# On exponential bistability of equilibrium profiles of nonisothermal axial dispersion tubular reactors

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***Abstract*—Sufficient conditions are established for the exponential stability/instability of the equilibrium profiles for a linearized model of nonisothermal axial dispersion tubular reactors. The considered reactors are assumed to involve a chemical reaction of the form $A \to B$, where $A$ and $B$ denote the reactant and the product, respectively, and where the Peclet numbers appearing in the energy and mass balance PDEs are assumed to be equal. First, different kinds of linearization of infinite-dimensional dynamical systems are presented. Then the considered linearized model around any equilibrium is shown to be well-posed. Moreover, by using a Lyapunov-based approach, exponential stability is adressed. In the case when the reactor can exhibit only one equilibrium, it is shown that the latter is always exponentially stable. When three equilibrium profiles are exhibited, bistability is established, i.e. the stability pattern "(exponentially) stable – unstable – stable" is proven for the linearized model. The results are illustrated by some numerical simulations.**

***Index Terms*—Nonisothermal tubular reactor – Nonlinear infinite-dimensional system – Lyapunov method – Equilibrium profile – Gâteaux-Fréchet derivatives**

## I. Introduction

The time evolution of temperature and concentration in nonisothermal axial dispersion tubular reactors is governed by the following nonlinear partial differential equations (PDE)

$$\begin{cases} \frac{\partial T}{\partial \tilde{t}} = -v\frac{\partial T}{\partial \tilde{z}} + \frac{\lambda_{ea}}{\rho C_p}\frac{\partial^2 T}{\partial \tilde{z}^2} - \frac{\Delta H}{\rho C_p}k_0 C e^{-\frac{E}{RT}} + \frac{4h}{\rho C_p d}(T_w - T), \\ \frac{\partial C}{\partial \tilde{t}} = -v\frac{\partial C}{\partial \tilde{z}} + D_{ma}\frac{\partial^2 C}{\partial \tilde{z}^2} - k_0 C e^{-\frac{E}{RT}}, \end{cases} \tag{1}$$

where $T(\tilde{t},\tilde{z})[K]$ and $C(\tilde{t},\tilde{z})[\mathrm{mol}/l]$ represent the temperature and the reactant concentration inside of the reactor at time $\tilde{t} \geq 0$ and position $\tilde{z} \in [0,L]$, respectively. The meaning and the units of the parameters are summarized in Table I. Note that, from a physical point of view, the variables $T$ and $C$ satisfy

$$0 \leq T(t,z),\ 0 \leq C(t,z) \leq C_{in}, \tag{2}$$

for $t \geq 0$ and $z \in [0,L]$. Intuitively speaking, the temperature has to remain above $0K$ (the absolute zero temperature) while the reactant concentration cannot exceed its value at the inlet and cannot be below 0, see e.g. [1]. To the PDEs (1) we associate some boundary conditions, known as the Danckwert's boundary conditions and expressed as $\frac{\lambda_{ea}}{\rho C_p}\frac{\partial T}{\partial \tilde{z}}(\tilde{t},0) = v(T(\tilde{t},0) - T_{in})$, $\frac{\partial T}{\partial \tilde{z}}(\tilde{t},L) = 0$ and $D_{ma}\frac{\partial C}{\partial \tilde{z}}(\tilde{t},0) = v(C(\tilde{t},0) - C_{in})$, $\frac{\partial C}{\partial \tilde{z}}(\tilde{t},L) = 0$. In order to work with a dimensionless model, we introduce the change of coordinates $t = \tilde{t}\frac{v}{L}, z = \frac{\tilde{z}}{L}$ together with $x_1 = (T - T_{in})/T_{in}, x_2 = (C_{in} - C)/C_{in}, x_w = (T_w - T_{in})/T_{in}$, which yields the following set of PDEs

$$\begin{cases} \frac{\partial x_1}{\partial t} = \frac{1}{Pe_h}\frac{\partial^2 x_1}{\partial z^2} - \frac{\partial x_1}{\partial z} + \gamma(x_w - x_1) + \delta\alpha(1 - x_2)e^{\frac{-\mu}{1+x_1}}, \\ \frac{\partial x_2}{\partial t} = \frac{1}{Pe_m}\frac{\partial^2 x_2}{\partial z^2} - \frac{\partial x_2}{\partial z} + \alpha(1 - x_2)e^{\frac{-\mu}{1+x_1}}, \\ \frac{\partial x_1}{\partial z}(t,0) = Pe_h x_1(t,0), \frac{\partial x_2}{\partial z}(t,0) = Pe_m x_2(t,0), \\ \frac{\partial x_1}{\partial z}(t,1) = 0, \frac{\partial x_2}{\partial z}(t,1) = 0, \end{cases} \tag{3}$$

TABLE I
System parameters.

| Constant | Unit | Description |
|---|---|---|
| $L$ | $m$ | Reactor length |
| $v$ | $\frac{m}{s}$ | Fluid superficial velocity |
| $\lambda_{ea}$ | $\frac{kJ}{m\,s\,K}$ | Axial energy dispersion coefficient |
| $D_{ma}$ | $\frac{m^2}{s}$ | Axial mass dispersion coefficient |
| $\Delta H$ | $\frac{kJ}{kg}$ | Heat transfer coefficient |
| $\rho$ | $\frac{kg}{m^3}$ | Fluid density |
| $C_p$ | $\frac{kJ}{kg\,K}$ | Specific heat |
| $k_0$ | $\frac{1}{s}$ | Kinetic constant |
| $E$ | $\frac{kJ}{kg}$ | Activation energy |
| $R$ | $\frac{kJ}{kg\,K}$ | Gaz constant |
| $h$ | $\frac{kJ}{m^2\,K\,s}$ | Wall heat transfer coefficient |
| $d$ | $m$ | Reactor diameter |
| $T_w$ | $K$ | Coolant temperature |
| $T_{in}$ | $K$ | Inlet temperature |
| $C_{in}$ | $\mathrm{mol}/l$ | Inlet reactant concentration |

where $x_1$ and $x_2$ are the dimensionless temperature and concentration, repsectively. The constants $\mu, \delta, \gamma$ and $\alpha = k_0 L v^{-1}$ depend on the model parameters, see e.g. [2], [3]. The key point in the analysis of that model lies in the relation between two specific numbers, $Pe_h$ and $Pe_m$. Those are the thermal and the mass Peclet numbers and represent the ratio between the convection transfer and the conduction transfer and the ratio between the convection transfer and the diffusion transfer, respectively, and are expressed as $Pe_h = \frac{vL\rho C_p}{\lambda_{ea}}$ and $Pe_m = \frac{vL}{D_{ma}}$. In the new coordinates, the variables $x_1$ and $x_2$ have to be constrained as follows:

$$-1 \leq x_1(t,z), 0 \leq x_2(t,z) \leq 1, \tag{4}$$

with $t \geq 0$ and $z \in [0,1]$, see (2). The variable $x_w$ denotes the dimensionless coolant temperature and is due to a heat exchanger that is modeled by the term $\gamma(x_w - x_1)$ in equations (3). In what follows, we shall consider adiabatic conditions, meaning that there is no heat exchange with the environment outside the reactor, or equivalently, $\gamma = 0$.

As it is highlighted in [2], such reactors can exhibit different numbers of equilibria (one to three), depending on the parameters of the system, more specifically on the conduction and diffusion coefficients.

Many questions concerning the stabilization of systems like (3) are of interest in process engineering. In particular, one could design a control law that stabilizes the system around an unstable equilibrium profile or even that improves the

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stablity margin of a stable one. In that perspective, the stability analysis of the equilibria of (3) is the first objective to achieve. The main difficulty comes from the nonlinearity, which is due to the Arrhenius law, that models the evolution of the rate of the reaction as a function of the temperature, namely $\alpha\,(1-x_2)\,e^{-\mu/(1+x_1)}$. Asymptotic stability has already been of concern in [3], [4] and also in [5], [6] and in [7] where the asymptotic bistability of the equilibrium profiles is shown, for equal Peclet numbers. Numerical methods to conclude stability are proposed e.g. in [8], [9] or [10]. These methods are based on the Galerkin Residuals Method for PDEs and consist of a finite dimension reduction of the system (3). The approach used here studies the exponential stability, instead of the asymptotic one, for the linearized parameter model. A complement to the previous references is also the well-posedness of the linearized model corresponding to (3).
The paper is organized as follows. In Section II, some changes of variables are introduced and a linearized model corresponding to Equations (3) is built around any equilibrium. Some useful properties of the equilibria are also developed in order to show that this linearized model is well-posed in the sense that the unbounded linear operator describing the dynamics of the system is the infinitesimal generator of a $C_0-$semigroup. In Section III, a Lyapunov–based method is developed in order to get sufficient conditions for an equilibrium profile to be exponentially stable. Furthermore bistability is established for the equilibria of (3). The last section of the paper is dedicated to the illustration of the most important results via numerical simulations. Note that equal Peclet numbers are considered in what follows, i.e. $Pe_h = Pe_m =: Pe =: vL/D$, where $D$ will be called the diffusion coefficient for the sake of simplicity. Note that $L$ is fixed to one (dimensionless model).

## II. Linearized model analysis

### A. Equilibrium profile preliminaries

In this section we aim at giving some introducing results concerning the existence, the multiplicity and the expression of the equilibria of (3) in the case of equal Peclet numbers and under adiabatic conditions, on the basis of [2, Section IV.A]. First note that an equilibrium pair $(x_1^e, x_2^e)$ of (3) is solution of the following two point boundary value problem:

$$\begin{cases} \frac{D}{v}\frac{d^2x_1^e}{dz^2} - \frac{dx_1^e}{dz} + \delta\alpha(1-x_2^e)e^{\frac{-\mu}{1+x_1^e}} = 0, \frac{dx_1^e}{dz}(0) - \frac{v}{D}x_1^e(0) = 0 = \frac{dx_1^e}{dz}(1), \\ \frac{D}{v}\frac{d^2x_2^e}{dz^2} - \frac{dx_2^e}{dz} + \alpha(1-x_2^e)e^{\frac{-\mu}{1+x_1^e}} = 0, \frac{dx_2^e}{dz}(0) - \frac{v}{D}x_2^e(0) = 0 = \frac{dx_2^e}{dz}(1). \end{cases} \quad (5)$$

First we have the following result that characterizes the existence and the multiplicity of the pair $(x_1^e, x_2^e)$, see [2, Lemma 4.1].

*Lemma 2.1:* For some values of the parameters $\mu$ and $\delta$, there exist $D^*$ large enough, $v_1^* > 0$ and $v_2^* >$ such that for all $D \geq D^*$; the system (5) has either

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

The proof of this result is based on perturbation theory (see e.g. [11]) that takes a small parameter into account, which is $1/D$ here. Since the diffusion phenomenon has to be considered large in the analysis, perturbation theory allows to study the existence and the multiplicity of the equilibria of (3) by looking at a simplified version with $1/D$ going to 0. This yields the following corollary that characterizes approximated solution of (5), that is solutions of (5) by taking $D$ tending to $+\infty$, see [2, Corollary 4.1].

*Corollary 2.1:* Taking into account the existence and the multiplicity of equilibrium profiles under the conditions of Lemma 2.1, approximated solutions of (5) are given by

$$x_1^\star(z) = a - \frac{k_0L(\delta-a)e^{\frac{-\mu}{1+a}}}{2D}(1-z)^2, x_2^\star(z) = x_1^\star(z)/\delta \quad (6)$$

where $a$ is a solution of the equation $v = k_0L(\delta-a)e^{\frac{-\mu}{1+a}}/a$ that corresponds to the approximated form of the velocity.

### B. Equilibrium profile bounds

We shall first introduce the following lemma that characterizes the boundedness of the approximated form of the equilibrium profiles of (3), given in (6). Note that, since we are considering equal energy and mass Peclet numbers, one finds the reaction invariant $x_1^e(z) - \delta x_2^e(z)$, that is $x_1^e(z) - \delta x_2^e(z) = 0$ a.e. on $[0,1]$, see e.g. [3]. In that way, only the temperature equilibrium, $x_1^e(z)$, will be considered. In the sequel, we denote that approximated form by $x_1^\star(z)$. The exact temperature equilibrium profile, introduced in the previous subsection, is denoted by $x_1^e(z)$.

*Lemma 2.2:* The approximated form $x_1^\star(z)$ of a temperature equilibrium profile for the nonisothermal axial dispersion tubular reactor (3) is such that $-1+\eta < x_1^\star(z) < \delta$, a.e. on $[0,1]$, for some positive constant $\eta$, whenever the diffusion coefficient $D$ is sufficiently large.

*Proof:* Remember that the function $x_1^\star(z)$ is defined as $x_1^\star(z) = a - \frac{k_0L(\delta-a)e^{\frac{-\mu}{1+a}}}{2D}(1-z)^2$ (see (6)) and the approximated form of the velocity is $v^\star = k_0L(\delta-a)e^{\frac{-\mu}{1+a}}/a$, see[1] Corollary 2.1, where perturbation theory has been used. Since we consider positive velocities and positive values of the parameter $a$, it follows that $\delta > a > 0$. Moreover, $0 \leq (1-z)^2 \leq 1$, which yields

$$a - k_0L(\delta-a)e^{\frac{-\mu}{1+a}}/2D \leq a - (k_0L(\delta-a)e^{\frac{-\mu}{1+a}}/2D)(1-z)^2 \leq a. \quad (7)$$

Consequently, $a - k_0L(\delta-a)e^{\frac{-\mu}{1+a}}/2D \leq x_1^\star(z) < \delta$. Furthermore, observe that, since $0 < e^{\frac{-\mu}{1+a}} < e^{\frac{-\mu}{1+\delta}}$ for all $a > 0$, it holds

$$\begin{aligned} x_1^\star(z) &\geq a - \frac{k_0L(\delta-a)e^{\frac{-\mu}{1+\delta}}}{2D} > \frac{2aD - k_0L\delta e^{\frac{-\mu}{1+\delta}} + 2D - 2D}{2D} \\ &> -1 + (2D - k_0L\delta e^{\frac{-\mu}{1+\delta}})/2D := -1+\eta. \end{aligned}$$

To ensure the positivity of $\eta$, $D$ has to be large enough, i.e. there must exist some $D^\star > 0$ such that $D \geq D^\star$. By "$D$ large enough", we mean $D^\star > k_0L\delta e^{\frac{-\mu}{1+\delta}}/2$. Note that $\eta \to 1$ as $D \to +\infty$, i.e. diffusion is sufficiently dominant. ■

A result that follows from the previous lemma is that $1/(1+x_1^\star) \in L^\infty(0,1)$ with $\|1/(1+x_1^\star)\|_\infty \leq 1/\eta$, where $\|f\|_\infty$ is given by $\inf\{M \geq 0 \,|\, |f(z)| \leq M$ a.e. on $[0,1]\}$ in our context, for $f \in L^\infty(0,1)$. In the next step, the exact form of the equilibrium

[1] Intuitively speaking, one could say that once the superficial fluid velocity $v^\star$ is fixed, $a$ is a parameter that is computed as a root of $v^\star - k_0L(\delta - a)e^{\frac{-\mu}{1+a}}/a$. The number of roots determines the number of equilibrium profiles, see subsection II-A and [2] for more details on the existence and the multiplicity of equilibrium profiles.

profile $x_1^e(z)$ will be characterized in a same manner as for the approximated one. First note the following result with the appropriate assumptions (2.1 and 2.2 below), known as the *Regular Perturbation Theorem*, see [11, Section 5.2].

Given a function $f: H \to H$ and an initial condition $\Theta \in \mathbb{R}^2$, we consider the initial value problem

$$\frac{dx}{dz} = f(z,x,\varepsilon), x(0) = \Theta(\varepsilon), \tag{8}$$

where $\varepsilon$ is a parameter. Assume that the following conditions are satisfied :

*Assumption 2.1:* For $\varepsilon = 0$, (8) has a unique solution on $0 \leq z \leq 1$, denoted by $x_0(z)$. Hence the latter satisfies the equations $\frac{dx_0}{dt} = f(z,x_0,0), x_0(0) = \Theta(0)$.

*Assumption 2.2:* The functions $f$ and $\Theta$ are smooth functions of their variables for $0 \leq z \leq 1$, $x$ near $x_0$, and $\varepsilon$ near 0. Specifically we suppose that $f$ and $\Theta$ are $\mathbf{n}+1$ times continuously differentiable in all their variables, so that $\Theta$ admits a series expansion of the form $\sum_{k=0}^{+\infty} \Theta_k \varepsilon^k$.

*Theorem 2.1:* (*Regular Perturbation Theorem*) Let Assumptions 2.1 and 2.2 hold. Then for sufficiently small $\varepsilon$ the perturbed problem (8) has a unique solution, which is $\mathbf{n}+1$ times differentiable with respect to $\varepsilon$. Moreover this solution admits a Taylor expansion $x(z,\varepsilon) = x_0(z) + x_1(z)\varepsilon + \cdots + x_{\mathbf{n}}(z)\varepsilon^{\mathbf{n}} + \mathcal{O}(\varepsilon^{\mathbf{n}+1})$, where the error estimate holds as $\varepsilon \to 0$ uniformly for $0 \leq z \leq 1$.

By the *Regular Perturbation Theorem*, it holds, in our case,

$$x_1^e(z,\varepsilon) = x_1^\star(z,\varepsilon) + \mathcal{O}(\varepsilon^2), \tag{9}$$

where $\varepsilon = 1/D$, see [2, Section IV. A.] for detailed arguments concerning the computation of $x_1^\star(z,\varepsilon)$. In order to bound the exact form of the temperature equilibrium profile, let us consider the following definition, see [11, Section 5.1.1, Gauge Functions].

*Definition 2.1:* Suppose that $f$ and $g$ are smooth functions of $\varepsilon$ for $\varepsilon$ near 0, say $0 < \varepsilon < \varepsilon_0$. We say that $f(\varepsilon) = \mathcal{O}(g(\varepsilon))$ as $\varepsilon \to 0$ if $f(\varepsilon)/g(\varepsilon)$ is bounded for all small $\varepsilon$. Thus there is a constant $K > 0$ and a sufficiently small constant $\varepsilon^\star > 0$ such that $|f(\varepsilon)| \leq K|g(\varepsilon)|$holds for all $\varepsilon \leq \varepsilon^\star$.

By using Theorem 2.1 and Definition 2.1 one gets the following theorem, which provides bounds on $x_1^e(z)$.

*Theorem 2.2:* The exact form of a temperature equilibrium profile for (3) satisfies

$$-1 + \tilde{\eta} < x_1^e(z) < \tilde{\delta}, \tag{10}$$

when the diffusion coefficient $D$ is sufficiently large, where $\tilde{\eta} = \eta - \frac{K}{D^2} > 0$ and $\tilde{\delta} = \delta + \frac{K}{D^2}$ for some positive constant $K$.

*Proof:* By taking (9) into account and the characterization of $\mathcal{O}$ in Definition 2.1, there exist $K > 0$ and $\varepsilon^\star > 0$ such that for a.e. $z \in [0,1]$, $|x_1^e(z,\varepsilon) - x_1^\star(z,\varepsilon)| \leq K\varepsilon^2$, for $\varepsilon \leq \varepsilon^\star$. This holds for a.e. $z \in [0,1]$ since the error estimate is valid uniformly for $0 \leq z \leq 1$. Consequently we have

$$x_1^\star(z,\varepsilon) - K\varepsilon^2 \leq x_1^e(z,\varepsilon) \leq x_1^\star(z,\varepsilon) + K\varepsilon^2. \tag{11}$$

By using Lemma 2.2, it follows that $-1 + \eta - K/D^2 < x_1^e(z,1/D) < \delta + K/D^2$, where we have been using the fact that $\varepsilon = 1/D$, which is equivalent to $-1 + \tilde{\eta} < x_1^e(z,1/D) < \tilde{\delta}$, where $\tilde{\eta} := \eta - K/D^2$and $\tilde{\delta} := \delta + K/D^2$. By considering sufficiently large diffusion, one gets that the constant $\tilde{\eta}$ is still positive. ■

Let us characterize the exact form of the velocity in a same manner as for the temperature equilibrium profile (that depends also on $\varepsilon$). By denoting by $v^\star$ the approximated form of the velocity and by $v^e$ the exact one, it holds $v^e = v^\star + \mathcal{O}(\varepsilon^2)$. Otherwise stated, there exist $\tilde{K} > 0$ and $\tilde{\varepsilon} > 0$ such that $|v^e - v^\star| \leq \tilde{K}\varepsilon^2$ for $\varepsilon \leq \tilde{\varepsilon}$, i.e.

$$v^\star - \tilde{K}\varepsilon^2 \leq v^e \leq v^\star + \tilde{K}\varepsilon^2, \tag{12}$$

for $\varepsilon \leq \tilde{\varepsilon}$. In order to get both inequalities (10) and (12) satisfied, the parameter $\varepsilon$ is chosen such that $\varepsilon \leq \min(\varepsilon^\star, \tilde{\varepsilon})$. In terms of the diffusion coefficient $D$, it has to satisfy $D \geq \max(D^\star, \tilde{D})$where $\varepsilon^\star = 1/D^\star$and $\tilde{\varepsilon} = 1/\tilde{D}$.

### C. Concepts and results on linearization

In order to build a linearized model of (3) around an equilibrium profile, denoted $(x_1^e, x_2^e)$, we introduce the following variables $\xi_1 = x_1 - x_1^e, \xi_2 = x_2 - x_2^e$. For the sake of simplicity in the notations, we introduce the product space $H = L^2(0,1) \times L^2(0,1)$and the function $g: \mathcal{D} \to L^2(0,1)$ defined by $g(x_1,x_2) = \alpha(1-x_2)e^{\frac{-\mu}{1+x_1}}$, where the invariant closed and convex domain $\mathcal{D}$ is defined as $\{(x_1,x_2) \in H | -1 \leq x_1, 0 \leq x_2 \leq 1 \text{ a.e. on } [0,1]\}$ and represents the physical constraints domain associated to (3) that are expressed in (4). When one deals with nonlinear infinite dimensional systems, different kinds of linearization are available. Those used here are based on *Gâteaux* and *Fréchet* derivatives. Roughly speaking, the Gâteaux derivative is the extension of the directional derivative (finite dimensional case) and the Fréchet derivative is a stronger concept that assumes that the Gâteaux derivative is the same in all directions. See e.g. [12] or [13, Pages 6, 7].

*Definition 2.2:* Let $F: \mathcal{D}(F) \subset X \to X$ be a (nonlinear) operator defined on the Banach space $X$. The operator $F$ is Gâteaux differentiable at $z_0 \in \mathcal{D}(F)$ if there exists a linear operator $dF(z_0): X \to X$ such that $\lim_{l \to 0} \frac{F(z_0+lh)-F(z_0)}{l} = dF(z_0)h$, for every $h \in \mathcal{D}(F)$ such that[2] $z_0 + lh \in \mathcal{D}(F)$.

The operator $F$ is said to be Fréchet differentiable at $z_0 \in \mathcal{D}(F)$ if there exists a bounded linear operator $DF(z_0): X \to X$ such that, $\lim_{h \to 0} \frac{\|F(z_0+h)-F(z_0)-DF(z_0)h\|_X}{\|h\|_X} = 0$. That is, for all $h \in X$ such that $z_0 + h \in \mathcal{D}(F)$, $F(z_0+h) - F(z_0) = DF(z_0)h + w(z_0,h)$, where $\lim_{\|h\|_X \to 0} \|w(z_0,h)\|_X / \|h\|_X = 0$.

Fréchet differentiability is often complicated to get, mainly due to technical difficulties or simply because many nonlinear operators are not Fréchet differentiable since they are unbounded. For the system (3), we shall linearize the nonlinear operator $g$ by using a Gâteaux derivative.

*Lemma 2.3:* The nonlinear operator $g$ introduced above is Gâteaux differentiable at $(x_1^e, x_2^e) \in \mathcal{D}$ and its Gâteaux derivative is given by the bounded linear operator $dg(x_1^e, x_2^e): H \to L^2(0,1)$defined for $(\xi_1 \; \xi_2)^T \in H$ by

$$dg(x_1^e, x_2^e)(\xi_1 \quad \xi_2)^T = \alpha \frac{\mu(1-x_2^e)}{(1+x_1^e)^2} e^{\frac{-\mu}{1+x_1^e}} \xi_1 - \alpha e^{\frac{-\mu}{1+x_1^e}} \xi_2.$$

*Proof:* Let us consider $\xi = (\xi_1 \; \xi_2)^T \in H$ and $x^e = (x_1^e, x_2^e) \in \mathcal{D}$. By computing $\lim_{l \to 0} \frac{g(x^e + l\xi) - g(x^e)}{l}$, it holds

$$dg(x_1^e, x_2^e)(\xi_1 \; \xi_2)^T = \lim_{l \to 0} \frac{\alpha(1-x_2^e)(e^{\frac{-\mu}{1+x_1^e+l\xi_1}} - e^{\frac{-\mu}{1+x_1^e}})}{l} - \lim_{l \to 0} \frac{\alpha l \xi_2 e^{\frac{-\mu}{1+x_1^e+l\xi_1}}}{l}$$

[2] Note that in the case where $\mathcal{D}(F)$ is convex, it is ensured that $az_0 + (1-a)(z_0 + lh) \in \mathcal{D}(F)$ for any $a \in [0,1]$ if so do $z_0$ and $z_0 + lh$.

$$= \alpha \frac{\mu\left(1-x_2^e\right)}{\left(1+x_1^e\right)^2} e^{\frac{-\mu}{1+x_1^e}} \xi_1 - \alpha e^{\frac{-\mu}{1+x_1^e}} \xi_2.$$

The linearity of the operator $dg(x^e)$ is obtained directly. Its boundedness is proven in the next subsection. ■

For a matter of convenience, we denote $\alpha\mu((1-x_2^e)/(1+x_1^e)^2)e^{-\mu/(1+x_1^e)}$by $g_{x_1}(z)$ and $-\alpha e^{-\mu/(1+x_1^e)}$by $g_{x_2}(z)$ in the following. Note that, with the definition of Fréchet differentiability introduced above, it can be shown that the nonlinear operator $g$ is not Fréchet differentiable when considering $L^2(0,1)$ as state space: see the Appendix. Before showing the well-posedness of the linearized model corresponding to (3), let us consider the following subsection that consists of making a step further to show the boundedness of the Gâteaux derivative of the operator $g$.

### D. Well-posedness of the linearized model

With the notations of Section II-C, the linearized model around an equilibrium profile is written in its abstract differential form as

$$\begin{cases} \dot{\xi} = A\xi + \begin{pmatrix} \delta dg(x^e)I & 0 \\ 0 & dg(x^e)I \end{pmatrix} \xi, \\ \xi(0) = \xi_0, \end{cases} \tag{13}$$

where $A$ is the unbounded linear operator defined as $A\xi = \begin{pmatrix} \frac{1}{Pe_h}\frac{d^2\xi_1}{dz^2} - \frac{d\xi_1}{dz} & \frac{1}{Pe_m}\frac{d^2\xi_2}{dz^2} - \frac{d\xi_2}{dz} \end{pmatrix}^T$ for $\xi = (\xi_1 \quad \xi_2)^T$in $D(A)$ given by

$$\left\{\xi \in (H^2(0,1))^2 \,|\, \frac{d\xi_1}{dz}(0) = Pe_h\xi_1(0), \frac{d\xi_1}{dz}(1) = 0, \frac{d\xi_2}{dz}(0) = Pe_m\xi_2(0), \frac{d\xi_2}{dz}(1) = 0\right\}, \tag{14}$$

with $\xi_1(t,z) = x_1(t,z) - x_1^e(z)$and $\xi_2(t,z) = x_2(t,z) - x_2^e(z)$. According to e.g. [1], it is well-known that this operator is the infinitesimal generator of a contraction $C_0-$semigroup. In order to show that the operator $A + \left(\delta dg(x^e) \; dg(x^e)\right)^T$ is still the generator of a $C_0-$semigroup, we show the boundedness of the operator $\left(\delta dg(x^e) \; dg(x^e)\right)^T$ and use the *Bounded Perturbation Theorem*, see [14, Bounded Perturbation Theorem]. That operator can be written as $A_1 + A_2$ where $A_1 = \begin{pmatrix} \delta g_{x_1}(z) & 0 \\ 0 & g_{x_2}(z) \end{pmatrix}$ and $A_2 = \begin{pmatrix} 0 & \delta g_{x_2}(z) \\ g_{x_1}(z) & 0 \end{pmatrix}$.

*Lemma 2.4:* The linear operator $A_1$ is bounded on $H$.

*Proof:* We have to show that there exists some constant $c > 0$ such that for every $\xi = (\xi_1 \; \xi_2)^T \in H, \|A_1\xi\|_H \leq c\|\xi\|_H$. By taking $\xi \in H$, a straightforward computation of $\|A_1\xi\|_H^2 = \|(A_1\xi)_1\|_{L^2}^2 + \|(A_1\xi)_2\|_{L^2}^2$ gives

$$\|A_1\xi\|_H^2 = \left\|\delta\alpha(1-x_2^e)e^{\frac{-\mu}{1+x_1^e}} \frac{\mu}{(1+x_1^e)^2}\xi_1\right\|_{L^2}^2 + \left\|\alpha e^{\frac{-\mu}{1+x_1^e}}\xi_2\right\|_{L^2}^2.$$

By using the fact that $(x_1^e \; x_2^e) \in \mathcal{D}$, it holds $0 \leq 1 - x_2^e \leq 1$ a.e on $[0,1]$ and $e^{-\mu/(1+x_1^e)} \leq 1$ a.e. on $[0,1]$. Hence,

$$\|A_1\xi\|_H^2 \leq \frac{\delta^2\alpha^2\mu^2}{\tilde{\eta}^4}\|\xi_1\|_{L^2}^2 + \alpha^2\|\xi_2\|_{L^2}^2,$$

where we have been using the inequality $\|1/(1+x_1^e)\|_\infty \leq \frac{1}{\tilde{\eta}}$ for the last inequality (see Theorem 2.2). In this way,

$$\|A_1\xi\|_H^2 \leq \max\left\{\frac{\delta^2\alpha^2\mu^2}{\tilde{\eta}^4}, \alpha^2\right\}\|\xi\|_H^2.$$

It follows that

$$\|A_1\|_{op} \leq \sqrt{\max\left\{\frac{\delta^2\alpha^2\mu^2}{\tilde{\eta}^4}, \alpha^2\right\}} = \alpha\max\left\{\frac{\delta\mu}{\tilde{\eta}^2}, 1\right\}.$$

■

The boundedness of $A_2$ is established by similar arguments. Hence the linearized model around an equilibrium, given by (13), is well-posed.

## III. Exponential stability

In this section, we shall apply a Lyapunov–type method, see e.g. [15, Chapters 4 and 5], in order to derive sufficient conditions for the exponential stability of equilibrium profiles for the linearized model of (3), i.e. (13). By exponential stability, we mean that the $L^2 \times L^2-$norm of the state trajectory of (13) decreases as fast as a decreasing exponential for any initial condition in the domain of the linear operator that describes the dynamics, i.e. there exists $\lambda > 0$ such that $\|\xi(t,\cdot)\|_{L^2\times L^2} \leq e^{-\lambda t}\|\xi_0(\cdot)\|_{L^2\times L^2}$ holds for every $\xi_0 \in D(A)$ given by (14).

Let us introduce the change of variables $\hat{\xi}_1(t,z) = e^{-\frac{Pe_h}{2}z}\xi_1(t,z), \hat{\xi}_2(t,z) = e^{-\frac{Pe_m}{2}z}\xi_2(t,z)$ and recall that we consider equal Peclet numbers. This allows to decouple the PDEs in the variables $\hat{\xi}_1$ and $\hat{\xi}_2$. Hence stability is adressed by looking at one parabolic PDE with variable coefficients instead of two, see [5, Section 2.5.2.1].

Let us define the asymptotic reaction invariant $\chi(t,z) = \hat{\xi}_1(t,z) - \delta\hat{\xi}_2(t,z)$ to obtain the two coupled systems

$$\begin{cases} \frac{\partial\chi}{\partial t} = \frac{1}{Pe}\frac{\partial^2\chi}{\partial z^2} - \frac{Pe}{4}\chi, \\ \frac{\partial\chi}{\partial z}(0) = \frac{Pe}{2}\chi(0), \; \frac{\partial\chi}{\partial z}(1) = -\frac{Pe}{2}\chi(1), \end{cases} \tag{15}$$

and

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

where $G_1(z) = g_{x_1}(x_1^e, x_2^e)$ and $G_2(z) = g_{x_2}(x_1^e, x_2^e)$. Let us define the linear operator $\mathfrak{A}\cdot := \frac{1}{Pe}\frac{d^2\cdot}{dz^2} - \frac{Pe}{4}I\cdot$ on the domain $D(\mathfrak{A})$ given by $\left\{\chi \in H^2(0,1), \frac{d\chi}{dz}(0) = \frac{Pe}{2}\chi(0), \frac{d\chi}{dz}(1) = -\frac{Pe}{2}\chi(1)\right\}$.The following proposition enables us to characterize exponential stability of the equilibrium profiles of (3) for the linearized dynamics on the basis of only one parabolic PDE.

*Proposition 3.1:* Let us consider the operator matrix $U = \begin{pmatrix} I & 0 \\ I & -\delta I \end{pmatrix} \in \mathcal{L}(H)$. The change of variables $\begin{pmatrix} \hat{\xi}_1 \\ \chi \end{pmatrix} = U\begin{pmatrix} \hat{\xi}_1 \\ \hat{\xi}_2 \end{pmatrix}$ yields a triangularization of (13). Moreover, the component $\chi$ in the new variables is expressed as

$$\chi(t,z) = \sum_{n=1}^{+\infty}\psi_n\phi_n(z)e^{-\left(\beta_n^2 + \frac{Pe}{4}\right)t}, \tag{16}$$

for $z \in [0,1], t \geq 0$ where $\psi_n = \int_0^1 f(z)\phi_n(z)dz$ and $f(z)$ denotes the initial condition of the variable $\hat{\xi}_1 - \delta\hat{\xi}_2$. The set $\{\phi_n\}_{n\geq 1}$ contains the eigenfunctions of the linear operator $\mathfrak{A}$, defined by $\phi_n(z) = K_n[\beta_n\sqrt{Pe}\cos(\beta_n\sqrt{Pe}z) + \frac{Pe}{2}\sin(\beta_n\sqrt{Pe}z)]$. Note that $\{K_n\}_{n\geq 1}$ is a set of normalization constants expressed as $K_n = \left(\frac{2}{\beta_n^2 Pe + Pe + Pe^2/4}\right)^{\frac{1}{2}}$ and $\{\beta_n\}_{n\geq 1}$ are the solutions of the resolvent equation $\tan(\beta\sqrt{Pe}) = \frac{4\beta\sqrt{Pe}}{4\beta^2 - Pe}$, see e.g. [16].

*Proof:* See e.g. [5, Section 2.5.2]. ■

Note that $U$ defines a similarity transformation, i.e. a Banach isomorphism on $H$. Then (13), which involves the variables $\begin{pmatrix} \hat{\xi}_1 \\ \hat{\xi}_2 \end{pmatrix}$, is equivalent to (13) written in the variables $\begin{pmatrix} \hat{\xi}_1 \\ \chi \end{pmatrix}$. Consequently, exponential stability of (13) can either be studied in the first set of variables or in the second one. Since $\{\phi_n\}_{n\in\mathbb{N}}$ is a Riesz-basis for $L^2(0,1)$, it follows from (11) that $\|\chi(\cdot,t)\|_{L^2} \leq$

$e^{-(\beta_1^2+Pe/4)t}\|f(\cdot)\|_{L^2}$, where $-(\beta_1^2+Pe/4)=\sup_{n\in\mathbb{N}}\{-(\beta_n^2+Pe/4)\}$is the growth constant of the semigroup generated by the Riesz-spectral operator that describes the dynamics (10). This means that $\|\chi(t,\cdot)\|_{L^2}$ converges exponentially fast to 0 as $t$ tends to $+\infty$. Moreover, by using the reaction invariant $x_1^e-\delta x_2^e$, the stability analysis is based on the following parabolic PDE

$$\begin{cases} \frac{\partial\hat{\xi}_1}{\partial t}=\frac{1}{Pe}\frac{\partial^2\hat{\xi}_1}{\partial z^2}-q(z)\hat{\xi}_1, \\ \frac{\partial\hat{\xi}_1}{\partial z}(0)=\frac{Pe}{2}\hat{\xi}_1(0),\ \frac{\partial\hat{\xi}_1}{\partial z}(1)=-\frac{Pe}{2}\hat{\xi}_1(1), \end{cases} \tag{17}$$

where $\hat{\xi}_1(z,t)=e^{\frac{-Pe}{2}z}(x_1(z,t)-x_1^e(z))$ and $q(z)=\frac{Pe}{4}+\frac{k_0L}{v^e}e^{\frac{-\mu}{1+x_1^e(z)}}-\delta\frac{k_0L}{v^e}\frac{\mu(1-x_2^e(z))}{(1+x_1^e(z))^2}e^{\frac{-\mu}{1+x_1^e(z)}}$. Let us choose as Lyapunov functional candidate the function $V:L^2(0,1)\to\mathbb{R}$, defined by $V(\hat{\xi}_1)=\frac{1}{2}\|\hat{\xi}_1\|_{L^2}^2$. By differentiating $V$ w.r.t. $t$ along the state trajectories corresponding to (17), one gets

$$\dot{V}(\hat{\xi}_1)=\frac{1}{2}\frac{d}{dt}\int_0^1\hat{\xi}_1^2dz=\int_0^1\hat{\xi}_1\left(\frac{1}{Pe}\frac{d^2\hat{\xi}_1}{dz^2}-q(z)\hat{\xi}_1\right)dz.$$

An integration by parts yields the following form for $\dot{V}(\hat{\xi}_1)$:

$$-\frac{1}{2}\hat{\xi}_1^2(1)-\frac{1}{2}\hat{\xi}_1^2(0)-\frac{1}{Pe}\int_0^1\left(\frac{d\hat{\xi}_1}{dz}\right)^2dz-\int_0^1q(z)\hat{\xi}_1^2dz.$$

According to the *Generalized Mean Value Theorem for Integrals*, see [17, Theorem 3.3], the first order time derivative of $V$ takes the form

$$-\frac{1}{2}\hat{\xi}_1^2(1)-\frac{1}{2}\hat{\xi}_1^2(0)-\frac{1}{Pe}\int_0^1\left(\frac{d\hat{\xi}_1}{dz}\right)^2dz-q(c)\int_0^1\hat{\xi}_1^2dz \tag{18}$$

for some $c\in(0,1)$. Before stating the main result, we shall prove the following lemma, obtained by exploiting a variation of *Wirtinger's Inequality*, see [18, Corollary 9].

*Lemma 3.1:* For any continuously differentiable function $w$ on $[0,1]$,

$$-\frac{1}{2}w^2(0)\le-\frac{1}{4\Lambda}\int_0^1w^2(z)dz+\frac{2}{\pi^2(2\Lambda-1)}\int_0^1w_z^2(z)dz, \tag{19}$$

for all $\Lambda>\frac{1}{2}$, where $w_z:=\frac{dw}{dz}$ for the ease of notation.

*Proof:* By [18, Corollary 9], it holds

$$\int_0^1(w(z)-w(0))^2dz\le\frac{4}{\pi^2}\int_0^1w_z(z)^2dz, \tag{20}$$

or equivalently

$$\int_0^1w^2(z)dz\le-w^2(0)+\int_0^12w(0)w(z)dz+\frac{4}{\pi^2}\int_0^1w_z^2(z)dz.$$

By using *Generalized Young's Inequality* [19], it follows that

$$\left(1-\frac{1}{2\Lambda}\right)\int_0^1w^2(z)dz\le(-1+2\Lambda)w^2(0)+\frac{4}{\pi^2}\int_0^1w_z^2(z)dz, \tag{21}$$

for some $\Lambda>0$. To ensure the positivity of $1-\frac{1}{2\Lambda}$, we have to assume that $\Lambda>\frac{1}{2}$. In this way, one can write (21) as

$$\int_0^1w^2(z)dz\le2\Lambda w^2(0)+\frac{8\Lambda}{\pi^2(2\Lambda-1)}\int_0^1w_z^2(z)dz.$$

■

Note that by applying similar arguments on the function $\tilde{w}$ defined by $\tilde{w}(z)=w(1-z),z\in[0,1]$, (19) holds also with $w(0)$ replaced by $w(1)$. We are now ready to give a bound on the time derivative of the Lyapunov functional. By considering (18) and by applying Lemma 3.1 to $\hat{\xi}_1$, $\dot{V}$ is bounded by

$$\left(\frac{-1}{2\Lambda}-q(c)\right)\int_0^1\hat{\xi}_1^2dz+\left(\frac{4}{\pi^2(2\Lambda-1)}-\frac{1}{Pe}\right)\int_0^1\left(\frac{d\hat{\xi}_1}{dz}\right)^2dz.$$

We shall now choose $\Lambda$ in such a way that $\frac{4}{\pi^2(2\Lambda-1)}-\frac{1}{Pe}=0$, which yields $\Lambda=\frac{1}{2}+\frac{2Pe}{\pi^2}>\frac{1}{2}$. Consequently

$$\frac{1}{2}\frac{d}{dt}\|\hat{\xi}_1\|_{L^2}^2\le-\left(\frac{\pi^2}{\pi^2+4Pe}+q(c)\right)\int_0^1\hat{\xi}_1^2dz.$$

By applying Grönwall's Lemma, see [20, Lemma A.6.7], one gets

$$\|\hat{\xi}_1(t,\cdot)\|_{L^2}\le e^{-\left(\frac{\pi^2}{\pi^2+4Pe}+q(c)\right)t}\|\hat{\xi}_1(0,\cdot)\|_{L^2}. \tag{22}$$

We are now ready to address the exponential stability of the equilibrium profiles.

*Theorem 3.1:* A sufficient condition for an equilibrium profile of (17) to be exponentially stable is that

$$\mu\le\tilde{h}^e(a), \tag{23}$$

where the function $\tilde{h}^e(a)$ is defined as $\frac{\left(1-\tilde{f}^e(a)\right)^2(r(\delta-a-al_D)+a)}{\left(\delta+\tilde{f}^e(a)\right)a}$ with $\tilde{f}^e(a)=\frac{k_0L(\delta-a)e^{\frac{-\mu}{1+a}}}{2D}-a+\frac{K}{D^2},r=\frac{\pi^2}{\pi^2+4Pe}+\frac{Pe}{4}$ and

$$l_D=\frac{\frac{k_0L(\delta-a)e^{\frac{-\mu}{1+a+\frac{K}{D^2}}}}{a}-\frac{k_0L(\delta-a)e^{\frac{-\mu}{1+a}}}{a}+\frac{\tilde{K}}{D^2}}{k_0Le^{\frac{-\mu}{1+a+\frac{K}{D^2}}}}, \tag{24}$$

where $K,\tilde{K}$ are the positive constants introduced in (10) and (12), respectively. Note that in the case where inequality (23) holds, exponential stability is obtained for all $D\ge\max(D^\star,\tilde{D})$ where $D^\star>0$ and $\tilde{D}>0$ are sufficiently large.

*Proof:* Starting from inequality (23), it holds

$$\frac{a\left(\mu\delta+\mu\tilde{f}^e(a)-\left(1-\tilde{f}^e(a)\right)^2\right)}{\delta-a-al_D}\le r\left(1-\tilde{f}^e(a)\right)^2. \tag{25}$$

It follows from inequalities (7) and (11) that $a-\frac{k_0L(\delta-a)e^{\frac{-\mu}{1+a}}}{2D}-\frac{K}{D^2}<x_1^e(z)<a+\frac{K}{D^2}$, a.e. on $(0,1)$, which can be written as

$$-\tilde{f}^e(a)<x_1^e(z)<a+K/D^2. \tag{26}$$

Since $x_1^e(z)<a+K/D^2$ a.e. on $(0,1)$, it follows that $e^{-\mu/(1+x_1^e(z))}<e^{-\mu/(1+a+\frac{K}{D^2})}$ a.e. on $(0,1)$. Combining (25), (26) and the previous inequality, it follows that

$$\frac{k_0Le^{\frac{-\mu}{1+x_1^e(z)}}}{k_0Le^{\frac{-\mu}{1+a+\frac{K}{D^2}}}}\frac{a\left(\mu\delta-\mu x_1^e(z)-\left(1+x_1^e(z)\right)^2\right)}{\delta-a-al_D}<r\left(1+x_1^e(z)\right)^2,$$

or equivalently

$$\frac{k_0Le^{\frac{-\mu}{1+x_1^e(z)}}\left(\mu\delta-\mu x_1^e(z)-\left(1+x_1^e(z)\right)^2\right)}{\frac{k_0L(\delta-a)e^{\frac{-\mu}{1+a+\frac{K}{D^2}}}}{a}-k_0Le^{\frac{-\mu}{1+a+\frac{K}{D^2}}}l_D}<r\left(1+x_1^e(z)\right)^2.$$

By plugging the expression of $l_D$ (24) in the previous inequality, it follows that

$$\frac{k_0Le^{\frac{-\mu}{1+x_1^e(z)}}}{v^\star-\frac{\tilde{K}}{D^2}}\left(\mu\delta-\mu x_1^e(z)-(1+x_1^e(z))^2\right)<r\left(1+x_1^e(z)\right)^2.$$

By taking into account inequalities (12), it holds $\frac{1}{v^e}\le\frac{1}{v^\star-\tilde{K}/D^2}$. Moreover, by dividing the last inequality by $(1+x_1^e(z))^2$, one obtains $-q(z)+Pe/4<r$ where we have been using $x_1^e(z)=\delta x_2^e(z)$. Hence $\frac{\pi^2}{\pi^2+4Pe}+q(z)>0$ for a.e. $z\in(0,1)$. In particular, $\frac{\pi^2}{\pi^2+4Pe}+q(c)>0$ for $c\in(0,1)$. By using the fact that (22) holds for all $t>0$, it follows that the equilibrium $x_1^e$ is exponentially stable. ■

*Remark 3.1:* Note that the condition "$D\geq\max(D^\star,\tilde{D})$" in the assumptions of Theorem 3.1 is needed in order to use both inequalities (11) and (12) that are valid for $D>D^\star$ and $D>\tilde{D}$, respectively.

The next step consists in showing that in the case of only one equilibrium profile, the latter is always exponentially stable and in the case of three equilibrium profiles, the pattern "exponentially stable–unstable–exponentially stable" is exhibited: see the two next corollaries.

*Corollary 3.1:* In the case where the nonisothermal axial dispersion tubular reactor (3) admits only one equilibrium profile, there exist $D^\star$ and $\tilde{D}$ sufficiently large such that this equilibrium profile is exponentially stable for all $D\geq\max(D^\star,\tilde{D})$.

*Proof:* First remember the approximated form of the velocity $v^\star$ given by $k_0L(\delta-a)e^{\frac{-\mu}{1+a}}/a$ and remember also that for a fixed value of $v^\star$ the number of equilibria is determined as the number of values of $a$ that reach $v^\star$, see the proof of Lemma 2.2. Hence, looking at $v^\star$ as a function of $a$, one has the following two options:

$$\mu\delta(\mu\delta-4\delta-4)<0, \tag{27}$$

$$\mu\delta(\mu\delta-4\delta-4)=0. \tag{28}$$

In the first situation, i.e. (27), the first order derivative of $v^\star(a)$ with respect to $a$ has no root, meaning that $v^\star$ has no extremum and is strictly decreasing, see [2, Section IV.A]. Only one value of $a$ can reach a fixed value $v^\star$ (one equilibrium). In the second case, i.e. (28), the first order derivative of $v^\star(a)$ with respect to $a$ vanishes only one time in the interval $]0,\delta[$, see [2, Section IV.A] and in particular [2, Equation (15)], wherein it is shown that the point where $\frac{dv^\star}{da}(a)$ vanishes is a point of inflexion, meaning that $v^\star$ is monotone on $]0,\delta[$ (only one value of $a$ can reach a fixed value of $v^\star$). To get exponential stability, by Theorem 3.1, one has to check that $\mu\leq\tilde{h}^e(a)$. This could be seen as challenging to show by looking at the expression of function $\tilde{h}^e(a)$. Therefore we shall use perturbation theory that consists of reformulating the problem with a (small) parameter and then looking at the problem by setting the parameter to 0, see e.g. [11, Regular Perturbation Theorem]. Hence, by introducing the parameter $\varepsilon=1/D$, the problem of finding values of $a$ such that $\mu\leq\tilde{h}^e(a)$ can be approached by a similar one by taking $\varepsilon=0$, i.e.[3] $\mu\leq\frac{\delta(1+a)^2}{a(\delta-a)}=:h(a)$. Equivalently we have

$$(\mu+\delta)a^2-\delta(\mu-2)a+\delta\geq0. \tag{29}$$

Let us look at the case for which (27) holds. The discriminant of the second order polynomial in (29), denoted by $\rho$, is equal to $\mu\delta(\mu\delta-4\delta-4)$, which is assumed to be negative here. Hence (29) is satisfied for all values of $a\in]0,\delta[$ and the corresponding equilibrium profiles are exponentially stable by Theorem 3.1. In the second case, see (28), the polynomial in (29) vanishes only one time when $a=\delta/(2+\delta):=a^\star$. For other values of the parameter $a$, it is positive, leading to exponential stability of the related equilibria. Note that the values of the function $h(a)$ characterize the speed of convergence to 0 (measured by the growth constant). Nearer $a$ is to 0 or $\delta$, faster the $L^2-$norm of the state trajectory $\hat{\xi}_1$ decreases exponentially fast to 0, as $t$ tends to $+\infty$. The reason behind is that nearer $a$ is to 0 or $\delta$, faster is the polynomial in (29) from 0. ■

[3] Setting $1/D$ to 0 implies that $l_D=0, r=1$ and $\tilde{f}^e(a)=-a$.

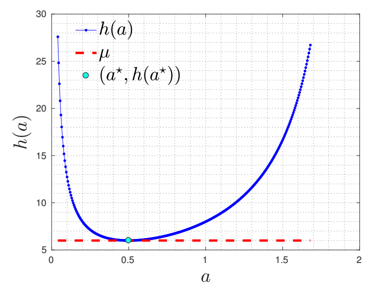


Fig. 1. Function $h(a)$ for $\mu=6$ and $\delta=2(\rho=0$, one equilibrium).

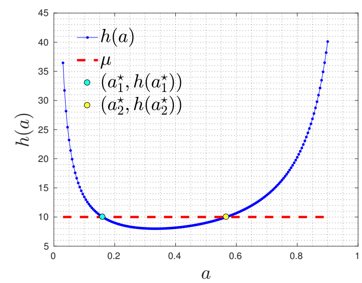


Fig. 2. Function $h(a)$ for $\mu=10$ and $\delta=1(\rho>0$, three equilibria).

The following corollary is dedicated to the case where three equilibria are exhibited.

*Corollary 3.2:* In the case where the nonisothermal axial dispersion tubular reactor admits three equilibrium profiles, there exist $D^\star$ and $\tilde{D}$ sufficiently large such that the pattern "exponentially stable – unstable – exponentially stable" holds for all $D\geq\max(D^\star,\tilde{D})$.

*Proof:* Similar arguments to those presented in the previous corollary are used here. In the case where the reactor can exhibit three equilibria, three values of $a$ can reach a fixed value of $v^\star$ meaning that $v^\star(a)$ has two extrema in the interval $]0,\delta[$. Mathematically there holds

$$\mu\delta(\mu\delta-4\delta-4)>0, \tag{30}$$

see the proof of Corollary 3.1 and [2, Section IV.A] for the reasoning and calculation details. Once more, exponential stability is obtained if (29) is satisfied. Since (30) holds, the second order polynomial in (29) possesses two roots that are given by $a_1^\star=\frac{\delta(\mu-2)}{2(\mu+\delta)}-\frac{1}{2(\mu+\delta)}\sqrt{\mu\delta(\mu\delta-4\delta-4)}$and $a_2^\star=\frac{\delta(\mu-2)}{2(\mu+\delta)}+\frac{1}{2(\mu+\delta)}\sqrt{\mu\delta(\mu\delta-4\delta-4)}$. Hence values of $a$ in the interval $]0,a_1^\star[$ or in $]a_2^\star,\delta[$ lead to exponentially stable equilibria. Since $a_1^\star$ and $a_2^\star$ are also roots of the first order derivative of $v^\star$, the intervals $]0,a_1^\star[,[a_1^\star,a_2^\star]$ and $]a_2^\star,\delta[$ denote the three zones where the first, the second and the third equilibrium profiles are located, respectively, see the expression and the shape of $v^\star(a)$. It follows that the first and the third equilibria are exponenially stable. For establishing the instability of the second equilibrium, we refer to [5, Section 2.5.2.]. ■

Illustrations of function $h(a)$ are depicted in Figures 1 and 2, for one equilibrium and three equilibria, respectively.

*Remark 3.2:* The convection-reaction-diffusion model is an intermediate model between the plug flow reactor model (when the diffusion coefficients are 0) and the CSTR model described by ODEs (the diffusion coefficients "are infinite"), see e.g. [21]. From [5], the plug flow reactor model can exhibit only one equilibrium profile while the CSTR may exhibit three. Intuitively, the reason why considering $D \geq \max(D^\star, \tilde{D})$ is quite natural here since there should exist a diffusion coefficient above which the tubular reactor can exhibit multiple equilibria and below which the reactor exhibit only one equilibrium, see [3]. Moreover, in the case where the diffusion coefficients vanish, the only equilibrium profile that is exhibited is exponentially stable, see e.g. [22].

## IV. Numerical simulations

This section is devoted to the illustration of the pattern highlighted above in the case when the reactor admits three equilibrium profiles. The parameters that have been chosen are the following : $\mu = 10, \delta = 1, v = 1, 1 * 10^{-3}, D = 10, k_0 = 1, L = 1$. The $L^2-$norm of the state trajectory $\hat{\xi}_1(t,\cdot)$ as a function of time is depicted in Figures 3, 4 and 5 for the three different equilibria, respectively, by using a numerical integration of the linearized PDE (17). Moreover, the relative error between the estimate found on the $L^2-$norm of the state trajectory $\hat{\xi}_1(t,\cdot)$, see (22), is also depicted in Figures 6, 7 and 8 (where RHS stands for Right-Hand Side), in order to illustrate the efficiency of the estimation.

## V. Conclusion and perspectives

In this paper, the stability analysis of a linearized model of a nonisothermal axial dispersion tubular reactor has been performed. After linearization, the model has been shown well-posed. Then sufficient conditions are given for an equilibrium profile of the linearized system to be exponentially stable. By characterizing the different equilibria, it has also been shown that, in the case when the reactor can exhibit only one equilibrium profile, the latter is always exponentially stable and in the case of three equilibria, the pattern "exponentially stable–unstable–exponentially stable" is highlighted, which is called bistability. The main contributions concern the well-posedness of the linearized model but mostly the type of stability that is proven and from this point of view, this paper extends previous results of [5, Section 2.5.2.].

Note that imposing the equality between the Peclet numbers $Pe_h$ and $Pe_m$ is quite a strong assumption since it entails that the condition $D_{ma} = \frac{\lambda_{ea}}{\rho C_p}$ holds true. This condition may be seen as restrictive from a physical point of view since $D_{ma}$ and $\lambda_{ea}$ are diffusion coefficients that model two completely different kinds of diffusion. However, studying exponential stability of the linearized system when the Peclet numbers are different is really challenging from a mathematical point of view. In this case, the asymptotic reaction invariant $\chi$ (see (16)) is not available anymore, which entails that no model reduction can be performed. Moreover, note that even the analysis of the existence and the multiplicity of the equilibrium profiles in the case of different Peclet numbers remained open for many years and is now quite a newly solved question, see [2]. To the best of our knowledge, the question of asymptotic stability in the case of different Peclet numbers is also still open. Hence the extension of the results on linearized stability to the case of different or close Peclet numbers could be considered for further research.

Furthermore, as indicated in Section II, one can linearize a nonlinear infinite-dimensional system either by means of a Gâteaux or a Fréchet derivate, but linearization with Fréchet derivative is not always possible, depending on the properties of the nonlinear operator. However Fréchet differentiability of the nonlinear operator with some more assumptions, see [12], could lead to conclusions on the stability of the nonlinear system (3). In that way, the next objective should be the investigation of local exponential stability or local instability of the nonlinear system by using such tools.

This analysis is a preliminary step before building control laws in order to stabilize the system around an equilibrium profile.

## VI. Acknowledgments

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## Appendix

Here we aim at showing that the nonlinear operator $g$ defined in Section II-C is not Fréchet differentiable at an equilibrium $x^e$. Therefore we shall consider the nonlinear operator $F : \mathcal{K} \to L^2(0,1)$ defined by $F(x) = (1-x)e^{\frac{-1}{1+x}}$ for $x$ in $\mathcal{K} := \{x \in L^2(0,1), 0 \leq x(z) \leq 1 \text{ a.e. on } [0,1]\}$. This nonlinear operator could be viewed as a simplification of $g$ in one direction with all the constants equal to 1 for the ease of calculation. Without loss of generality, we shall consider the null function of $L^2(0,1)$ as equilibrium profile. In the following result, it is shown that $F$ is not Fréchet differentiable at 0. This is the main reason of considering a Gâteaux linearization of the nonlinear operator $g$ in Section II-C.

*Proposition A.1:* The nonlinear operator $F$ is not Fréchet differentiable at 0.

*Proof:* Suppose, for the sake of a contradiction, that $F$ is Fréchet differentiable at 0. Since it is also Gâteaux differentiable at 0 (see Lemma 2.3) the corresponding derivatives are equal. Remark that the Gâteaux derivative of $F$ at $x^e$ in the direction $h \in L^2(0,1)$ is given by $dF(x^e)h = \left(-e^{\frac{-1}{1+x^e}} + \frac{1-x^e}{(1+x^e)^2}e^{\frac{-1}{1+x^e}}\right)h$. By looking at that derivative for $x^e \equiv 0 \in L^2(0,1)$, one gets that $dF(0) \equiv 0 \in \mathcal{L}(L^2(0,1))$. It follows that the corresponding Fréchet derivative $DF(0)$ is the null operator on $L^2(0,1)$. Because of the Fréchet differentiability of $F$ at 0, the relation $\lim_{\|h\|_{L^2} \to 0} \frac{\|F(0+h)-F(0)-DF(0)h\|_{L^2}}{\|h\|_{L^2}} = 0$ holds for every $h \in \mathcal{K}$, i.e.

$$\lim_{\|h\|_{L^2} \to 0} \|(1-h)e^{\frac{-1}{1+h}} - e^{-1}\chi_{[0,1]}\|_{L^2} / \|h\|_{L^2} = 0, \tag{31}$$

where $\chi_{[0,1]}$ denotes the characteristic function of the interval $[0,1]$. Let us consider the sequence of $L^2(0,1)-$functions $\{h_n\}_{n\in\mathbb{N}}$ defined by $h_n(z) = \frac{1}{n}\chi_{[0,1-\frac{1}{n}]}(z) + \chi_{[1-\frac{1}{n},1]}(z)$, for $n \in \mathbb{N}$. Remark that $h_n \in \mathcal{K}$ for each $n \in \mathbb{N}$. Moreover,

$$\|h_n\|_{L^2}^2 = \int_0^{1-\frac{1}{n}} \frac{1}{n^2} dz + \int_{1-\frac{1}{n}}^1 dz = \frac{n^2+n-1}{n^3}. \tag{32}$$

It is obvious that $\lim_{n\to+\infty} \|h_n\|_{L^2}^2 = 0$. Hence (31) implies that

$$\lim_{n\to+\infty} \frac{\|(1-h_n)e^{\frac{-1}{1+h_n}} - e^{-1}\chi_{[0,1]}\|_{L^2}}{\|h_n\|_{L^2}} = 0. \tag{33}$$

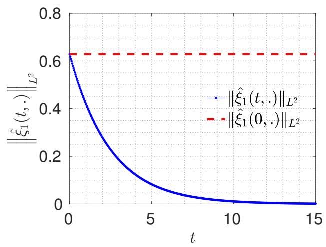


Fig. 3. $L^2-$norm of $\hat{\xi}_1$ for $a = 0.079$ (1st eq.).

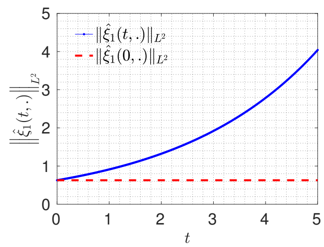


Fig. 4. $L^2-$norm of $\hat{\xi}_1$ for $a = 0.328$ (2nd eq.).

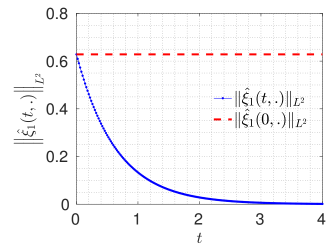


Fig. 5. $L^2-$norm of $\hat{\xi}_1$ for $a = 0.749$ (3rd eq.).

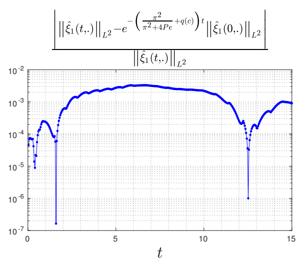


Fig. 6. Relative error between the RHS of (22) and the $L^2-$norm of $\hat{\xi}_1$ for $a = 0.079$ (1st eq.).

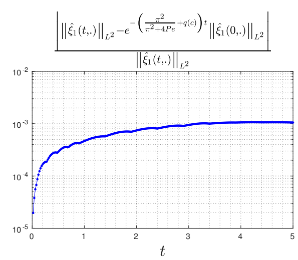


Fig. 7. Relative error between the RHS of (22) and the $L^2-$norm of $\hat{\xi}_1$ for $a = 0.328$ (2nd eq.).

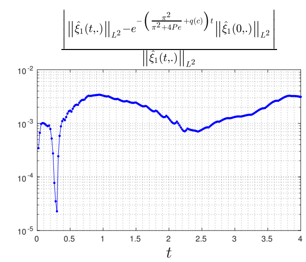


Fig. 8. Relative error between the RHS of (22) and the $L^2-$norm of $\hat{\xi}_1$ for $a = 0.749$ (3rd eq.).

Let us compute $\|(1-h_n)e^{\frac{-1}{1+h_n}} - e^{-1}\chi_{[0,1]}\|^2_{L^2} =: S_n$. It holds

$$\begin{aligned} S_n &= \int_0^1 \left( e^{\frac{-1}{1+h_n(z)}} - e^{-1}\chi_{[0,1]}(z) - e^{\frac{-1}{1+h_n(z)}} h_n(z) \right)^2 dz \\ &= \int_0^{1-\frac{1}{n}} \left( e^{\frac{-1}{1+\frac{1}{n}}} - e^{-1} - e^{\frac{-1}{1+\frac{1}{n}}} \frac{1}{n} \right)^2 dz + \int_{1-\frac{1}{n}}^1 \left( e^{\frac{-1}{2}} - e^{-1} - e^{\frac{-1}{2}} \right)^2 dz \\ &= e^{-2} + e^{\frac{-2n}{1+n}} \frac{(n-1)^3}{n^3} - \frac{2e^{-2+\frac{1}{1+n}}(n-1)^2}{n^2}. \end{aligned} \tag{34}$$

Combining (34) with (32) yields

$$\frac{\|(1-h_n)e^{\frac{-1}{1+h_n}} - e^{-1}\chi_{[0,1]}\|^2_{L^2}}{\|h_n\|^2_{L^2}} = \frac{n^3 e^{-2} + (n-1)^3 e^{\frac{-2n}{1+n}} - 2n(n-1)^2 e^{-2+\frac{1}{1+n}}}{n^2+n-1}.$$

It follows that $\lim_{n\to+\infty} \frac{\|(1-h_n)e^{\frac{-1}{1+h_n}} - e^{-1}\chi_{[0,1]}\|_{L^2}}{\|h_n\|_{L^2}} = e^{-1}$, which is a contradiction since (33) holds. ■

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