the TRAD for equal Peclet numbers

1 Fix m, the number of terms in the trial solution

2 Compute β_i, $i = 1,\dots,m$ solutions of $\tan\left(\beta\sqrt{Pe}\right) = \frac{4\beta\sqrt{Pe}}{4\beta^2 - Pe}$

3 Compute $\phi_i(z)$ and C_i, $i = 1,\dots,m$ such that $\phi_i(z) = \beta_i\sqrt{Pe}\cos\left(\beta_i\sqrt{Pe}\,z\right) + \frac{Pe}{2}\sin\left(\beta_i\sqrt{Pe}\,z\right)$ and $\langle\phi_i,\phi_i\rangle_{L^2(0,1)} = C_i$

4 Compute $q(z) = \frac{Pe}{4} - G_2(z) - \delta G_1(z)$ where

$$G_2(z) = -\frac{k_0 L}{v}e^{\frac{-\mu}{1+x_1^\star(z)}}, G_1(z) = -\frac{G_2(z)\left(1-x_2^\star(z)\right)\mu}{\left(1+x_1^\star(z)\right)^2}$$

and where $x_1^\star(z)$ and $x_2^\star(z)$ are the approximated expressions of the equilibrium profiles given by (4.15)

5 Compute $F(i,j), i,j = 1,\dots,m$ by

$$\int_0^1 q(z)\phi_i(z)\phi_j(z)dz$$

6 Compute the matrix $\mathbb{A} \in \mathbb{R}^{m\times m}$ whose entries are given by $\mathbb{A}_{ij} = -\beta_i^2\delta_{ij} - \frac{1}{C_i}F(i,j)$, $i,j = 1,\dots,m$

7 Compute

$$\lambda^\star = \max_{\lambda\in\sigma(\mathbb{A})} \mathfrak{Re}(\lambda)$$

where $\sigma(\mathbb{A})$ is the set of eigenvalue of the matrix $\mathbb{A}$

8 If $\lambda^\star < 0$, the equilibrium profile is exponentially stable. Else, it is unstable.

To illustrate all these theoretical and numerical considerations, we present different numerical simulations, both in the case of only one equilibrium profile and in the case of three equilibrium profiles.

5.4.1 Numerical simulations : one equilibrium profile

By (Varma and Aris, 1977, Section 2.5.2.1.), it is well-known that in the case of only one equilibrium profile ($\rho = 0$, see equation (4.8)), the latter is always exponentially stable. We will take a set of parameters wich gives only one equilibrium profile and see what happens in this case with the different tools presented here before to study the stability. The first test we present is the representation of function $\hat{\xi}_1$ as a function of t and z and the representation of $\left\|\hat{\xi}_1(t,.)\right\|_{L^2}$ as a function of t. The stability can already be detected by these considerations. We take $\mu = 6$ and $\delta = 2$ such that $\rho = 0$ (see equation (4.8), it means that the system can exhibit only one equilibrium profile). We choose as velocity 0.02 and as diffusion coefficient 0.1 such that $Pe = 0.2$. In this case, the value of a for this equilibrium is 1.685. The functions $\hat{\xi}_1(t,z)$ and $\left\|\hat{\xi}_1(t,.)\right\|_{L^2}$ are depicted in Figures 5.1 and 5.2 respectively. Note also that the choosen initial condition is $\hat{\xi}_1(0,z) = -\sin(4\pi z) + 1$.

At the sight of these two graphs, it can be easily seen that the considered equilibrium profile is exponentially stable. To support this first idea, we use Theorem 10. The representation of function $p(z)$ can

be seen on figure 5.3. Furthermore, the value $\frac{dp}{dz}(1) + \frac{Pe}{2}p(1)$ is 1.07 in this case. With these two new elements, it appears that the equilibrium profile is exponentially stable.

The last test that was established was the computation of $\lambda^\star$ (see Algorithm 1). This value is equal to -4.478 which means that once again, the equilibrium profile is detected as exponentially stable.

5.4.2 Numerical simulations : three equilibrium profiles

In this section, we will establish the same tests as in the previous one : the numerical integration of the PDE (5.23) with appropriated boundary conditions, the use of Theorem 10 and the execution of Algorithm 1. All these tests will be performed on each of the three equilibria ($\rho > 0$, see equation (4.8)). Notice also that the same quantities as before are represented in this section. By (Varma and Aris, 1977, Section 2.5.2.1.), in the case of three equilibria, they are alternatively exponentially stable and unstable, with the pattern « stable - unstable - stable ». We take as parameters $\mu = 9, \delta = 3 (\rho = 297)$. The velocity v is fixed at 0.00815 and the diffusion coefficient D is equal set to 0.1. In such a way, $Pe = 0.0815$. The first value of a that reaches the choosen value of v is 0.098 (this value corresponds to the first equilibrium profile). The choosen initial condition is the same as in the case of only one equilibrium profile, $\hat{\xi}_1(0,z) = -\sin(4\pi z) + 1$.

Looking at the Figures 5.4 and 5.5, it can be seen that the first equilibrium is detected as exponentially stable by the numerical integration. Using Theorem 10 and by looking at Figure 5.6, it turns out that this equilibrium is exponentially stable. Computing the value $\frac{dp}{dz}(1) + \frac{Pe}{2}p(1)$, we obtain 0.0264. We conclude the exponentially stability by Theorem 10. Finally, executing Algorithm 1 on this equilibrium, the value $\lambda^\star$ found is -0.3183 which supports once again the exponential stability.

The second value of a that reaches the velocity is 0.0244 and caracterizes the second equilibrium profile. All other parameters remain unchanged. The numerical integration reveals an unstable behaviour (see Figures 5.7 and 5.8). Using Theorem 10 and looking only at the graph of $p(z)$ (see Figure 5.9), one cannot conclude the unstability but the value $\frac{dp}{dz}(1) + \frac{Pe}{2}p(1)$ is -0.0248, which provides unstability of this equilibrium profile. Computing the value $\lambda^\star$ of Algorithm 1, one finds 0.3021 which means that at least one eigenvalue of (5.23) is positive. Hence, the equilibrium profile is unstable.

As exposed in (Varma and Aris, 1977, Section 2.5.2.1.), the last equilibrium profile is expected to be exponentially stable. In this case, the value of a is 2.753. Firstly, Figures 5.10 and 5.11 (numerical integration) point in this direction. Applying Theorem 10, function $p(z)$ is strictly positive on the interval $[0,1]$ (see Figure 5.12) and the value $\frac{dp}{dz}(1) + \frac{Pe}{2}p(1)$ is 0.9295. The Theorem confirms exponential stability. The dominant eigenvalue $\lambda^\star$ is equal to -9.8844, which means the same conclusion. Note also that $\lambda^\star$ tells us information on the speed of convergence or divergence of the state trajectories. More negative this value is, faster the state trajectory goes exponentially fast to 0 and more positive it is, faster the state diverges.

In conclusion, one can say with relatively high certainty that both numerical and theoretical results agree and are also consistent with the theory first presented in (Amundson, 1965) and recalled in (Varma and Aris, 1977, Section 2.5.2.1.).

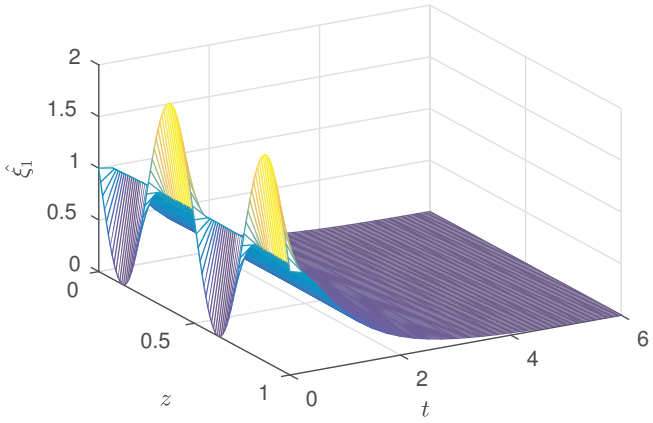

Fig. 5.1 – Function $\hat{\xi}_1(t,z)$ for $\mu = 6, \delta = 2, a = 1.685$.

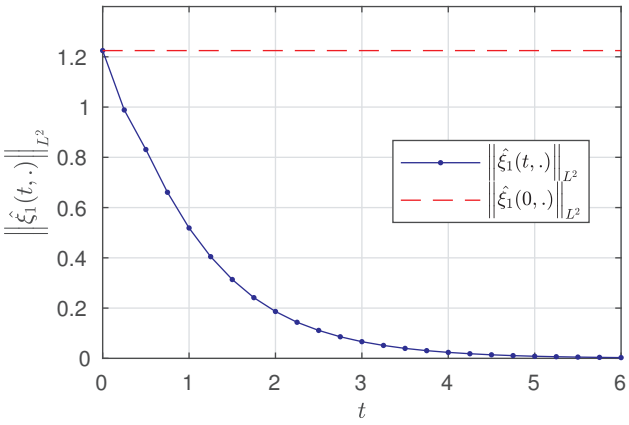

Fig. 5.2 – L^2-norm of $\hat{\xi}_1(t,.)$ for $\mu = 6, \delta = 2, a = 1.685$.

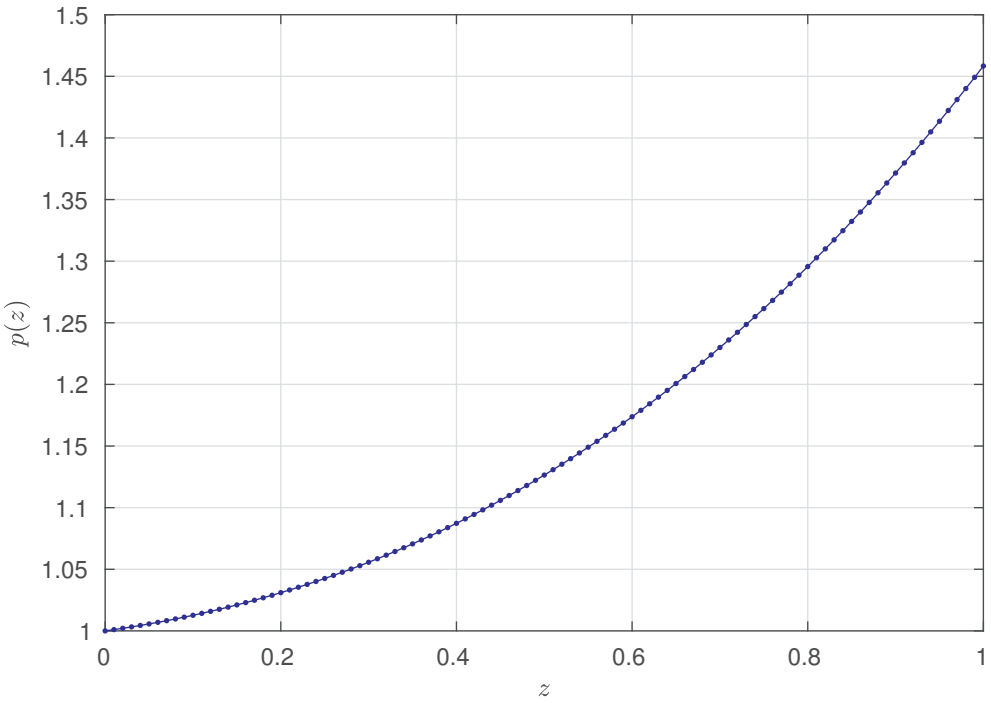

Fig. 5.3 – The function $p(z)$ of Theorem 10 for $\mu = 6, \delta = 2, a = 1.685$.

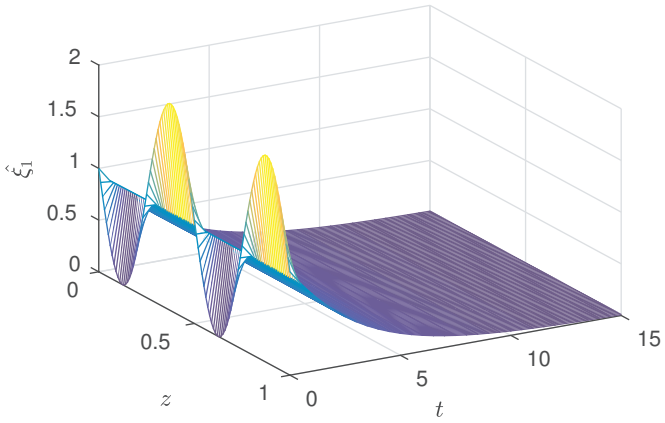

Fig. 5.4 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 0.098$.

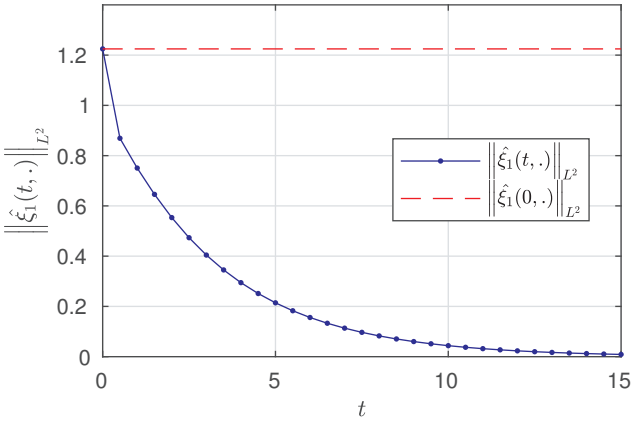

Fig. 5.5 – L^2-norm of $\hat{\xi}_1(t,.)$ for $\mu = 9, \delta = 3, a = 0.098$.

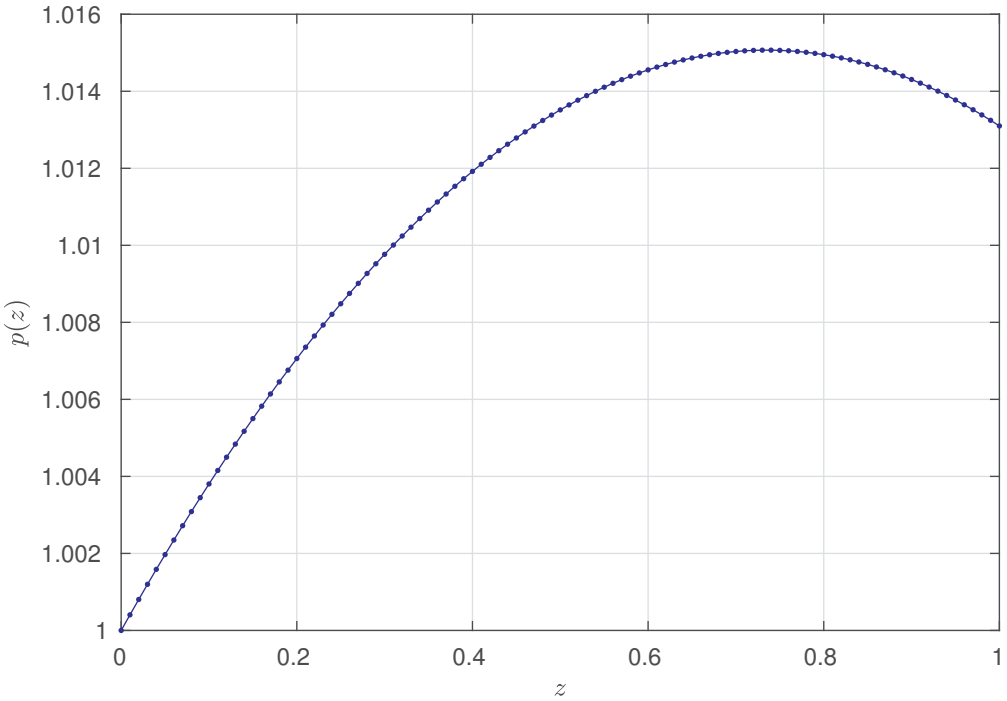

Fig. 5.6 – The function $p(z)$ of Theorem 10 for $\mu = 9, \delta = 3, a = 0.098$.

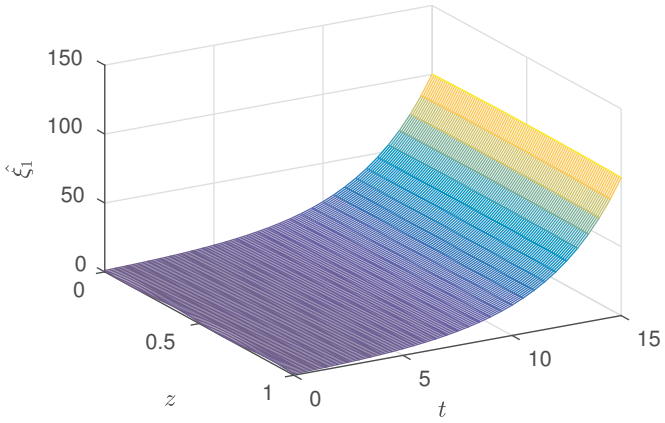

Fig. 5.7 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 0.244$.

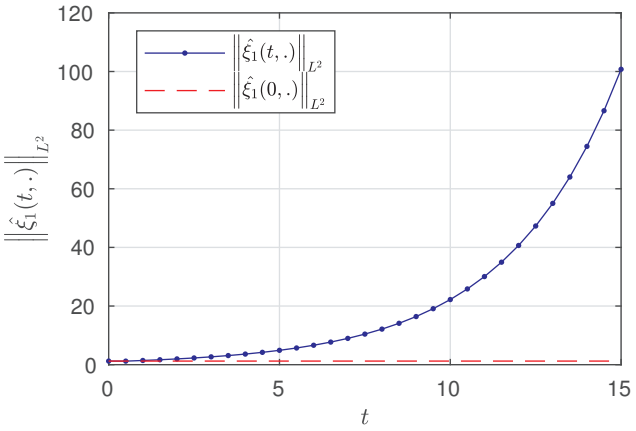

Fig. 5.8 – L^2-norm of $\hat{\xi}_1(t,.)$ for $\mu = 9, \delta = 3, a = 0.244$.

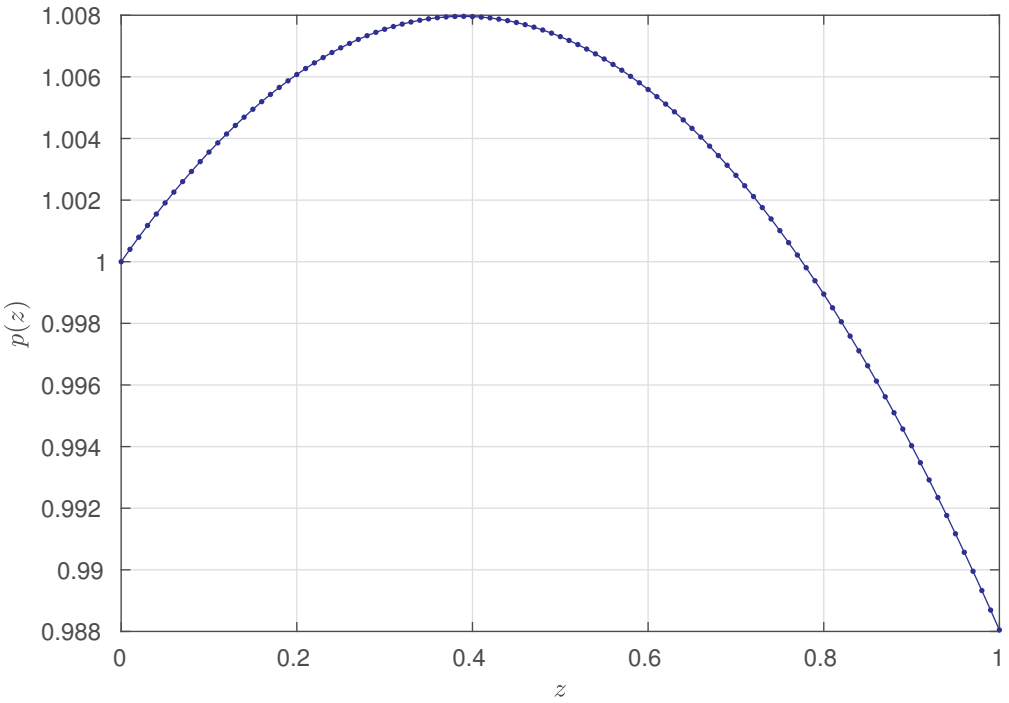

Fig. 5.9 – The function $p(z)$ of Theorem 10 for $\mu = 9, \delta = 3, a = 0.244$.

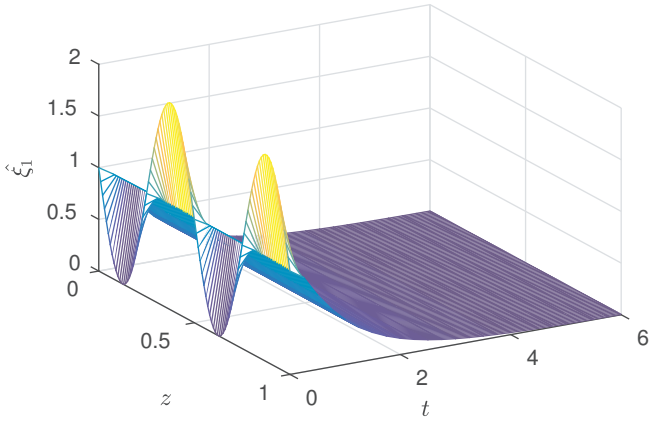

Fig. 5.10 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 2.753$.

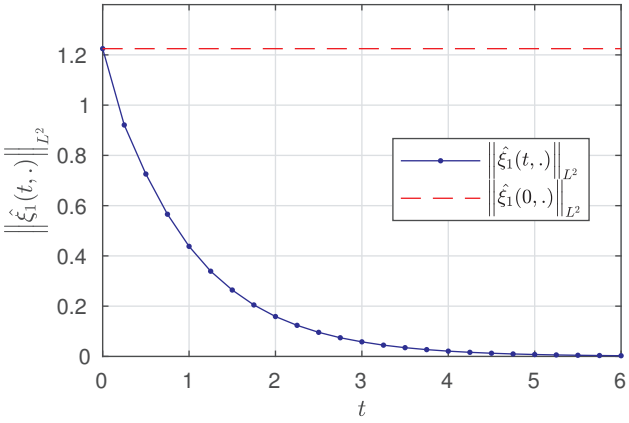

Fig. 5.11 – L^2-norm of $\hat{\xi}_1(t,.)$ for $\mu = 9, \delta = 3, a = 2.753$.

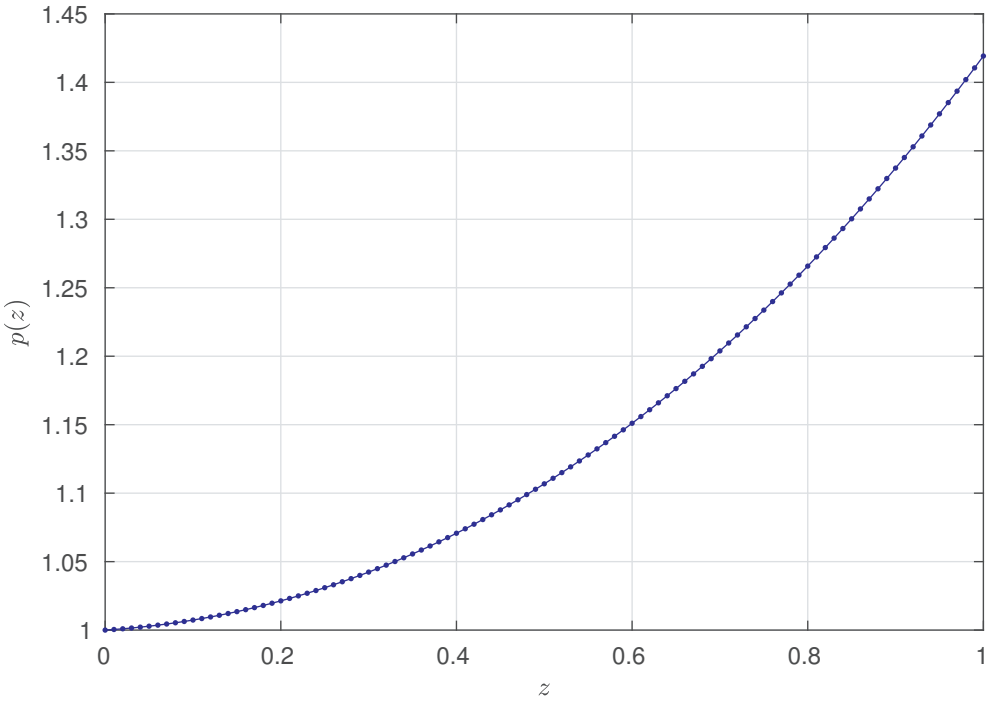

Fig. 5.12 – The function $p(z)$ of Theorem 10 for $\mu = 9, \delta = 3, a = 2.753$.

5.5 Case 2 : $Pe_h \neq Pe_m$

In this section, the same analysis as in the previous section is presented but with different Peclet numbers. The first big difference is that, as for the existence of equilibrium profiles, the change of variables (5.17) is no more possible and one has to consider the whole system (5.14) for the stability analysis. However, the eigenvalues approach is preserved since (5.14) is a coupled parabolic system of PDEs. In the same way of Theorem 10, we present a result from (Nishimura and Matsubara, 1969, Theorem 3) to get exponential stability. The problem is that this result provides only sufficient conditions which require numerical simulations that can be very expensive. In such a way, this will not be computed in practice

in this section. The two remaining approaches will be the numerical integration of (5.14) and the numerical Galerkin's method presented for the case $Pe_h = Pe_m$. Therefore, we extend the method to a more technical one, especially due to the fact that one has two coupled PDEs instead of only one (necessarily uncoupled). Some numerical simulations will be presented and it will notably be shown that the previous pattern of « stable - unstable - stable » is not necessarily satisfied in the case of different Peclet numbers.

We start by stating sufficient conditions which provide exponential stability of an equilibrium profile, see (Nishimura and Matsubara, 1969, Theorem 3).

Theorem 11. *Let $v_1(z)$ and $v_2(z)$ be the solutions of the linear ODE*

$$P\frac{dv}{dz} - Q(z)v = 0,\ z \in [0,1] \tag{5.41}$$

with initial conditions

$$v_1(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \frac{dv_1}{dz}(0) = \begin{bmatrix} \frac{Pe_h}{2} \\ 0 \end{bmatrix} \tag{5.42}$$

and

$$v_2(0) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \frac{dv_2}{dz}(0) = \begin{bmatrix} 0 \\ \frac{Pe_m}{2} \end{bmatrix}, \tag{5.43}$$

where

$$P = \begin{bmatrix} \frac{1}{Pe_h} & 0 \\ 0 & \frac{1}{Pe_m} \end{bmatrix} \text{ and } Q(z) = \begin{bmatrix} \frac{Pe_h}{4} - \delta G_1(z) & -\delta \hat{G}_2(z) \\ -\hat{G}_1(z) & \frac{Pe_m}{4} - G_2(z) \end{bmatrix}, \tag{5.44}$$

where $G_1, \hat{G}_1, G_2$ and $\hat{G}_2$ are the functions whose expressions are given by (5.15) and (5.16). Let $V(z)$ be the matrix composed as $\begin{bmatrix} v_1 & v_2 \end{bmatrix}$. Then, a sufficient condition for the equilibrium profile under consideration to be exponentially stable is that both of the following conditions hold simultaneously.

- *$V(z)$ is nonsingular on $z \in [0,1]$,*
- *$V'(1) + AV(1) \geq 0$ where $A = diag\left(\frac{Pe_h}{2}, \frac{Pe_m}{2}\right)$.*

This result is not proven here. We notice the similarity of this result with Theorem 10. It comes mainly from the fact that stability is still addressed by an eigenvalue problem. Theorem 11 is the vectorial extension of Theorem 10. We notice also that the numerical computation of this theorem will not be performed, for the reason that it is relatively expensive from an algorithmic point of view, especially the first condition. It requires the test of the nonsingularity of the matrix $V(z)$ for each $z \in [0,1]$, which is impossible to do. Even for a discrete set of points in the interval $[0,1]$, this can be very hard to perform in many cases.

In this way, we shall consider the previous Galerkin's method extended to different Peclet numbers. As previously said, the change of variable (5.17) is no more possible and the functions $\hat{G}_1$ and $\hat{G}_2$ cannot be simplified. In order to develop the Galerkin's method for different Peclet numbers, we still approximate

the solutions $\hat{\xi}_1$ and $\hat{\xi}_2$ of equations (5.14) by trial ones, noted $\tilde{\xi}_1, \tilde{\xi}_2$ and given by

$$\tilde{\xi}_1(z,t) = \sum_{n=1}^{m} \alpha_1^n(t)\phi_1^n(z)$$
$$\tilde{\xi}_1(z,t) = \sum_{n=1}^{m} \alpha_2^n(t)\phi_2^n(z),$$

where the functions $\alpha_1^n(t)$ and $\alpha_2^n(t)$ are expressed as $e^{-\lambda_1^n t}$ and $e^{-\lambda_2^n t}$ up to a multiplicative constant where $\{\lambda_1^n\}_{n=1}^m, \{\lambda_2^n\}_{n=1}^m$ are the set of eigenvalues associated to $\tilde{\xi}_1^n$ and $\tilde{\xi}_2^n$ respectively. As for equal Peclet numbers, the functions ϕ_1^n and ϕ_2^n are the eigenfunctions associated to λ_1^n and λ_2^n respectively and are given by

$$\phi_1^n(z) = \beta_1^n\sqrt{Pe_h}\cos\left(\beta_1^n\sqrt{Pe_h}z\right) + \frac{Pe_h}{2}\sin\left(\beta_1^n\sqrt{Pe_h}z\right)$$
$$\phi_2^n(z) = \beta_2^n\sqrt{Pe_m}\cos\left(\beta_2^n\sqrt{Pe_m}z\right) + \frac{Pe_m}{2}\sin\left(\beta_2^n\sqrt{Pe_m}z\right),$$

where $\{\beta_1^n\}_{n=1}^m$ and $\{\beta_1^n\}_{n=1}^m$ are solutions of the resolvent equations

$$\tan\left(\beta\sqrt{Pe_h}\right) = \frac{4\beta\sqrt{Pe_h}}{4\beta^2 - Pe_h}$$
$$\tan\left(\beta\sqrt{Pe_m}\right) = \frac{4\beta\sqrt{Pe_m}}{4\beta^2 - Pe_m}$$

respectively. For different Peclet numbers, the equations (5.14) reduce to a matrix system of the form

$$\dot{x} = \mathbb{A}x$$

but the matrix $\mathbb{A}$ is now a real $2m \times 2m$ matrix [5] and the vector x is $\begin{pmatrix}\alpha_1^1(t) & \dots & \alpha_1^m(t) & \alpha_2^1(t) & \dots & \alpha_2^m(t)\end{pmatrix}$. The target is still to estimate the dominant real part of eigenvalues of matrix $\mathbb{A}$. If it is negative, the equilibrium profile under consideration will be stable. Otherwise, it will be unstable. We shall follow the same steps as for equal Peclet numbers, i.e. developing the orthogonality between the error residuals associated to $\tilde{\xi}_1$ and $\tilde{\xi}_2$ with the eigenvector ϕ_1^n and ϕ_2^n respectively. The matrix $\mathbb{A}$ will be computed using these considerations. Formally, we first explicit the error residuals due to the approximations of functions $\hat{\xi}_1$ and $\hat{\xi}_2$. These are noted $\Gamma_{\hat{\xi}_1}(z), \Gamma_{\hat{\xi}_2}(z)$ and given by

$$\begin{aligned}\Gamma_{\hat{\xi}_1}(z) &= \frac{\partial\tilde{\xi}_1}{\partial t} - \frac{1}{Pe_h}\frac{\partial^2\tilde{\xi}_1}{\partial z^2} + \frac{Pe_h}{4}\tilde{\xi}_1 - \delta G_1(z)\tilde{\xi}_1 - \delta\hat{G}_2(z)\tilde{\xi}_2 \\ &= \sum_{n=1}^{m}\frac{d\alpha_1^n}{dt}(t)\phi_1^n(z) - \frac{1}{Pe_h}\sum_{n=1}^{m}\alpha_1^n(t)\frac{d^2\phi_1^n}{dz^2}(z) + \frac{Pe_h}{4}\sum_{n=1}^{m}\alpha_1^n(t)\phi_1^n(z) - \delta G_1(z)\sum_{n=1}^{m}\alpha_1^n(t)\phi_1^n(z) \\ &\qquad - \delta\hat{G}_2(z)\sum_{n=1}^{m}\alpha_2^n(t)\phi_2^n(z)\end{aligned}$$

5. Because of the fact that the considered PDEs are coupled and cannot be uncoupled since the change of variables (5.17) makes no sense.

and

$$\begin{aligned}\Gamma_{\hat{\xi}_2}(z) &= \frac{\partial\tilde{\xi}_2}{\partial t} - \frac{1}{Pe_m}\frac{\partial^2\tilde{\xi}_2}{\partial z^2} + \frac{Pe_m}{4}\tilde{\xi}_2 - \hat{G}_1(z)\tilde{\xi}_1 - G_2(z)\tilde{\xi}_2 \\ &= \sum_{n=1}^{m}\frac{d\alpha_2^n}{dt}(t)\phi_2^n(z) - \frac{1}{Pe_m}\sum_{n=1}^{m}\alpha_2^n(t)\frac{d^2\phi_2^n}{dz^2}(z) + \frac{Pe_m}{4}\sum_{n=1}^{m}\alpha_2^n(t)\phi_2^n(z) - \hat{G}_1(z)\sum_{n=1}^{m}\alpha_1^n(t)\phi_1^n(z) \\ &\qquad - G_2(z)\sum_{n=1}^{m}\alpha_2^n(t)\phi_2^n(z).\end{aligned}$$

The orthogonality between $\Gamma_{\hat{\xi}_1}(z), \Gamma_{\hat{\xi}_2}(z)$ and $\phi_1^n(z)$ and $\phi_2^n(z)$ is expressed as $\left\langle \Gamma_{\hat{\xi}_1}, \phi_1^n \right\rangle_{L^2(0,1)} = 0$ and $\left\langle \Gamma_{\hat{\xi}_2}, \phi_2^n \right\rangle_{L^2(0,1)} = 0$. Developing the first orthogonality relation with the $i-$th eigenvector yields

$$\begin{aligned}&\int_0^1 \left[\sum_{n=1}^{m}\frac{d\alpha_1^n}{dt}(t)\phi_1^n(z)\right]\phi_1^i(z)dz - \frac{1}{Pe_h}\int_0^1\left[\sum_{n=1}^{m}\alpha_1^n(t)\frac{d^2\phi_1^n}{dz^2}(z)\right]\phi_1^i(z)dz \\ &+ \frac{Pe_h}{4}\int_0^1\left[\sum_{n=1}^{m}\alpha_1^n(t)\phi_1^n(z)\right]\phi_1^i(z)dz - \int_0^1\left[\delta G_1(z)\sum_{n=1}^{m}\alpha_1^n(t)\phi_1^n(z)\right]\phi_1^i(z)dz \\ &- \int_0^1\left[\delta\hat{G}_2(z)\sum_{n=1}^{m}\alpha_2^n(t)\phi_2^n(z)\right]\phi_1^i(z)dz = 0.\end{aligned} \tag{5.45}$$

Taking into account the expression of the eigenvector $\phi_1^n(z)$, the relation

$$\frac{d^2\phi_1^n}{dz^2}(z) = -\left(\beta_1^n\right)^2 Pe_h\phi_1^n(z) \tag{5.46}$$

holds. Noticing that $\{\phi_1^n\}_{n=1}^m$ forms an orthogonal basis of functions with respect to the inner product in $L^2(0,1)$, (5.45) becomes

$$\begin{aligned}&\sum_{n=1}^{m}\frac{d\alpha_1^n}{dt}(t)\int_0^1\phi_1^n(z)\phi_1^i(z)dz = \frac{1}{Pe_h}\sum_{n=1}^{m} -\left(\beta_1^n\right)^2\alpha_1^n(t)\int_0^1\phi_1^n(z)\phi_1^i(z)dz - \frac{Pe_h}{4}\sum_{n=1}^{m}\alpha_1^n(t)\int_0^1\phi_1^n(z)\phi_1^i(z)dz \\ &\qquad + \delta\sum_{n=1}^{m}\alpha_1^n(t)\int_0^1 G_1(z)\phi_1^n(z)\phi_1^i(z)dz + \delta\sum_{n=1}^{m}\alpha_2^n(t)\int_0^1\hat{G}_2(z)\phi_2^n(z)\phi_1^i(z)dz \\ &\Leftrightarrow \sum_{n=1}^{m}\frac{d\alpha_1^n}{dt}(t)C_1^i\delta_{ni} = \frac{1}{Pe_h}\sum_{n=1}^{m} -\left(\beta_1^n\right)^2\alpha_n(t)C_1^i\delta_{ni} - \frac{Pe_h}{4}\sum_{n=1}^{m}\alpha_n(t)C_1^i\delta_{ni} \\ &\qquad \delta\sum_{n=1}^{m}\alpha_1^n(t)\int_0^1 G_1(z)\phi_1^n(z)\phi_1^i(z)dz + \delta\sum_{n=1}^{m}\alpha_2^n(t)\int_0^1\hat{G}_2(z)\phi_2^n(z)\phi_1^i(z)dz \\ &\Leftrightarrow \frac{d\alpha_i}{dt}(t) = -\left[\frac{\left(\beta_1^i\right)^2}{Pe_h} + \frac{Pe_h}{4}\right]\alpha_i(t) + \delta\sum_{n=1}^{m}G_1(i,n)\alpha_1^n(t) + \delta\sum_{n=1}^{m}\hat{G}_2(i,n)\alpha_2^n(t),\end{aligned} \tag{5.47}$$

where

$$\left\langle\phi_1^i,\phi_1^n\right\rangle_{L^2(0,1)} = C_1^i\delta_{in}, G_1(i,n) = \frac{1}{C_1^i}\int_0^1 G_1(z)\phi_1^n(z)\phi_1^i(z)dz, \hat{G}_2(i,n) = \frac{1}{C_1^i}\int_0^1\hat{G}_2(z)\phi_2^n(z)\phi_2^i(z)dz.$$

Holding a similar reasoning for the equation $\left\langle \Gamma_{\hat{\xi}_2}, \phi_2^n \right\rangle_{L^2(0,1)} = 0$ gives us

$$\frac{d\alpha_2^i}{dt} = -\left[\frac{\left(\beta_2^i\right)^2}{Pe_m} + \frac{Pe_m}{4}\right]\alpha_2^i(t) + \sum_{n=1}^{m} \hat{G}_1(i,n)\alpha_1^n(t) + \sum_{n=1}^{m} G_2(i,n)\alpha_2^n(t), \tag{5.48}$$

where

$$\left\langle \phi_2^i, \phi_2^n \right\rangle_{L^2(0,1)} = C_2^i \delta_{in}, \hat{G}_1(i,n) = \frac{1}{C_2^i}\int_0^1 \hat{G}_1(z)\phi_1^n(z)\phi_2^i(z)dz, G_2(i,n) = \frac{1}{C_2^i}\int_0^1 G_2(z)\phi_2^n(z)\phi_2^i(z)dz.$$

The equations (5.47) and (5.48) can be written in the form $\dot{x}(t) = \mathbb{A}x(t)$ where

$$x(t) = \begin{pmatrix} \alpha_1^1(t) & \dots & \alpha_1^m(t) & \alpha_2^1(t) & \dots & \alpha_2^m(t) \end{pmatrix}$$

and

$$\mathbb{A} = \begin{bmatrix} \delta G_1(1,1) & \dots & \delta G_1(1,m) & \delta \hat{G}_2(1,1) & \dots & \delta \hat{G}_2(1,m) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \delta G_1(m,1) & \dots & \delta G_1(m,m) & \delta \hat{G}_2(m,1) & \dots & \delta \hat{G}_2(m,m) \\ \hat{G}_1(1,1) & \dots & \hat{G}_1(1,m) & G_2(1,1) & \dots & G_2(1,m) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \hat{G}_1(m,1) & \dots & \hat{G}_1(m,m) & G_2(m,1) & \dots & G_2(m,m) \end{bmatrix}$$

$$+ \operatorname{diag}\left(-\left(\frac{\left(\beta_1^1\right)^2}{Pe_h} + \frac{Pe_h}{4}\right) \quad \dots \quad -\left(\frac{\left(\beta_1^m\right)^2}{Pe_h} + \frac{Pe_h}{4}\right) \quad -\left(\frac{\left(\beta_2^1\right)^2}{Pe_m} + \frac{Pe_m}{4}\right) \quad \dots \quad -\left(\frac{\left(\beta_2^m\right)^2}{Pe_m} + \frac{Pe_m}{4}\right)\right). \tag{5.49}$$

As for equal Peclet numbers, the Galerkin's method is recalled in an algorithm (see Algorithm 2) in order to implement it.

Notice that this numerical method provides necessary and sufficient conditions to prove exponential stability. The method has been computed for different sets of parameters, notably for either one equilibrium profile or three. Therefore, numerical simulations are available in the next section.

5.5.1 Numerical simulations : one equilibrium profile

In this section, we shall present numerical simulations for which the reactor can exhibit only one equilibrium profile. In particular, it is shown, as in the case of equal Peclet numbers, that the equilibrium profile is exponentially stable. We choosed as parameters $\mu = 6, \delta = 2$. The velocity of the chemical reaction is fixed to $v = 0.015$, the diffusion coefficients are $D_1 = 0.1$ and $D_2 = 10$, and the coefficient $k_p := \rho C_p$ is equal to 15 such that $Pe_h = 2.25$ and $Pe_m = 0.0015$. The two first represented quantities are $\hat{\xi}_1$ and $\hat{\xi}_2$ as functions of the spatial variable z and the temporal variable t. We represent also the $L^2 \times L^2-$norm of the vector $\hat{\xi} = \begin{bmatrix} \hat{\xi}_1 & \hat{\xi}_2 \end{bmatrix}^T$. Notice that the functions $\hat{\xi}_1$ and $\hat{\xi}_2$ are the one introduced in (5.14). The initial

Algorithm 2: Galerkin's method applied to the TRAD for different Peclet numbers

1 Fix all the parameters, i.e. $\mu, \delta, v, k_0, L, D_1, D_2, k_p$

2 Compute the quantity $\rho = \mu\delta(\mu\delta - 4\delta - 4)$. If it is 0, the reactor can exhibit only one equilibrium profile. Else, if it is strictly positive, one can observe three equilibria. In both cases, compute the value(s) of a such that

$$\frac{k_0 L(\delta - a)\, e^{\frac{-\mu}{1+a}}}{a} = v$$

3 Compute the Peclet numbers like $Pe_h = \frac{vk_p}{D_1}, Pe_m = \frac{v}{D_2}$

4 Fix m, the number of terms in the trial solution

5 Compute $\beta_1^i, \beta_2^i,\ i = 1, \ldots, m$ solutions of $\tan\left(\beta\sqrt{Pe_h}\right) = \frac{4\beta\sqrt{Pe_h}}{4\beta^2 - Pe_h}$ and $\tan\left(\beta\sqrt{Pe_m}\right) = \frac{4\beta\sqrt{Pe_m}}{4\beta^2 - Pe_m}$ respectively

6 Compute $\phi_1^i(z), \phi_2^i, C_1^i$ and $C_2^i,\ i = 1, \ldots, m$ such that

$$\begin{aligned}
\phi_1^i(z) &= \beta_1^i\sqrt{Pe_h}\cos\left(\beta_1^i\sqrt{Pe_h}\,z\right) + \frac{Pe_h}{2}\sin\left(\beta_1^i\sqrt{Pe_h}\,z\right),\\
\phi_2^i(z) &= \beta_2^i\sqrt{Pe_m}\cos\left(\beta_2^i\sqrt{Pe_m}\,z\right) + \frac{Pe_m}{2}\sin\left(\beta_2^i\sqrt{Pe_m}\,z\right),\\
&\langle\phi_1^i, \phi_1^i\rangle_{L^2(0,1)} = C_1^i \text{ and } \langle\phi_2^i, \phi_2^i\rangle_{L^2(0,1)} = C_2^i
\end{aligned}$$

7 Compute $G_1(z), \hat{G}_1(z), G_2(z)$ and $\hat{G}_2(z)$ where

$$\begin{aligned}
G_2(z) &= -\frac{k_0 L}{v} e^{\frac{-\mu}{1+x_1^\star(z)}}, G_1(z) = -\frac{G_2(z)\,(1 - x_2^\star(z))\,\mu}{(1 + x_1^\star(z))^2}\\
\hat{G}_1(z) &= G_1(z) e^{\frac{(Pe_h - Pe_m)z}{2}}, \hat{G}_2(z) = G_2(z) e^{\frac{(Pe_m - Pe_h)z}{2}}
\end{aligned}$$

and where $x_1^\star(z)$ and $x_2^\star(z)$ are the approximated expressions of the equilibrium profiles given by (4.25)

8 Compute $G_1(i,j), \hat{G}_1(i,j), G_2(i,j)$ and $\hat{G}_2(i,j), i,j = 1, \ldots, m$ by

$$\begin{aligned}
G_1(i,j) &= \frac{1}{C_1^i}\int_0^1 G_1(z)\phi_j(z)\phi_i(z)dz, \hat{G}_1(i,j) = \frac{1}{C_2^i}\int_0^1 \hat{G}_1(z)\phi_1^j(z)\phi_2^i(z)dz,\\
G_2(i,j) &= \frac{1}{C_2^i}\int_0^1 G_2(z)\phi_2^j(z)\phi_2^i(z)dz, \hat{G}_2(i,j) = \frac{1}{C_1^i}\int_0^1 \hat{G}_2(z)\phi_2^j(z)\phi_1^i(z)dz.
\end{aligned}$$

9 Compute the matrix $\mathbb{A} \in \mathbb{R}^{2m\times 2m}$ whose entries are given by

$$\mathbb{A}_{ij} = \begin{cases}
\delta G_1(i,j) - \left(\frac{\left(\beta_1^i\right)^2}{Pe_h} + \frac{Pe_h}{4}\right)\delta_{ij}, & 1 \le i,j \le m\\
\delta\hat{G}_2(i, j-m), & 1 \le i \le m, m+1 \le j \le 2m\\
\hat{G}_1(i-m, j), & m+1 \le i \le 2m, 1 \le j \le m\\
G_2(i-m, j-m) - \left(\frac{\left(\beta_2^i\right)^2}{Pe_m} + \frac{Pe_m}{4}\right)\delta_{ij}, & m+1 \le i,j \le 2m
\end{cases} \tag{5.50}$$

10 Compute

$$\lambda^\star = \max_{\lambda\in\sigma(\mathbb{A})} \mathfrak{Re}(\lambda)$$

where $\sigma(\mathbb{A})$ is the set of eigenvalue of the matrix $\mathbb{A}$

11 If $\lambda^\star < 0$, the equilibrium profile is exponentially stable. Else, it is unstable.

conditions for the simulation are $\hat{\xi}_1(0,z) = -\sin(8\pi z)+1$ and $\hat{\xi}_2(0,z) = -\cos(4\pi z)+1$. The value of a that reaches the velocity is 1.7683.

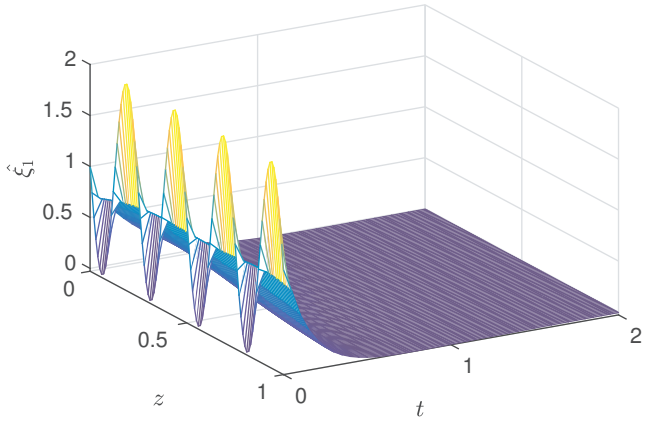

Fig. 5.13 – Function $\hat{\xi}_1(t,z)$ for $\mu = 6, \delta = 2, a = 1.7683$.

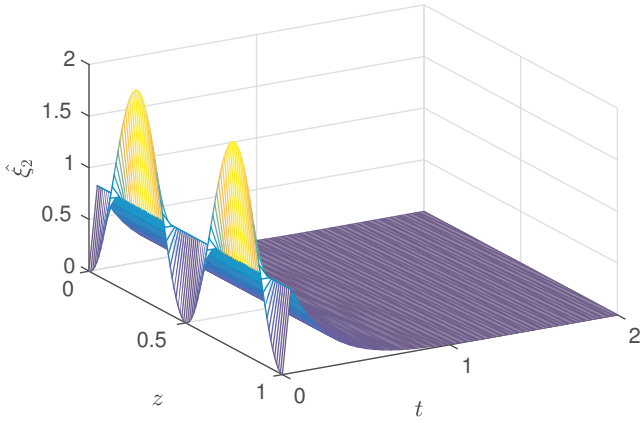

Fig. 5.14 – Function $\hat{\xi}_2(t,z)$ for $\mu = 6, \delta = 2, a = 1.7683$.

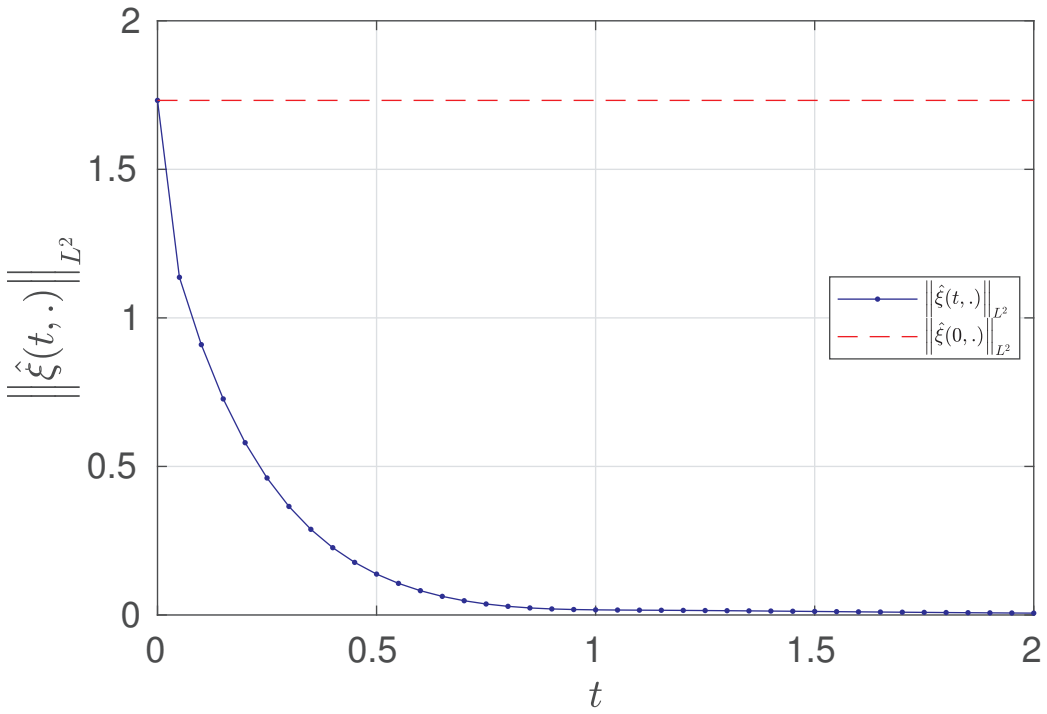

Fig. 5.15 – $L^2 \times L^2-$norm of $\hat{\xi}(t,\cdot)$ for $\mu = 6, \delta = 2, a = 1.7683$.

At the sight of these graphs, it is quite evident that the considered equilibrium profiles is exponentially stable. To confort this idea, the value $\lambda^\star$ has been computed following Algorithm 2. It is equal to -2.1474 in that case, which provides again exponential stability. More numerical simulations has been treated but only one is shown for a matter of convenience and all of these simulations exhibited exponential stability, like in the case of equal Peclet numbers.

5.5.2 Numerical simulations : three equilibrium profiles

Unlike the case of equal Peclet numbers, there is no predetermined pattern for the stability of the equilibrium profiles for different Peclet numbers. However, in the performed numerical simulations, one can observe two different behaviors : « stable – unstable – stable » (like for equal Peclet numbers) or « stable – stable – stable ». We do not have theoretical results to support these phenomena but we will give the intuition to reach one pattern rather than another.

Notice that we show the same quantities as in the previous section with different parameters. We shall present first a set of simulations for which the Peclet numbers are far apart. Then, we will change the diffusion coefficients and the value of k_p to get closer Peclet numbers but still well different. The initial conditions remain also the same as previously. The choosen coefficients are $\mu = 9, \delta = 3, \nu = 0.0015$. The three values of a that reach the velocity of the reaction are $0.0984, 0.244$ and 2.753 respectively. For the first set of simulations, the diffusion coefficients D_1 and D_2 and the value of k_p are $0.1, 20$ and 12 respectively such that $Pe_h = 0.978$ and $Pe_m = 0.0004075$.

In that case, the three equilibria are detected as exponentially stable by the numerical integration, see Figures 5.16, 5.17, 5.18 for the first equilibrium ($a = 0.0984$), Figures 5.19, 5.20, 5.21 for the second one ($a = 0.244$) and Figures 5.22, 5.23, 5.24 for the last one ($a = 2.753$). That pattern could not be found in the case of equal Peclet numbers. The exponential stability of the middle equilibrium is due to the « distance » between the Peclet numbers, which is quite considerable in this case. We will show with the next set of parameters, choosen to bring the Peclet numbers closer, that the middle equilibrium is unstable, like in the case of equal Peclet numbers. Notice also that this is just an intuition and that no theoretical result can assure that behaviour. Like for only one equilibrium, the value of $\lambda^\star$ has been computed for the three equilibria. These are given respectively by $-0.0797, -0.0156$ and -1.5013, which is coherent with the numerical integration and also with the speed of exponential convergence of the trajectories to 0, see therefore the different figures in question in the begining of this paragraph. More $\lambda^\star$ is negatively large, more the trajectories converge fast to 0.

We shall now consider the second set of parameters which gives us the other pattern of stability for the equilibrium profiles, « stable – unstable – stable », the same as that for equal Peclet numbers. The parameters μ, δ and ν remains unchanged. In this way, the three values of a that reach the velocity remain also unchanged. As regards the diffusion coefficients and the coefficient k_p, these are set at $0.1, 0.2$ and 3 respectively such that the Peclet numbers are $Pe_h = 0.2445$ and $Pe_m = 0.0407$. One can see that in this case, they are quite closer than in the previous one and this is the main reason for which the middle equilibrium is unstable. More the Peclet numbers are close, more the change of variables (5.17) is feasible and the conclusion of the case of equal Peclet numbers can be recovered. These considerations are depicted on Figures 5.25, 5.26, 5.27 for the first equilibrium (exponentially stable), Figures 5.28, 5.29, 5.30 for the second equilibrium (unstable) and Figures 5.31, 5.32, 5.33 for the last one (exponentially stable). Like in the previous cases, the values $\lambda^\star$ were computed for each equilibrium. These are given by $-0.3580, 0.2362$ and -1.0435 respectively, which bring us to the same conclusion for the stability.

Remark also that these values are coherent with the speed of convergence/divergence.

All the previous remarks and conclusions are summarized in Table 5.1.

5.5.2.1 First pattern

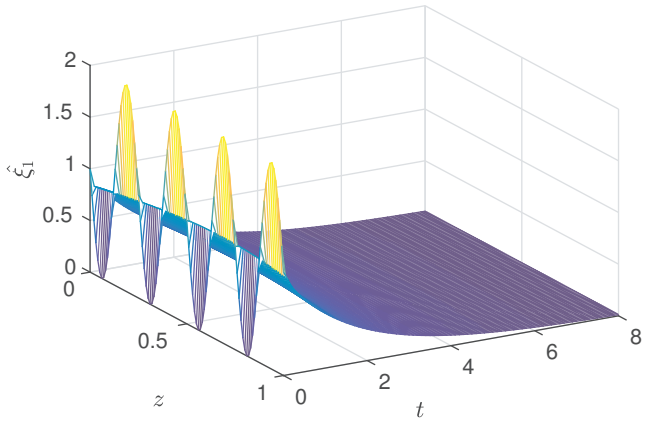

Fig. 5.16 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 0.0984$, first pattern.

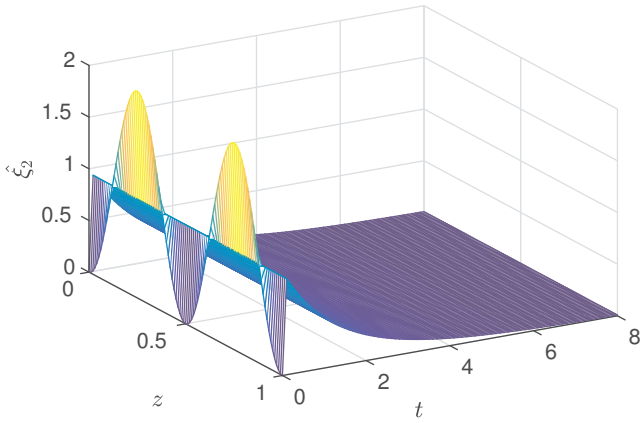

Fig. 5.17 – Function $\hat{\xi}_2(t,z)$ for $\mu = 9, \delta = 3, a = 0.0984$, first pattern.

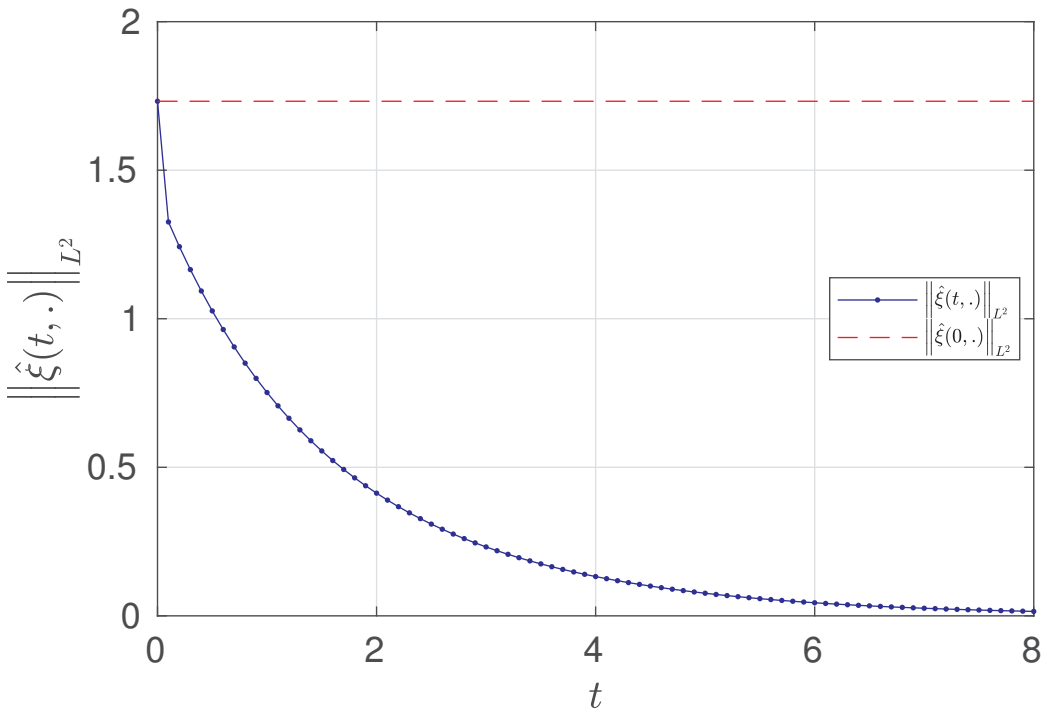

Fig. 5.18 – $L^2 \times L^2-$norm of $\hat{\xi}(t,\cdot)$ for $\mu = 9, \delta = 3, a = 0.0984$, first pattern.

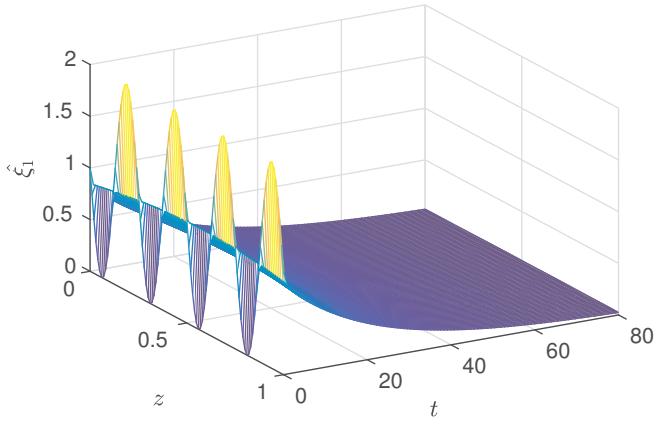

Fig. 5.19 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 0.244$, first pattern.

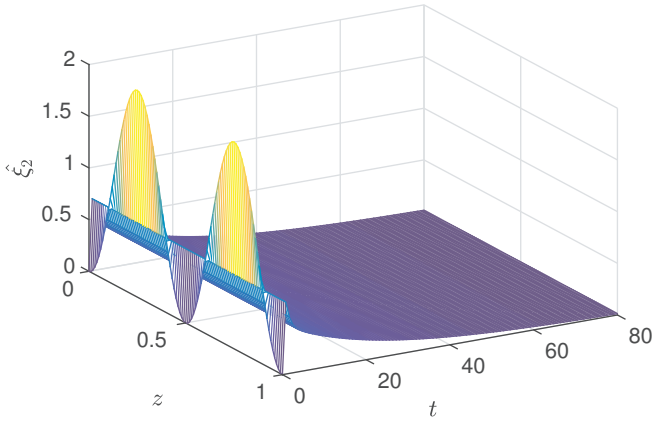

Fig. 5.20 – Function $\hat{\xi}_2(t,z)$ for $\mu = 9, \delta = 3, a = 0.244$, first pattern.

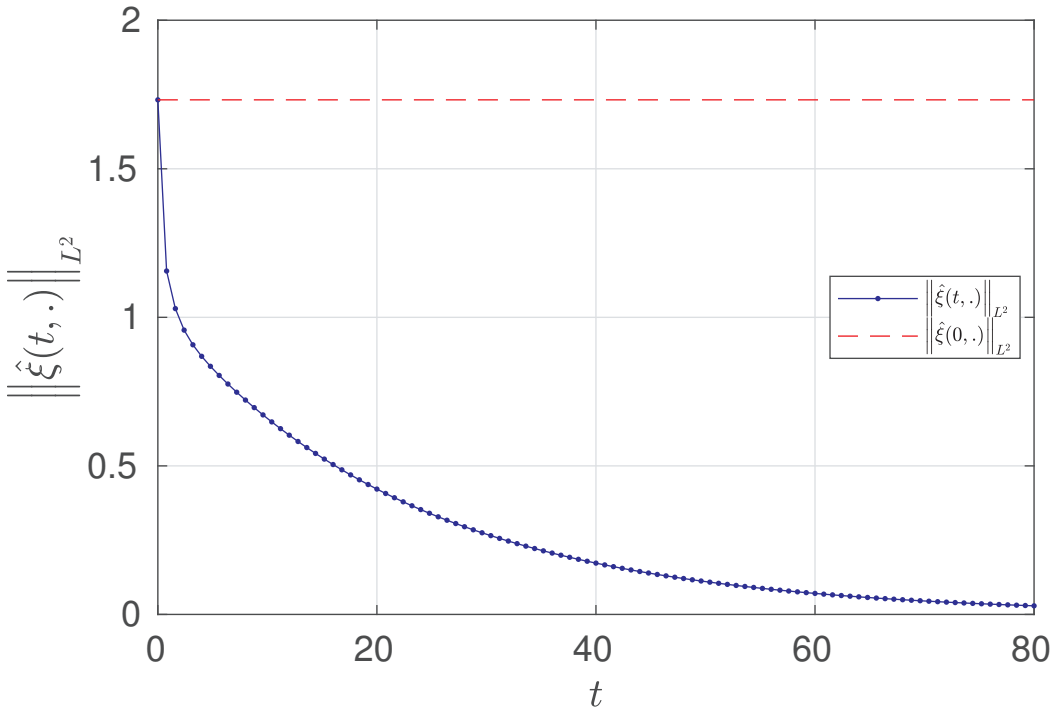

Fig. 5.21 – $L^2 \times L^2-$norm of $\hat{\xi}(t,\cdot)$ for $\mu = 9, \delta = 3, a = 0.244$, first pattern.

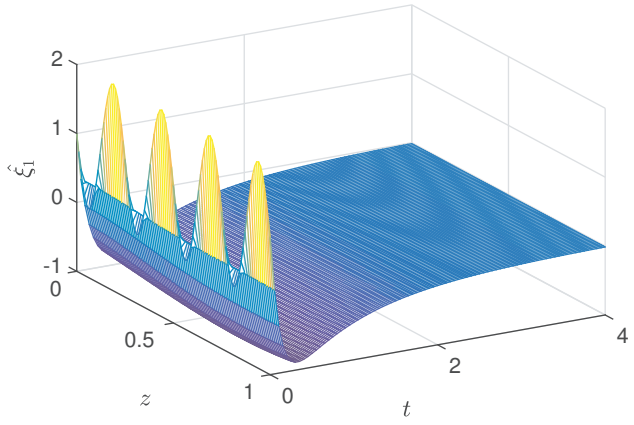

Fig. 5.22 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 2.753$, first pattern.

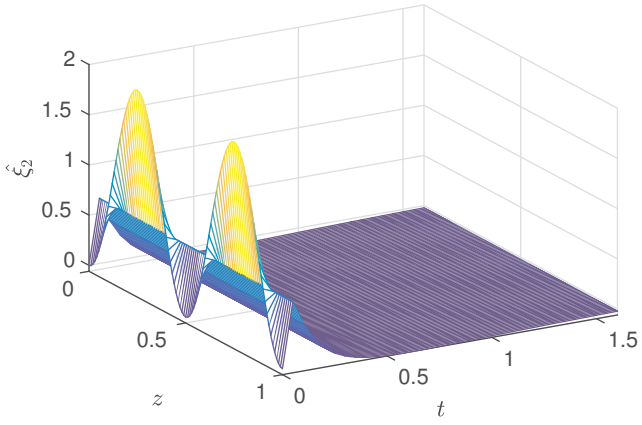

Fig. 5.23 – Function $\hat{\xi}_2(t,z)$ for $\mu = 9, \delta = 3, a = 2.753$, first pattern.

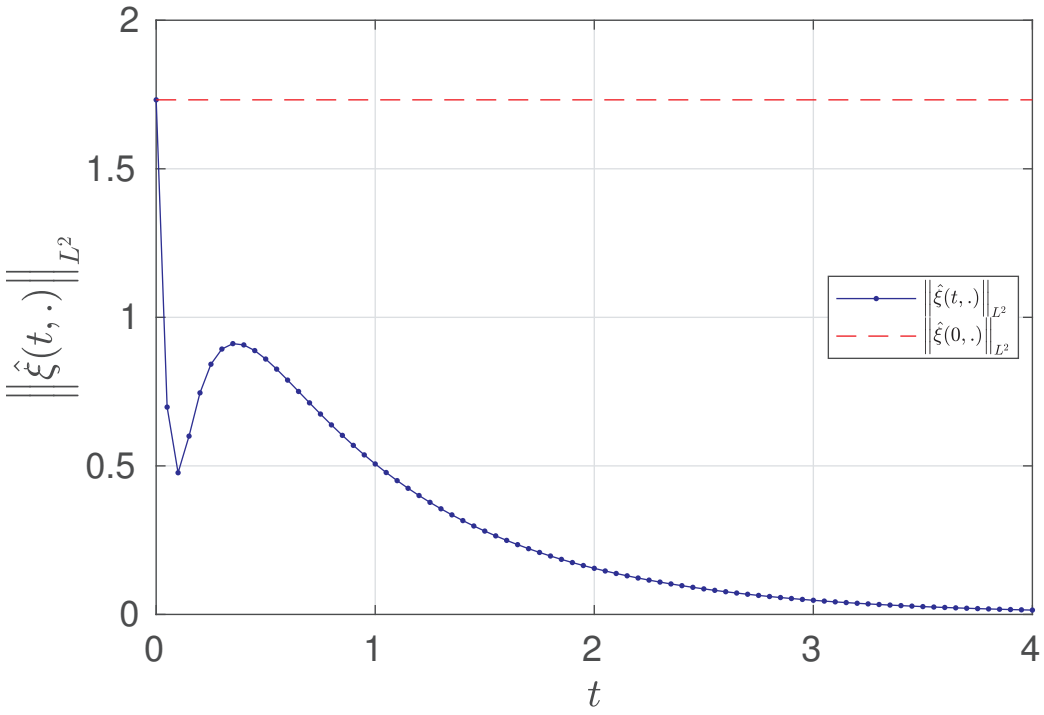

Fig. 5.24 – $L^2 \times L^2-$norm of $\hat{\xi}(t,\cdot)$ for $\mu = 9, \delta = 3, a = 2.753$, first pattern.

5.5.2.2 Second pattern

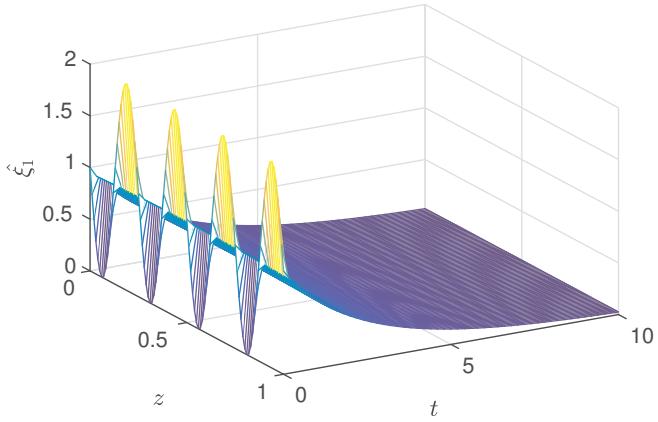

Fig. 5.25 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 0.0984$, second pattern.

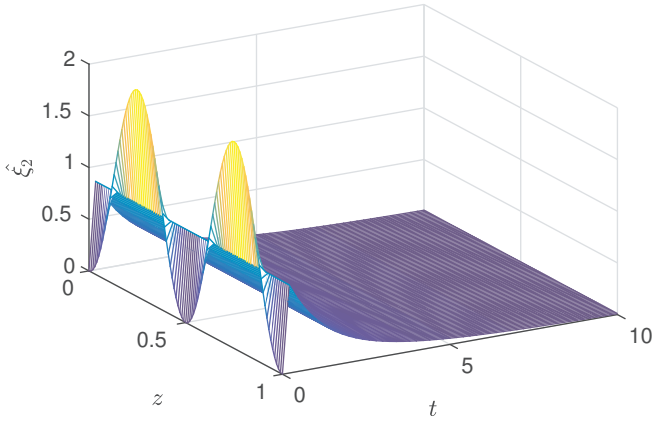

Fig. 5.26 – Function $\hat{\xi}_2(t,z)$ for $\mu = 9, \delta = 3, a = 0.0984$, second pattern.

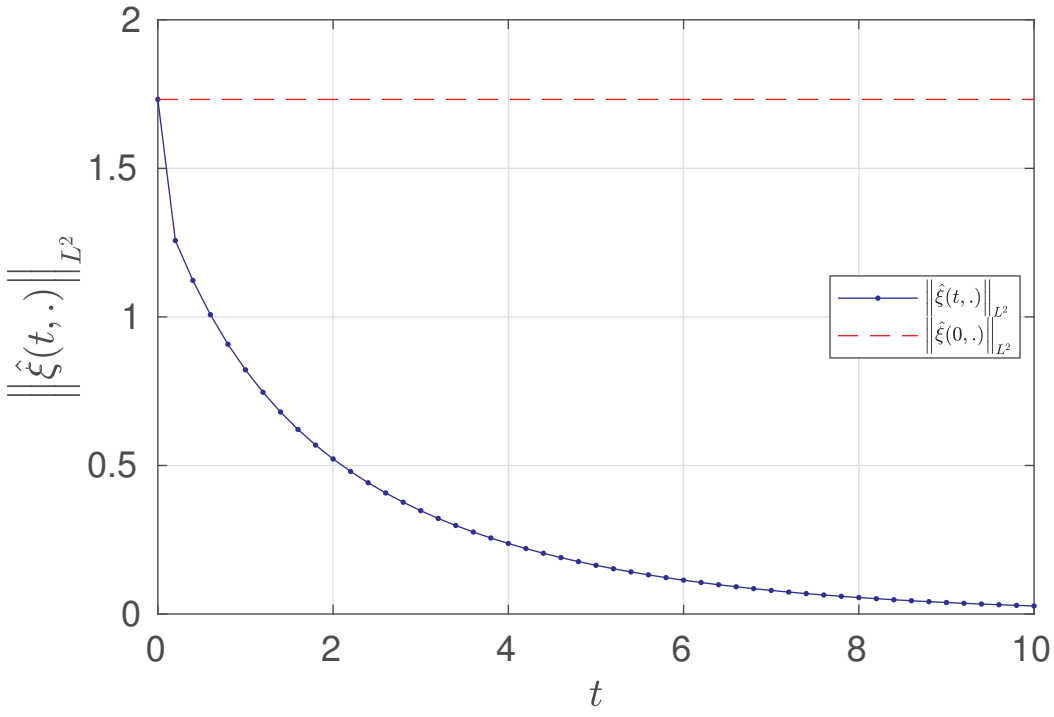

Fig. 5.27 – $L^2 \times L^2-$norm of $\hat{\xi}(t,\cdot)$ for $\mu = 9, \delta = 3, a = 0.0984$, second pattern.

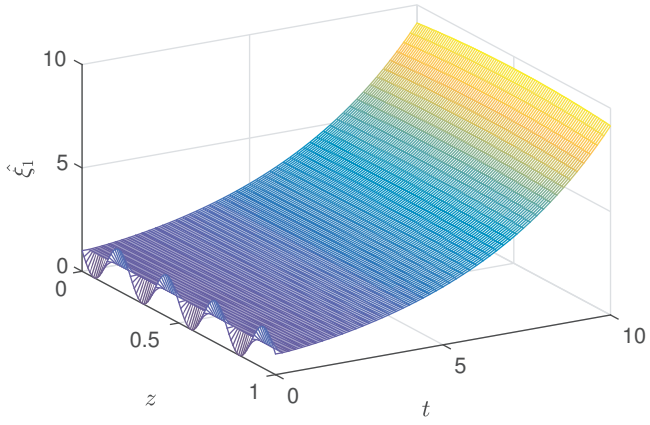

Fig. 5.28 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 0.244$, second pattern.

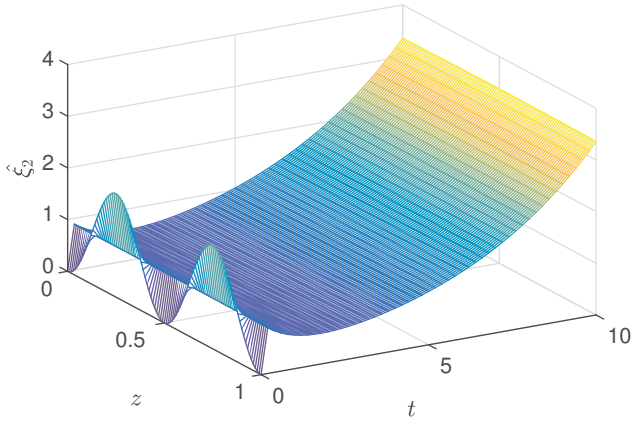

Fig. 5.29 – Function $\hat{\xi}_2(t,z)$ for $\mu = 9, \delta = 3, a = 0.244$, second pattern.

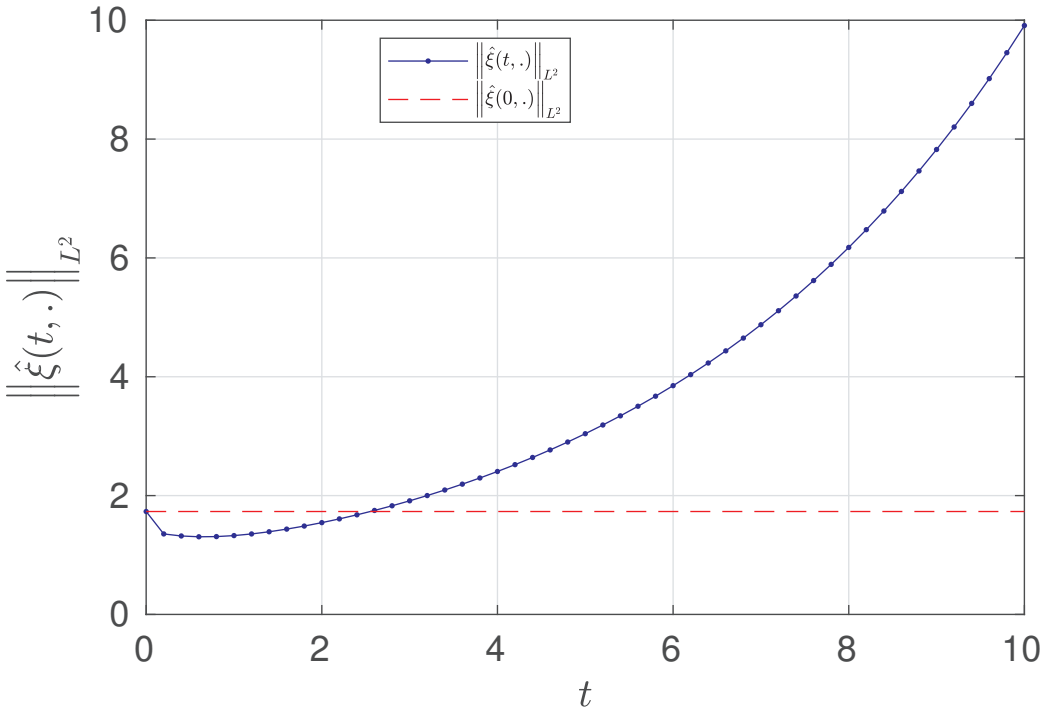

Fig. 5.30 – $L^2 \times L^2-$norm of $\hat{\xi}(t,\cdot)$ for $\mu = 9, \delta = 3, a = 0.244$, second pattern.

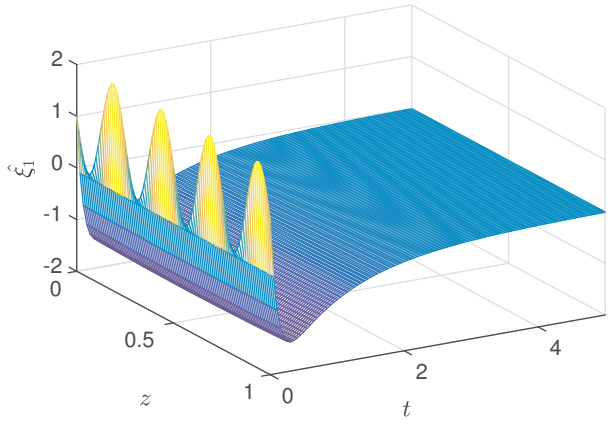

Fig. 5.31 – Function $\hat{\xi}_1(t,z)$ for $\mu = 9, \delta = 3, a = 2.753$, second pattern.

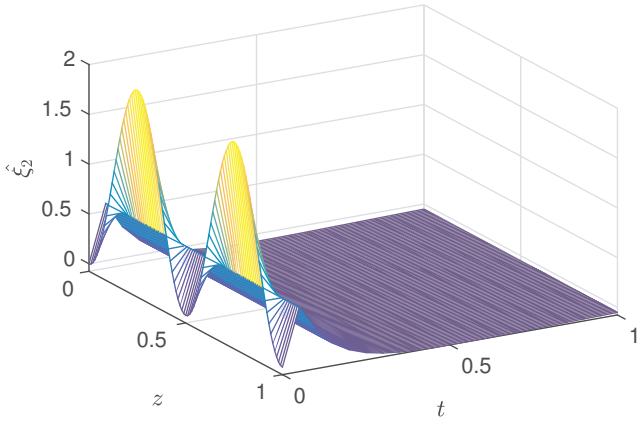

Fig. 5.32 – Function $\hat{\xi}_2(t,z)$ for $\mu = 9, \delta = 3, a = 2.753$, second pattern.

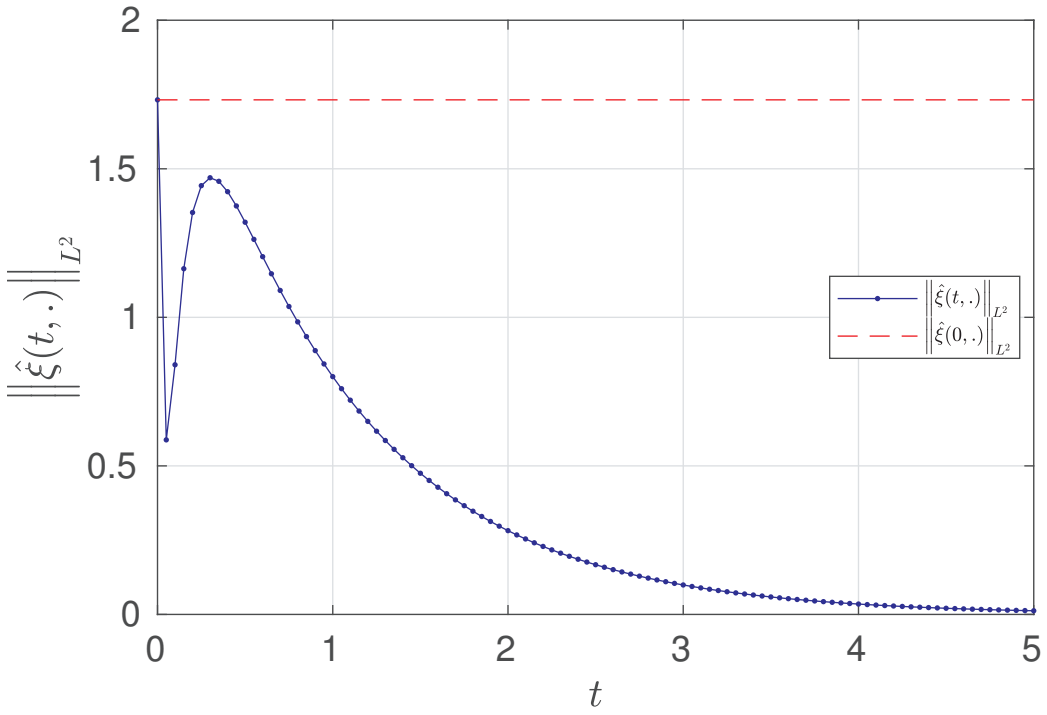

Fig. 5.33 – $L^2 \times L^2-$norm of $\hat{\xi}(t,\cdot)$ for $\mu = 9, \delta = 3, a = 2.753$, second pattern.

		Num. int.	$\lambda^\star$ **(Alg. 2)**
$\mu = 6, \delta = 2$ (**1 eq.**)		exp. stable	-2.1472 (exp. stable)
$\mu = 9, \delta = 3$ (**3 eq.**)	$Pe_h = 0.978$ $Pe_m = 4.075e-4$ (1st pattern)	exp. stable	-0.0797 (exp.stable)
		exp.stable	-0.0156 (exp.stable)
		exp. stable	-1.5013 (exp.stable)
	$Pe_h = 0.2445$ $Pe_m = 0.0407$ (2nd pattern)	exp.stable	-0.3580 (exp.stable)
		unstable	0.2362 (unstable)
		exp.stable	-1.0435 (exp.stable)

TABLE 5.1 – Summary of the stability of equilibrium profiles for different Peclet numbers.

5.6 Case 3 : $Pe_h = Pe_m + \eta$

As for the existence of the equilibrium profiles in Chapter 4, the stability analysis for close Peclet numbers can be reduced to the same analysis as for different Peclet numbers. However, the change of variables (5.17) is no more possible and only the Galerkin's method is developed. We do not recall it. Notice also that the numerical integration of the PDEs governing the model is still feasible in this case but reduces also to the same case as for different Peclet numbers. The numerical simulations are not shown anymore. However, as mentionned in the previous section (different Peclet numbers), the more the Peclet numbers are close, i.e. the more η is close to 0, but still different, the more the central equilibrium (in the case of three equilibrium profiles) is unstable and the more the case of equal Peclet is recovered. Due to these similarities, we do not insist more on the exponential stability of equilibrium profiles for close Peclet numbers.

To conclude this chapter, we would like to insist on the fact that most of the techniques used to detect stability in a tubular reactor are numerical methods, especially for different Peclet numbers. An important remark is that all the simulations made are coherent through each of the methods that are exposed. As for equal Peclet numbers, an objective (and even a challenge) could be to investigate theoretical results that provide necessary or sufficient conditions for which an equilibrium profile is exponentially stable or unstable in the case of different Peclet numbers.

Conclusion and perspectives

Conclusion

In this master's thesis, a dynamical analysis of a nonisothermal axial dispersion tubular reactor has been envisaged. First, some concepts and basic notions of chemical engineering were recalled to get the reader more familar with the framework. Then, the first part of the dynamical analysis, the well-posedness, has been treated. A state space representation of the model has been constructed and the resulting abstract differential equation has been shown to be well-posed, i.e. there exists a unique mild solution to it. The port-Hamiltonian formalism has been notably addressed to show well-posedness of the linear part.

Next, the concepts of Riesz basis, Riesz spectral operators, Sturm-Liouville systems have been defined and it has been shown that the system under study is exponentially stable using these different tools, i.e. the norm of the state trajectory generated by the linear operator converges to zero exponentially fast.

The last part that has been considered is the analysis of the equilibrium profiles and can be decomposed in two distinct ones. First, one addressed the existence and the multiplicity of these equilibrium profiles, developing notably new theorems for the case of different or close Peclet numbers. To illustrate these results, numerical simulations were also provided. Some approximated analytical forms of the equilibrium profiles have been computed using perturbation theory. Then, the question of the stability of the equilibrium profiles was investigated. A linearized model around an equilibrium was build and in particular, it was shown that it is well-posed. Next, some theoretical results concerning the stability in the case of equal Peclet numbers were recalled and proven. A numerical method, known as Galerkin's residuals method, was also studied, first for equal Peclet numbers and secondly, an extension of this method was developed for the case of different Peclet numbers. Numerical integration of the PDEs that describe the dynamic was also performed and numerical simulations were depicted.

Perspectives

A non limited list of perspectives is provided below, in the continuity of this master's thesis.

- The first perspective that could be investigated is the consolidation of additional theoretical results to address the asymptotic or exponential stability of the equilibrium profiles. This is most for the case of different Peclet numbers where more numerical methods are up to now envisaged. For example, an indirect Lyapunov method could be considered, for which the theoretical foundations are consolidated and clarified in (Al Jamar and Morris, 2018) for controlled dynamical systems whose state space is an infinite-dimensional space.
- Another perspective is to look at the stability of the equilibrium profiles of the nonlinear PDEs describing the dynamic of the system under study. Unfortunately, an asymptotically or exponentially

stable equilibrium of the linearized model is not necessarily a stable one for the nominal system. Theoretical tools would be developed to lead such a study, mainly based on (Al Jamar and Morris, 2018), where the question is considered and where some results are already highlighted.

- This perspective is more challenging and consists in the conception of a control law for a class of nonlinear distributed parameters systems described by reaction-convection-diffusion equations and in particular for a nonisothermal chemical reactor with axial dispersion. The designed control law would minimize the following cost functional

$$J(u,x,\infty) = \frac{1}{2}\int_0^\infty \left[\|Cx(t)\|^2 + u(t)^* Qu(t)\right] dt,$$

where u denotes the control, x the state trajectory, C is the observation operator and Q is a positive-definite weighting matrix. This kind of control is called LQ-optimal control. Due to the nonisothermal behavior of the system under considerations, the quantity that has to be controlled here is the temperature. Under suitable assumptions, the LQ-optimal control law is known to be stabilizable. The objectives are multiple. For example, one could stabilize an unstable equilibrium or change the behavior of a stable one in order to have a higher margin of stability or to improve the robustness, ... In order to implement such a law, different approaches have to be envisaged. First, we distinguish the action on the system : boundary control (control that acts on the border of the domain) or distributed control (control that takes part of the dynamic, along the spatial domain). These two controls are in this case the inlet temperature at the entrance of the reactor and the cooling temperature along the reactor respectively. Secondly, two methods can be studied to compute the LQ-optimal control : one in the temporal domain based on the operatorial Riccati equation and another in the frequency domain, the spectral factorization method. The main interests of these two methods is that they make it possible to compute an optimal control law by state feedback and the optimal corresponding cost. In that way, preliminary steps have also to be envisaged. One of them is the well-posedness analysis of the linearized model around an equilibrium, which has already been done in this master's thesis. Further analysis as the study of the accessibility/controlability, the exponential stabilizability, the observability or the exponential detectability have to be envisaged.

This perspective would be an extension of many works that are present in the litterature. One can find control (LQ-optimal) on a reaction – convection system with the nonlinearity but without axial dispersion in (Aksikas et al., 2007). The control law is there computed via the Riccati equation and the spectral factorization method. LQ-optimal control has also been studied in (Dehaye and Winkin, 2016; Dehaye, 2015) where the model of reaction – convection – diffusion is considered without nonlinearities and where the spectral factorization is privileged. In particular, the boundary control for the whole model could be treated as an extension of the works made in (Dehaye and Winkin, 2016) by injecting it in the dynamic using a Dirac delta function in order to render homogeneous the boundary conditions. An analysis of the well-posedness would also be made in this case.

This project would be first analysed for the nonisothermal axial dispersion tubular reactor and then, it could be interesting to extend all the results on a whole class of distributed parameters systems described by reaction – convection – diffusion PDEs with an additional nonlinearity, including for example bioreactor models based on a kinetic of type « Haldane generalized ».

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Nomenclature

List of abbreviations

a.c.	absolutely continuous
a.e.	almost everywhere
CDR	convection-diffusion-reaction
LQ	linear quadratic
ODE	ordinary differential equation
PDE	partial differential equation
TRAD	tubular reactor axial despersion

List of notations

$\dot{x}(t)$	The time derivative of x with respect to t
$(\lambda I - A)^{-1}$	The resolvent operator of the operator A, with $\lambda \in \rho(A)$
$(T(t))_{t\geq 0}$	C_0-semigroup of bounded linear operators
$\mathbb{A}$	The matrix $\mathbb{A}$
$\mathbb{C}$	The set of complex numbers
$\mathbb{R}$	The set of real numbers
$\mathcal{L}(X,Y)$	The vector space of all bounded operators from X to Y
$\mathcal{L}(X)$	The vector space of all bounded operators from X to X
$\rho(A)$	The resolvent set of the operator A
$\sigma(A)$	The spectrum of the operator A
A	The linear (unbounded) operator A
$A^\star$	The topological adjoint of the operator A
$D(A)$	The domain of the operator A
$H^1([a,b],W)$	The Sobolev space of $W-$valued square integrable functions defined on $[a,b]$ and whose first order derivative is in $L^2([a,b],W)$

$H^1(a,b)$	The Sobolev space of complex-valued square integrable functions defined on $[a,b]$ and whose first order derivative is in $L^2(a,b)$
I	The identity operator
$L^2([a,b],W)$	The Lebesgue space of $W-$valued square integrable functions defined on $[a,b]$
$L^\infty([a,b],W)$	The Lebesgue space of W-valued essentially bounded functions defined on $[a,b]$
$L^\infty(a,b)$	The Lebesgue space of complex-valued essentially bounded functions on $[a,b]$
$L^p(a,b)$	The Lebesgue space of complex-valued $p-$integrable functions defined on $[a,b]$
N	The nonlinear operator N

Appendices

Chapter A

Dissipativity of the operator A

Directly linked with Proposition 1, we give more details about the computation of $\mathfrak{Re}\langle (Ax)_2, x_2\rangle$ for $x \in D(A)$. Keeping in mind (2.9) and (2.10), we have

$$\begin{aligned}
\mathfrak{Re}\langle (Ax)_2, x_2\rangle &= \mathfrak{Re}\left(\int_0^1 (Ax)_2(\zeta)x_2(\zeta)d\zeta\right) \\
&= \mathfrak{Re}\left(\int_0^1 \left(\begin{pmatrix} \beta_1\frac{d^2}{d\zeta^2} - \frac{d}{d\zeta} - \gamma I & 0 \\ 0 & \beta_2\frac{d^2}{d\zeta^2} - \frac{d}{d\zeta}\end{pmatrix}\begin{pmatrix} x_1 \\ x_2\end{pmatrix}\right)_2 (\zeta)x_2(\zeta)d\zeta\right) \\
&= \mathfrak{Re}\left(\int_0^1 \left(\beta_2\frac{d^2x_2}{d\zeta^2}(\zeta) - \frac{dx_2}{d\zeta}(\zeta)\right)(x_2(\zeta))d\zeta\right) \\
&= \underbrace{\mathfrak{Re}\left(\int_0^1 \beta_2 x_2(\zeta)\frac{d^2x_2}{d\zeta^2}(\zeta)d\zeta\right)}_{(a)} - \underbrace{\mathfrak{Re}\left(\int_0^1 x_2(\zeta)\frac{dx_2}{d\zeta}(\zeta)d\zeta\right)}_{(b)}.
\end{aligned}$$

(a) Denoting $f = x_2$ and $\frac{dg}{d\zeta} = \frac{d^2x_2}{d\zeta^2}$, we have $\frac{df}{d\zeta} = \frac{dx_2}{d\zeta}$ and $g = \frac{dx_2}{d\zeta}$. Integration by parts yields

$$\begin{aligned}
\int_0^1 \beta_2 x_2(\zeta)\frac{d^2x_2}{d\zeta^2}(\zeta)d\zeta &= \left[\beta_1 x_2(\zeta)\frac{dx_2}{d\zeta}(\zeta)\right]_0^1 - \int_0^1 \beta_2\left(\frac{dx_2}{d\zeta}(\zeta)\right)^2 d\zeta \\
&= \dots \\
&= -\beta_2^2\left(\frac{dx_2}{d\zeta}(0)\right)^2 - l_1^2
\end{aligned}$$

where

$$l_1^2 = \int_0^1 \beta_2\left(\frac{dx_2}{d\zeta}(\zeta)\right)^2 d\zeta.$$

(b) Let $f = x_2$ and $\frac{dg}{d\zeta} = \frac{dx_2}{d\zeta}$. Hence, $\frac{df}{d\zeta} = \frac{dx_2}{d\zeta}$ and $g = x_2$ hold. It follows that

$$\int_0^1 x_2(\zeta)\frac{dx_2}{d\zeta}(\zeta)d\zeta = \frac{\left[x_2^2(\zeta)\right]_0^1}{2}.$$

Consequently, one has

$$\begin{aligned}
\mathfrak{Re}\langle (Ax)_2, x_2\rangle &= -\beta_2^2\left(\frac{dx_2}{d\zeta}(0)\right)^2 - l_1^2 - \frac{\left[x_2^2(\zeta)\right]_0^1}{2} \\
&= -\beta_2^2\left(\frac{dx_2}{d\zeta}(0)\right)^2 - l_1^2 - \frac{x_2^2(1)}{2} + \frac{x_2^2(0)}{2} \\
&\overset{(2.10)}{=} -\beta_2^2\frac{1}{2}\left(\frac{dx_2}{d\zeta}(0)\right)^2 - l_1^2 - \frac{x_2^2(1)}{2} \\
&\leq 0.
\end{aligned}$$

Chapter B

Resolvent operator

This appendix is dedicated to the computation of the integral form of the resolvent operator of operator A defined by (2.9) and (2.10). We first fix $y = (y_1 \quad y_2)^T \in H = L^2(0,1) \times L^2(0,1)$ and $\lambda \in \rho(A)$ defined by (3.17). Then, we will search $x = (x_1 \quad x_2)^T \in D(A)$ such that

$$(\lambda I - A)x = y. \tag{B.1}$$

We first notice the similarity of this problem with the surjectivity of $I - A$, established in Chapter 2. In particular, this similarity will be seen in the solution of (B.1). Developing that equation, one has

$$\begin{aligned}
(\lambda I - A)x = y &\Leftrightarrow \left(\begin{pmatrix} \lambda I & 0 \\ 0 & \lambda I \end{pmatrix} - \begin{pmatrix} \beta_1 \frac{d^2}{d\zeta^2} - \frac{d}{d\zeta} - \gamma I & 0 \\ 0 & \beta_2 \frac{d^2}{d\zeta^2} - \frac{d}{d\zeta} \end{pmatrix} \right) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \\
&\Leftrightarrow \begin{pmatrix} -\beta_1 \frac{d^2}{d\zeta^2} + \frac{d}{d\zeta} + (\gamma + \lambda) I & 0 \\ 0 & -\beta_2 \frac{d^2}{d\zeta^2} + \frac{d}{d\zeta} + \lambda I \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \\
&\Leftrightarrow \begin{cases} -\beta_1 \frac{d^2 x_1}{d\zeta^2} + \frac{dx_1}{d\zeta} + (\gamma + \lambda) x_1 = y_1 \\ -\beta_2 \frac{d^2 x_2}{d\zeta^2} + \frac{dx_2}{d\zeta} + \lambda x_2 = y_2. \end{cases}
\end{aligned}$$

Once again, each of these second order ODEs is treated separately. Looking at the first one, which is given by

$$-\beta_1 \frac{d^2 x_1}{d\zeta^2} + \frac{dx_1}{d\zeta} + (\gamma + \lambda) x_1 = y_1, \tag{B.2}$$

we note $u = \frac{dx_1}{d\zeta}$ and $v = x_1$. The second order ODE can be expressed as a system of two first order ODEs, whose expression is

$$\frac{d}{d\zeta} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \frac{1}{\beta_1} & \frac{\gamma + \lambda}{\beta_1} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} -\frac{1}{\beta_1} \\ 0 \end{pmatrix} y_1. \tag{B.3}$$

Let us denote by $A_{1\lambda}$ the matrix

$$\begin{pmatrix} \frac{1}{\beta_1} & \frac{\gamma + \lambda}{\beta_1} \\ 1 & 0 \end{pmatrix}$$

and by B_1 the vector $\begin{pmatrix} -\frac{1}{\beta_1} & 0 \end{pmatrix}^T$. Hence, by using (Winkin, 2017, Chapter 2, page 45), one finds

$$\begin{pmatrix} u(\zeta) \\ v(\zeta) \end{pmatrix} = \exp(A_{1\lambda}\, \zeta) \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \int_0^\zeta \exp(A_{1\lambda}\, (\zeta - z)) B_1 y_1(z) dz.$$

It remains to adapt the vector $\begin{pmatrix} u_0 & v_0 \end{pmatrix}^T$ taking the boundary conditions into account, whose are given by $D(A)$, i.e. by (2.10). It can be easily deduced from (2.10) that

$$\beta_1 u_0 = v_0. \tag{B.4}$$

Next, we evaluate the vector $\begin{pmatrix} u(\zeta) & v(\zeta) \end{pmatrix}^T$ in $\zeta = 1$, which gives us

$$\begin{pmatrix} u(1) \\ v(1) \end{pmatrix} = \exp(A_{1\lambda}) \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \int_0^1 \exp(A_{1\lambda}\,(1-z)) B_1 y_1(z) dz. \tag{B.5}$$

For a sake of readability, the matrix $\exp(A_{1\lambda})$ is denoted by

$$\begin{pmatrix} a_{\lambda\,11} & a_{\lambda\,12} \\ a_{\lambda\,21} & a_{\lambda\,22} \end{pmatrix}$$

and the notation $w_{\lambda\,1} = \begin{pmatrix} w_{\lambda\,11} & w_{\lambda\,12} \end{pmatrix}^T$ is introduced to express the vector

$$\int_0^1 \exp(A_{1\lambda}\,(1-z)) B_1 y_1(z) dz.$$

All these considerations allow us to rewrite the first component of (B.5) as

$$0 = a_{\lambda\,11} u_0 + a_{\lambda\,12} v_0 + w_{\lambda\,11}. \tag{B.6}$$

Putting (B.4) and (B.6) together yields

$$\begin{cases} u_0 = -\frac{w_{\lambda\,11}}{a_{\lambda\,11} + a_{\lambda\,12}\beta_2}, \\ v_0 = -\frac{\beta_1 w_{\lambda\,11}}{a_{\lambda\,11} + a_{\lambda\,12}\beta_2}. \end{cases}$$

Taking into account that only the component $v(\zeta)$ is usefull to express the solution of (B.2), one has

$$v(\zeta) = x_1(\zeta) = -M_{\lambda\zeta_{21}} \frac{w_{\lambda\,11}}{a_{\lambda\,11} + a_{\lambda\,12}\beta_1} - M_{\lambda\zeta_{22}} \frac{\beta_1 w_{\lambda\,11}}{a_{\lambda\,11} + a_{\lambda\,12}\beta_1} + \mathcal{W}(\zeta)_{\lambda 12}$$

where

$$\exp(A_{1\lambda}\,\zeta) = \begin{pmatrix} M_{\lambda\zeta_{11}} & M_{\lambda\zeta_{12}} \\ M_{\lambda\zeta_{21}} & M_{\lambda\zeta_{22}} \end{pmatrix}$$

and

$$\int_0^\zeta \exp(A_{1\lambda}\,(\zeta - z)) B_1 y_1(z) dz = \begin{pmatrix} \mathcal{W}(\zeta)_{\lambda 11} \\ \mathcal{W}(\zeta)_{\lambda 12} \end{pmatrix}.$$

With regards to the equation

$$-\beta_2 \frac{d^2 x_2}{d\zeta^2} + \frac{dx_2}{d\zeta} + \lambda x_2 = y_2, \tag{B.7}$$

we allow ourselves not to repeat all the developments, these being similar to those previously exposed

for the resolution of (B.2). However, the solution of (B.7) is given by

$$x_2(\zeta) = -N_{\lambda\zeta_{21}} \frac{w_{\lambda 21}}{b_{\lambda 11} + b_{\lambda 12}\beta_2} - N_{\lambda\zeta_{22}} \frac{\beta_2 w_{\lambda 21}}{b_{\lambda 11} + b_{\lambda 12}\beta_2} + \mathcal{W}(\zeta)_{\lambda 12}$$

where

$$A_{2\lambda} = \begin{pmatrix} \frac{1}{\beta_1} & \frac{\gamma+\lambda}{\beta_1} \\ 1 & 0 \end{pmatrix}, w_{\lambda 2} = \begin{pmatrix} w_{\lambda 21} & w_{\lambda 22} \end{pmatrix}^T = \int_0^1 \exp(A_{2\lambda}(1-z)) B_2 y_2(z) dz,$$

$$\exp(A_{2\lambda}\zeta) = \begin{pmatrix} N_{\lambda\zeta_{11}} & N_{\lambda\zeta_{12}} \\ N_{\lambda\zeta_{21}} & N_{\lambda\zeta_{22}} \end{pmatrix} \text{ and } \int_0^\zeta \exp(A_{2\lambda}(\zeta - z)) B_2 y_2(z) dz = \begin{pmatrix} \mathcal{W}(\zeta)_{\lambda 11} \\ \mathcal{W}(\zeta)_{\lambda 12} \end{pmatrix}.$$

Hence, the solution of (B.1) is given by

$$x(\zeta) = \begin{pmatrix} x_1(\zeta) \\ x_2(\zeta) \end{pmatrix} = \begin{pmatrix} -M_{\lambda\zeta_{21}} \frac{w_{\lambda 11}}{a_{\lambda 11} + a_{\lambda 12}\beta_1} - M_{\lambda\zeta_{22}} \frac{\beta_1 w_{\lambda 11}}{a_{\lambda 11} + a_{\lambda 12}\beta_1} + \mathcal{W}(\zeta)_{\lambda 12} \\ -N_{\lambda\zeta_{21}} \frac{w_{\lambda 21}}{b_{\lambda 11} + b_{\lambda 12}\beta_2} - N_{\lambda\zeta_{22}} \frac{\beta_2 w_{\lambda 21}}{b_{\lambda 11} + b_{\lambda 12}\beta_2} + \mathcal{W}(\zeta)_{\lambda 12} \end{pmatrix}.$$

Chapter C

Existence of equilibrium profiles

In this appendix, more detailed arguments are provided to the reader for the derivation of the main results in Chapter 4.

C.1 Case 1 : $Pe_h = Pe_m$

First at all, we will develop only once the transition from Equations (4.1) to Equations (4.3). Note that we denote Pe_h and Pe_m by Pe for simplicity of notation. The first change of variables is

$$y_1 = x_1, \qquad y_2 = x_1 - \delta x_2.$$

The first equation of (4.1) takes the form

$$\frac{1}{Pe}\frac{d^2y_1}{dz^2} - \frac{dy_1}{dz} + \alpha(\delta - y_1 + y_2)\, e^{\frac{\mu y_1}{1+y_1}} = 0$$

and the second one becomes

$$\frac{d^2y_2}{dz^2} - Pe\frac{dy_2}{dz} = 0.$$

The related boundary conditions are

$$\frac{dy_1}{dz}(0) - Pey_1(0) = \frac{dy_1}{dz}(1) = 0$$

and

$$\frac{dy_2}{dz}(0) - Pey_2(0) = \frac{dy_2}{dz}(1) = 0.$$

Using these conditions, it follows that y_2 is the null function. Therefore,

$$\frac{1}{Pe}\frac{d^2y_1}{dz^2} - \frac{dy_1}{dz} + \alpha(\delta - y_1)\, e^{\frac{\mu y_1}{1+y_1}} = 0. \tag{C.1}$$

Now let us introduce the functions

$$u(z) = y_1(1-z), \qquad w = \frac{dy_1}{dz}(1-z),$$

with a view to rewrite (C.1) as a system of two first order differential equations. Using the relation $Pe = \frac{v}{D}$, one gets

$$\frac{du}{dz} = -\frac{dy_1}{dz} = -w$$

and

$$\begin{aligned}\frac{dw}{dz} &= -\frac{d^2y_1}{dz} \\ &= -\frac{v}{D}\frac{dy_1}{dz} + \frac{v}{D}\alpha(\delta - y_1)e^{\frac{\mu y_1}{1+y_1}} \\ &= -\frac{1}{D}(vw - g(u)),\end{aligned}$$

where the function g is defined by

$$g(x) = v\alpha(\delta - x)e^{\frac{\mu x}{1+x}}.$$

In addition, the boundary conditions are derived as follows :

$$\begin{aligned}u(0) &= y_1(1) =: a, \\ w(0) &= \frac{dy_1}{dz}(1) = 0, \\ w(1) &= \frac{dy_1}{dz}(0) = Pey_1(0) = \frac{v}{D}u(1).\end{aligned}$$

In the proof of Proposition 1, when $\rho > 0$, for a matter of simplicity, an interval where the extrema are located is considered in order to avoid the study of the second order derivative of the function v. It entails three possibilities :

- $a_1^* < -1$ and $a_2^* < -1$;
- $-1 < a_1^*$ and $a_2^* < 0$;
- $0 < a_1^*$ and $0 < a_2^*$.

Developing each of these inequations, it can be deduced that the two first possibilities lead to a contradiction, and thus the only possibility is the third one. To find the sets of feasible parameters, we combine this double inequality with the positivity of ρ. Two cases should be distinguished :

- $\mu\delta > 0$ and $\mu\delta - 4\delta - 4 > 0$;
- $\mu\delta < 0$ and $\mu\delta - 4\delta - 4 < 0$.

This leads to the fact that μ (which should be positive, see Chapter 2) and δ have to satisfy either

$$\delta > 0, \mu > 4, \delta(\mu - 4) > 4 \tag{C.2}$$

or

$$\delta < -2, \mu > 2, \mu + \delta < 0, \delta(\mu - 4) < 4. \tag{C.3}$$

Noting that the coefficient of a^2 in the first order derivative of v is $-(\mu + \delta)$, it is obvious that, in the case (C.2), a_1^* corresponds to a minimum and a_2^* to a maximum and vice-versa for the case (C.3).

Now we take a look at the last part of the proof of Lemma 1 concerning the case $\rho = 0$. Since the product $\mu\delta$ cannot be zero from a physical point of view, it follows that

$$\mu\delta - 4\delta - 4 = 0,$$

which is equivalent to

$$\delta = \frac{4}{\mu - 4}. \tag{C.4}$$

Putting the identity (C.4) into the polynomial factor in the second order derivative of v yields the following expression :

$$\frac{2(\mu-2)^2}{\mu-4}a^4 + \frac{(2-\mu)\left(\mu^2-4\mu+16\right)}{\mu-4}a^3 + \frac{4\mu^2-24\mu+48}{\mu-4}a^2 - 8a + \frac{8}{\mu-4}.$$

C.2 Case 2 : $Pe_h \neq Pe_m$

The arguments for deducing a necessary form of function v are similar to the case $Pe_h = Pe_m$. We take the solutions

$$\begin{aligned} u_{\varepsilon_1}(z) &= a_1, \qquad & w_{\varepsilon_1}(z) &= k_p\delta g(a_1,a_2)z, \\ u_{\varepsilon_2}(z) &= a_2, \qquad & w_{\varepsilon_2}(z) &= g(a_1,a_2)z \end{aligned}$$

and we used the boundary conditions

$$\begin{aligned} w_{\varepsilon_1}(1) &= vk_p u_{\varepsilon_1}(1), \\ w_{\varepsilon_2}(1) &= vu_{\varepsilon_2}(1). \end{aligned}$$

We find

$$\begin{cases} k_p\delta g(a_1,a_2) = vk_p a_1 \\ g(a_1,a_2) = va_2. \end{cases}$$

Taking the difference of these equations, we have

$$(1-\delta)\, g(a_1,a_2) = v\,(a_2 - a_1)\,.$$

Therefore, the function v satisfies

$$v(a_1,a_2,0,0) = (1-\delta)\,\frac{g(a_1,a_2)}{a_2-a_1}.$$

Note that this expression is a necessary form of function v.
The last point we discuss is related to the Hessian matrix of function v. This matrix is symmetric, there-

fore its eigenvalues are real and its determinant satisfies

$$\det \mathscr{H} = \prod_{i=1}^{2} \lambda_i, \tag{C.5}$$

where $\{\lambda_i\}_{i=1}^{2}$ denotes the set of eigenvalues of $\mathscr{H}$. Since the matrix $\mathscr{H}$ evaluated at (a_1^*, a_2^*) is given by

$$\mathscr{H}\left(1, \frac{\mu-4}{\mu}\right) = k_0 L (1-\delta) e^{\frac{-\mu}{2}} \begin{pmatrix} -\frac{\mu^2}{16} + \frac{\mu}{16} & \frac{\mu^2}{16} \\ \frac{\mu^2}{16} & 0 \end{pmatrix},$$

we deduce that

$$\det \mathscr{H}\left(1, \frac{\mu-4}{\mu}\right) = -k_0^2 L^2 (1-\delta)^2 e^{-\mu} \left(\frac{\mu^2}{16}\right)^2 < 0.$$

Using (C.5), we find that $\lambda_1 \lambda_2 < 0$, which means that $\mathscr{H}$ is indefinite. The point (a_1^*, a_2^*) is therefore a saddle point.