Analysis of the existence of equilibrium profiles in nonisothermal axial dispersion tubular reactors

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***Abstract*—This paper deals with the analyis of the nonisothermal axial dispersion tubular reactor. The existence of equilibrium profiles is investigated. In particular, for equal Peclet numbers, it is shown that one or three equilibria can be exhibited, depending on the parameters of the system, especially on the diffusion coefficient. In addition, different and close Peclet numbers are also considered. In these cases, it is also shown that the reactor has one or three equilibrium profiles. Some numerical simulations support the theoretical results.**

***Index Terms*—Nonisothermal tubular reactor - Equilibrium profile - Positive semigroup - Nonlinear infinite-dimensional systems**

I. Introduction

The dynamics of tubular reactors are governed by nonlinear partial differential equations (PDEs) derived from mass and energy balance equations. This includes plug flow and axial dispersion reactor models. Nonlinearities in the dynamics are typically located in the kinetic terms and are based notably on the Arrhenius law for nonisothermal reactors, see [1].

From [2], tubular reactors are known to be well-posed, i.e. there exist unique state trajectories describing the temperature and the reactant concentration's evolution. Some results of [2] are recalled here and some further remarks are made. The well-posedness analysis relies on the semigroup approach; see e.g. [3] or [4] for an overview.

The multiplicity and the stability of equilibrium profiles have been widely studied over the years, see for instance [5] and [6]. More particularly, for biochemical reactor distributed parameter models, a study of the existence and the multiplicity of equilibria was performed in [7].

It is also important to note that many control problems for tubular reactors have also been studied over the years. Even though a majority of works was devoted to lumped parameters systems (see [8] and references therein), one observes an increasing number of contributions for PDE models over the last decades. This includes the challenging issues of controlling and stabilizing PDE models of tubular reactors around unstable equilibrium profiles. For instance, the sliding mode control approach was developed in [9] and applied to the stabilization of both plug flow and tubular reactors, backstepping was studied in [10] and adaptive extremum-seeking control in [11]. An optimal Linear Quadratic (LQ) regulation problem has also been investigated in [1].

More recently, in [13] an analysis of the multiplicity of equilibrium profiles of a tubular reactor with equal energy and mass Peclet numbers was performed. 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). The main contribution of this paper is to extend this study to the case of different or close Peclet numbers.

The aim of this paper is to study the existence of equilibrium profiles for nonisothermal tubular reactors and to derive multiplicity criteria for these equilibrium profiles. It is shown that such reactors can exhibit different numbers of equilibrium profiles depending on parameters of the system, particularly on the diffusion coefficient. A further contribution is to give a clarification of the analysis developed in [13] for equal Peclet numbers.

The paper is organized as follows. In Section II the system under study is introduced together with the reduced model (dimensionless model). Section III is devoted to the study of the well-posedness. In Section IV three different cases, based on the Peclet numbers, for the study of existence of equilibrium profiles in such reactors are analyzed. The approach used here is purely qualitative and consists of an an extension of the analysis developed in [13, Section 3]. The theory is illustrated by some numerical simulations. Note that all the parameter values that are used in the simulations are based on conditions that were used in previous works, see e.g. [10], [7], [12], [11], [14], [9], [5].

II. Model description

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 thickness dz during an infinitesimal time dt as depicted in Figure 1. They are given by

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

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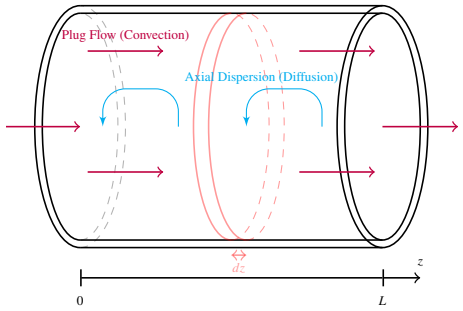

Fig. 1. Profile view of a tubular reactor.

where $T(t,z)$ and $C(t,z)$ denote the temperature in the reactor and the concentration of the reactant respectively in the reactor at time t and position z. Such equations are usually called diffusion-reaction-convection equations. The meaning and the units of the parameters are summarized in Table I.

To the PDEs (1), we associate specific boundary conditions, known as the Danckwerts'conditions [15], which are given by

$$\frac{\lambda_{ea}}{\rho C_p}\frac{\partial T}{\partial z}(t,0) = v(T(t,0)-T_{in}), \frac{\partial T}{\partial z}(t,L) = 0$$

and

$$D_{ma}\frac{\partial C}{\partial z}(t,0) = v(C(t,0)-C_{in}), \frac{\partial C}{\partial z}(t,L) = 0.$$

Observe that Equations (1) together with the above boundary conditions describe a system of controlled PDEs. We distinguish two types of control actions : on one hand, the model takes distributed control into account, symbolized by the variable T_w, which is due to a heat exchanger that acts along the whole spatial domain. On the other hand, the boundary control variables $T_{in}(t)$ and $C_{in}(t)$ can be fixed at the inlet of the reactor.In order to introduce the corresponding dimensionless model, we consider the following change of coordinates

$$\tilde{t} = t\frac{v}{L}, \qquad \tilde{z} = \frac{z}{L}.$$

Applying this change of coordinates to (1) yields the following equivalent PDEs:

$$\begin{cases} \frac{\partial T}{\partial \tilde{t}} = -\frac{\partial T}{\partial \tilde{z}} + \frac{1}{Pe_h}\frac{\partial^2 T}{\partial \tilde{z}^2} - \frac{\Delta H}{\rho C_p}\frac{k_0 L}{v}Ce^{-\frac{E}{RT}} + \frac{4hL}{\rho C_p dv}(T_w - T), \\ \frac{\partial C}{\partial \tilde{t}} = -\frac{\partial C}{\partial \tilde{z}} + \frac{1}{Pe_m}\frac{\partial^2 C}{\partial \tilde{z}^2} - \frac{k_0 L}{v}Ce^{-\frac{E}{RT}}, \end{cases} \tag{2}$$

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

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

The corresponding boundary conditions are given by

$$\frac{\partial T}{\partial \tilde{z}}(\tilde{t},0) = Pe_h(T(\tilde{t},0)-T_{in}), \frac{\partial T}{\partial \tilde{z}}(\tilde{t},1) = 0$$

and

$$\frac{\partial C}{\partial \tilde{z}}(\tilde{t},0) = Pe_m(C(\tilde{t},0)-C_{in}), \frac{\partial C}{\partial \tilde{z}}(\tilde{t},1) = 0.$$

TABLE I
SYSTEM PARAMETERS.

Constant	Unit	Description
L	m	Reactor 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	$\frac{kJ}{kgK}$	Gaz constant
h	$\frac{kJ}{m^2Ks}$	Wall heat transfer coefficient
d	m	Reactor diameter
T_w	K	Coolant temperature
T_{in}	K	Input temperature
C_{in}	$\frac{kg}{m^3}$	Input reactant concentration

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

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

which yields the following PDEs with their associated boundary conditions

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

where

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

For a matter of convenience, the notation $t := \tilde{t}, z := \tilde{z}$ is adopted hereafter.

Remark 2.1: Observe that the description of the dynamics of the product concentration requires an additionnal PDE. However, following the approach of [1], the latter is not considered here, since the evolution of the product concentration is fully determined by the knowledge of the temperature and the reactant concentration.

III. WELL-POSEDNESS

By well-posedness, we mean that (3) has a unique mild solution on $[0,\infty)$. In this section we assume that $T_w = T_{in}$, which entails that $x_w = 0$. Let us define the linear unbounded

operator

$$Ax = \begin{pmatrix} \frac{1}{Pe_h}\frac{d^2}{dz^2} - \frac{d}{dz} - \gamma I & 0 \\ 0 & \frac{1}{Pe_m}\frac{d^2}{dz^2} - \frac{d}{dz} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \tag{4}$$

on the domain

$$D(A) = \left\{ x = (x_1, x_2)^T \in H : \frac{dx}{dz} \in H \text{ a.c. }, \frac{d^2x}{dz^2} \in H \right. \\ \left. \beta_i \frac{dx_i}{dz}(0) - x_i(0) = 0 = \beta_i \frac{dx_i}{dz}(1), i = 1,2 \right\}$$

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

$$\beta_1 = \frac{1}{Pe_h} \text{ and } \beta_2 = \frac{1}{Pe_m}$$

is adopted. Moreover, the nonlinear operator $N : \mathcal{D} \to H$ is defined as

$$N(x) := (\alpha\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}}, \alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}})^T$$

on the domain

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

Using these operators, the system (3) with initial condition can be described equivalently by the following abstract differential equation:

$$\dot{x}(t) = Ax(t) + N(x(t)), \qquad x(0) = x_0. \tag{5}$$

The following result is stated in [2].

Theorem 3.1: For every $x_0 \in \mathcal{D}$, the Cauchy problem (5) admits a unique mild solution $x(t) = S(t)x_0$ for all $t \ge 0$ and $x_0 \in \mathcal{D}$, where $S(t)$ is the nonlinear semigroup on $\mathcal{D}$ whose infinitesimal generator is the operator $A+N$.
Furthermore, the C_0-semigroup $(T(t))_{t\ge 0}$ generated by A is positive.

Proof: See [2], where arguments based on [16] and [3, Theorem 2.3.5] are used to prove that A is the infinitesimal generator of a C_0-semigroup $(T(t))_{t\ge 0}$. The posivity of $(T(t))_{t\ge 0}$ is established in [2, Proposition 5.1]. Furthermore, the fact that $A+N$ generates a nonlinear semigroup on $\mathcal{D}$ is proved by means of [17, Theorem 5.1]. ■

Remark 3.1:

1) Instead of using the Riesz-spectral property of A as in [16], note that the generation of a C_0-semigroup by A can also be obtained by a straightforward application of Lumer-Philipps Theorem separately to both operators A_1 and A_2, see [18, Theorem 6.1.7].
2) One can show that operators A_1 and A_2 describe first order port-Hamiltonian systems with dissipation, see [19, Chapter 6]. Thus the generation of a C_0-semigroup can also be easily deduced by applying [19, Theorem 6.9]. See also [18].

IV. Existence and Multiplicity of equilibrium profiles

In this section, the existence and the multiplicity of equilibrium profiles are investigated in three different cases depending on the link between the Peclet numbers. As in [13], 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 [20, Regular Perturbation Theorem]. Firstly, we consider the case $Pe_h = Pe_m \overset{\text{not.}}{=} Pe$ for which the analysis of [13, 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 (3) at the equilibrium, which read as follows

$$\begin{cases} \frac{1}{Pe_h}\frac{d^2x_1}{dz^2} - \frac{dx_1}{dz} + \alpha\delta(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = 0, \\ \frac{1}{Pe_m}\frac{d^2x_2}{dz^2} - \frac{dx_2}{dz} + \alpha(1-x_2)e^{\frac{\mu x_1}{1+x_1}} = 0, \\ \frac{dx_1}{dz}(0) - Pe_h x_1(0) = 0 = \frac{dx_1}{dz}(1), \\ \frac{dx_2}{dz}(0) - Pe_m x_2(0) = 0 = \frac{dx_2}{dz}(1). \end{cases} \tag{6}$$

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

Considering the change of variables

$$y_1 = x_1, \qquad y_2 = x_1 - \delta x_2, \tag{7}$$

it follows from the second equation and the last boundary conditions of (6) that $y_2 \equiv 0$ (y_2 formally corresponds to a reaction invariant, see [21] and [22]). Moreover, by using the functions u and w defined by

$$u(z) = y_1(1-z), \qquad w(z) = \frac{dy_1}{dz}(1-z), \tag{8}$$

the first equation of (6) with the associated boundary conditions takes the form

$$\begin{cases} \frac{du}{dz} = -w, \\ \frac{dw}{dz} = -\frac{1}{D}(vw - g(u)), \\ u(0) = a, w(0) = 0, w(1) = \frac{v}{D}u(1), \end{cases} \tag{9}$$

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

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

Calculation details are provided in Appendix A. Note that, since $\alpha = \frac{k_0 L}{v}e^{-\mu}$, the function g is equivalently given by

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

Lemma 4.1: 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 $D \ge D^*$, the set of equations (9) 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.

Remark 4.1: We are not interested in finding a solution to (9) but in finding a function $v(a, D)$ such that the final condition $w(1) = \frac{v}{D}u(1)$ is satisfied. Whereas, from the modeling point

of view, v is a (fixed) parameter, in the proof of Lemma 4.1 below, it is interpreted as a function for analysis purposes. It is indeed well known in chemical engineering [14] that the convection-diffusion-reaction model is an intermediate model between the plug flow reactor model (when the diffusion coefficients are equal to zero) and the CSTR (Continuous Stirred Tank Reactor) model (described by ODEs) (when these coefficients tend to $+\infty$). As it was already pointed out in [5], it is obvious that the plug flow reactor can generate only one equilibrium profile since the latter is the solution of a set of first-order differential equations with fixed initial values. And, at the other extreme, it is well known that the CSTR can exhibit three different equilibrium points. Therefore one could conclude intuitively that there should be a value of the diffusion coefficients above which the tubular reactor model can exhibit multiple equilibrium profiles (and below which there is only one equilibrium profile). In this context it is important to note that the (dimensionless) Peclet numbers allow to evaluate the relative importance of convection (characterized by v) versus diffusion (characterized by D). Thus, if there are $a_1 \neq a_2$ and $D > 0$ such that $v(a_1, D) = v(a_2, D)$, the equations (9) have at least two solutions. To reach this goal, we use pertubation theory [20, Regular Perturbation Theorem], which consists of disturbing the equations with a small parameter ε. Then if a solution can be found to the disturbed equations with $\varepsilon = 0$ (see [20, Section 5.2.1., Hypothesis H2]), perturbation theory guarantees that the system has a solution for small ε (this is the reason why we consider a large diffusion coefficient (D^* large enough)), under a few assumptions, especially continuity conditions (see [20, Section 5.2.1., Hypothesis H3]). Furthermore, the solution can be identified to its Taylor expansion of powers of ε.

Proof: Let us introduce the following notations:

$$\varepsilon = \frac{1}{D}, \qquad u_\varepsilon = u, \qquad w_\varepsilon = \frac{1}{\varepsilon} w, \tag{10}$$

where D satisfies $D \geq D^*$ for D^* sufficiently large such that ε is small enough. Equations (9) can be rewritten as

$$\begin{cases} \frac{du_\varepsilon}{dz} = -\varepsilon w_\varepsilon, \\ \frac{dw_\varepsilon}{dz} = -\left(v\varepsilon w_\varepsilon - g(u_\varepsilon)\right), \\ u_\varepsilon(0) = a, w_\varepsilon(0) = 0, w_\varepsilon(1) = v u_\varepsilon(1), \end{cases} \tag{11}$$

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,

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

Hence, the analytical expression of the function v is given for $\varepsilon = 0$ by

$$v(a, 0) = \frac{g(a)}{a} = \frac{k_0 L (\delta - a) e^{\frac{-\mu}{1+a}}}{a}. \tag{12}$$

In order to determine how many values of a can reach a given value of function v, one has to look at the extrema of v. Hence, let us search if v has minima and/or maxima by computing its first and second order derivatives. They are given by[1]

$$\frac{dv}{da}(a, 0) = k_0 L e^{\frac{-\mu}{1+a}} \left[\frac{-(\mu + \delta) a^2 + \delta(\mu - 2) a - \delta}{a^2 (1+a)^2} \right] \tag{13}$$

and

$$\begin{aligned} &\frac{d^2 v}{da^2}(a, 0) = \\ &\frac{k_0 L e^{\frac{-\mu}{1+a}}}{a^3 (1+a)^4} [(2\delta + 2\mu) a^4 + \left(2\mu - \mu^2 - 4\delta\mu + 8\delta\right) a^3 \\ &+ \left(12\delta + \delta\mu^2 - 6\delta\mu\right) a^2 + (8\delta - 2\delta\mu) a + 2\delta], \end{aligned}$$

respectively. The stationary points of $v(a, 0)$ (found by setting its first order derivative equal to 0) are thus characterized by the following equation:

$$-(\mu + \delta) a^2 + \delta(\mu - 2) a - \delta = 0. \tag{14}$$

The discriminant of (14) is given by

$$\rho = \mu\delta(\mu\delta - 4\delta - 4) \tag{15}$$

and is first considered to be positive. The roots of (14) are then given by

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

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

$$\delta > 0, \qquad \mu > 4, \qquad \delta(\mu - 4) > 4$$

or

$$\delta < -2, \qquad \mu > 2, \qquad \mu + \delta < 0, \qquad \delta(\mu - 4) < 4.$$

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 $\left(\min\{v_1^*, v_2^*\}, \max\{v_1^*, v_2^*\}\right)$, 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 [23, Theorem 17.3, p. 192], the functions u_ε and w_ε are

[1] Further calculation details about the first order derivative are available in Appendix A.

both continuous with respect to ε. Observe also that the last boundary condition in (11) 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 is strictly decreasing or strictly increasing since the coefficient $-(\mu+\delta)$ of a^2 in (13) is either negative or positive. Hence, 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 (15) that

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

which yields

$$a^* = \frac{2}{\mu-2}. \tag{16}$$

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

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

See Appendix A for further details. Using (16), this polynomial can be factorized as

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

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 4.1 can be found in Figure 2 for $\rho = 0$ and in Figure 3 for $\rho > 0$.

We present now a corollary of Lemma 4.1 that provides approximated solutions to equations (11). Moreover, with these solutions, one can also find solutions of equations (6) for equal Peclet numbers using the appropriate change of variables. The method used is based on perturbation theory [20, Regular Perturbation Theorem].

Corollary 4.1: Taking into account the existence of equilibrium profiles under the conditions of Lemma 4.1, approximated

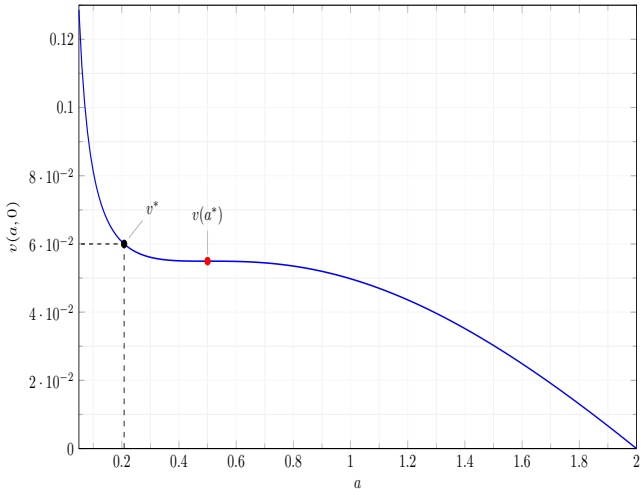

Fig. 2. Illustration of Lemma 4.1 with $\mu = 6$ and $\delta = 2$ ($\rho = 0$).

solutions of equations (11) 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

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

Proof: According to Perturbation theory (see [20, Regular Perturbation Theorem]), a function $f_\varepsilon(z)$ that depends on the disturbing parameter ε has always the form

$$f_\varepsilon(z) = \sum_{n=0}^{+\infty} f_n(z)\varepsilon^n \tag{17}$$

for sufficiently small ε. Applying the same decomposition to the functions $u_\varepsilon(z)$ and $w_\varepsilon(z)$, both depending on ε, yields the following identities:

$$u_\varepsilon(z) = u_0(z) + u_1(z)\varepsilon + \mathcal{O}(\varepsilon^2), \tag{18}$$
$$w_\varepsilon(z) = w_0(z) + w_1(z)\varepsilon + \mathcal{O}(\varepsilon^2), \tag{19}$$

where $\mathcal{O}(\varepsilon^2)$ includes all the polynomial terms of the form $u_n(z)\varepsilon^n, n \geq 2$. By using similar arguments for function v_ε (also depending on ε), one finds

$$v_\varepsilon = v_0 + v_1\varepsilon + \mathcal{O}(\varepsilon^2). \tag{20}$$

In the sequel of the proof, note that all the terms including ε^2 or higher order of ε are considered to be negligible. By plugging (18) and (19) in equations (11), one gets

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

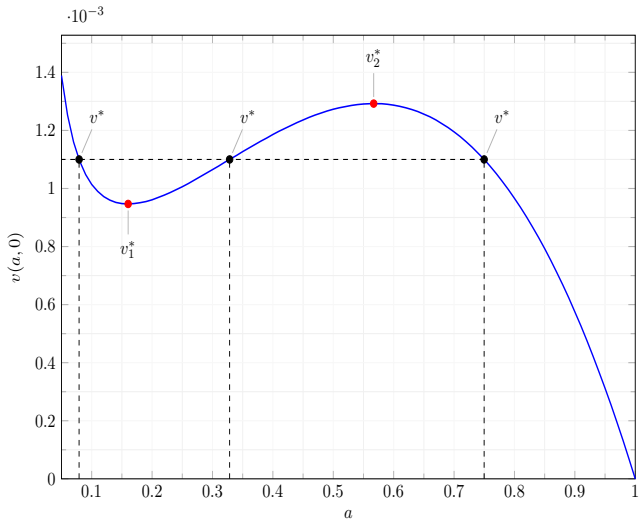

Fig. 3. Illustration of Lemma 4.1 with $\mu = 10$ and $\delta = 1$ ($\rho > 0$).

By identification[2], and by using the approximation $g(u_0 + u_1\varepsilon) \approx g(u_0)$ for sufficiently small ε, we have

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

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 expressions of functions u_ε and w_ε and using the decomposition of v_ε, provided by (20), 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 $\frac{g(a)}{a}$, which corresponds to the same expression as function v for $\varepsilon = 0$, see (12) (because v_1 is identically zero). ■

To estimate the form of solutions of equations (6), one has to consider Corollary 4.1, relations (7), (8) and (10). This leads to

$$x_1(z) \simeq a - \frac{g(a)}{2D}(1-z)^2,$$
$$x_2(z) \simeq \frac{a}{\delta} - \frac{g(a)}{2\delta D}(1-z)^2,$$

which are approximated solutions to equilibrium equations for equal Peclet numbers[3]. 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 since D_{ma} and λ_{ea} are diffusion coefficients that model two completely different kinds of diffusion, namely axial mass dispersion (D_{ma}), that is related to the diffusion of the reactant, and axial energy dispersion (λ_{ea}), that is linked to the diffusion of temperature in the reactor. This leads us to consider the case $Pe_h \neq Pe_m$ in the next section.

B. 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 (9) with a two variable auxiliary function g : see (22) below. Considering that Pe_h and Pe_m are different, a change of variables as (7) 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 a new 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

$$\begin{cases} D_1 \frac{d^2x_1}{dz^2} - vk_p\frac{dx_1}{dz} + k_p\delta g(x_1,x_2) = 0, \\ D_2 \frac{d^2x_2}{dz^2} - v\frac{dx_2}{dz} + g(x_1,x_2) = 0, \\ D_1\frac{dx_1}{dz}(0) - vk_p x_1(0) = 0 = \frac{dx_1}{dz}(1), \\ D_2\frac{dx_2}{dz}(0) - vx_2(0) = 0 = \frac{dx_2}{dz}(1). \end{cases} \tag{21}$$

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

$$\begin{cases} \frac{du_1}{dz} = -w_1, \\ \frac{dw_1}{dz} = -\frac{k_p}{D_1}(vw_1 - \delta g(u_1,u_2)), \\ \frac{du_2}{dz} = -w_2, \\ \frac{dw_2}{dz} = -\frac{1}{D_2}(vw_2 - g(u_1,u_2)), \\ u_1(0) = a_1, w_1(0) = 0, w_1(1) = \frac{vk_p}{D_1}u_1(1), \\ u_2(0) = a_2, w_2(0) = 0, w_2(1) = \frac{v}{D_2}u_2(1). \end{cases} \tag{22}$$

Once again we have to find $v(a_1,a_2,D_1,D_2)$ such that $w_1(1) = \frac{vk_p}{D_1}u_1(1)$ and $w_2(1) = \frac{v}{D_2}u_2(1)$ hold. A similar argument as for

[2]Two polynomials are equal if they have the same coefficients (the variable of the polynomials is ε).

[3]The change of variables (10) allows to write u and w as functions of $u_\varepsilon, w_\varepsilon$ and ε (which is replaced by $\frac{1}{D}$). Furthermore, the other changes of variables (7) and (8) make the link between u, w and x_1, x_2.

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 (22) has at least two solutions. In order to find the function v, Perturbation theory is applied to (22). 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. These conditions come once again from Perturbation theory (see [20, Regular Perturbation Theorem]). Thus, the system (22) takes the form

$$\begin{cases}\frac{du_{\varepsilon_1}}{dz}=-\varepsilon_1 w_{\varepsilon_1},\\ \frac{dw_{\varepsilon_1}}{dz}=-\left(k_p v\varepsilon_1 w_{\varepsilon_1}-k_p\delta g(u_{\varepsilon_1},u_{\varepsilon_2})\right),\\ \frac{du_{\varepsilon_2}}{dz}=-\varepsilon_2 w_{\varepsilon_2},\\ \frac{dw_{\varepsilon_2}}{dz}=-\left(v\varepsilon_2 w_{\varepsilon_2}-g(u_{\varepsilon_1},u_{\varepsilon_2})\right),\\ u_{\varepsilon_1}(0)=a_1, w_{\varepsilon_1}(0)=0, w_{\varepsilon_1}(1)=vk_p u_{\varepsilon_1}(1),\\ u_{\varepsilon_2}(0)=a_2, w_{\varepsilon_2}(0)=0, w_{\varepsilon_2}(1)=vu_{\varepsilon_2}(1),\end{cases}\tag{23}$$

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

$$v(a_1,a_2,0,0)=(1-\delta)k_0L\frac{(1-a_2)e^{\frac{-\mu}{1+a_1}}}{a_2-a_1},\tag{24}$$

which is a necessary form for the function v. The reader is referred to Appendix B 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

$$v=\frac{w_{\varepsilon_1}(1)}{k_p u_{\varepsilon_1}(1)}\text{ and }v=\frac{w_{\varepsilon_2}(1)}{u_{\varepsilon_2}(1)}\tag{25}$$

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 [23, 17.3, p. 192]). Keeping in mind that our study of equilibrium is qualitative, we first give the gradient of function v:

$$\begin{aligned}&\overrightarrow{\nabla}v(a_1,a_2,0,0)\\&=(1-\delta)k_0Le^{\frac{-\mu}{1+a_1}}\begin{pmatrix}\frac{(1-a_2)\left((1+a_1)^2+\mu(a_2-a_1)\right)}{(a_2-a_1)^2(1+a_1)^2}\\ \frac{a_1-1}{(a_2-a_1)^2}\end{pmatrix}.\end{aligned}\tag{26}$$

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

$$\begin{aligned}\mathcal{H}_{11}(a_1,a_2)&=\frac{1-a_2}{a_2-a_1}(1-\delta)k_0Le^{\frac{-\mu}{1+a_1}}\tilde{\mathcal{H}}_{11},\\ \mathcal{H}_{12}(a_1,a_2)&=\mathcal{H}_{21}(a_1,a_2)=(1-\delta)k_0Le^{\frac{-\mu}{1+a_1}}\tilde{\mathcal{H}}_{12},\\ \mathcal{H}_{22}(a_1,a_2)&=\frac{-2(a_1-1)}{(a_2-a_1)^3}(1-\delta)k_0Le^{\frac{-\mu}{1+a_1}},\end{aligned}$$

where

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

and

$$\begin{aligned}\tilde{\mathcal{H}}_{11}=&\frac{2}{(a_2-a_1)^2}+\frac{2\mu}{(a_2-a_1)(1+a_1)^2}-\frac{2\mu}{(1+a_1)^3}\\&+\frac{\mu^2}{(1+a_1)^4}.\end{aligned}$$

Setting (26) to 0, we find that the only possibility is

$$(a_1,a_2)=\left(1,\frac{\mu-4}{\mu}\right):=(a_1^*,a_2^*).\tag{27}$$

Plugging (27) in $\mathcal{H}$, we obtain that

$$\mathcal{H}\left(1,\frac{\mu-4}{\mu}\right)=k_0L(1-\delta)e^{\frac{-\mu}{2}}\begin{pmatrix}-\frac{\mu^2}{16}+\frac{\mu}{16} & \frac{\mu^2}{16}\\ \frac{\mu^2}{16} & 0\end{pmatrix}.$$

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

$$v^*=(1-\delta)k_0L\frac{1-a_2}{a_2-a_1}e^{\frac{-\mu}{1+a_1}}.$$

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

$$\mathcal{C}_{v^*}=\left\{(a_1,a_2)\in\mathbb{R}^2:a_1\neq a_2, a_2=\frac{(1-\delta)k_0Le^{\frac{-\mu}{1+a_1}}+a_1v^*}{v^*+(1-\delta)k_0Le^{\frac{-\mu}{1+a_1}}}\right\}.$$

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 4.2: 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 (22) 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.

Proof: Function v (see (24)) in the direction $a_2=\alpha a_1+\beta$ becomes

$$v(a_1,\alpha a_1+\beta,0,0)=\frac{(1-\delta)k_0L(1-\beta-\alpha a_1)e^{\frac{-\mu}{1+a_1}}}{(\alpha-1)a_1+\beta}\tag{28}$$

and its first order derivative is given by

$$\frac{dv}{da_1}(a_1,\alpha a_1+\beta,0,0)=$$
$$\frac{(1-\delta)k_0Le^{\frac{-\mu}{1+a_1}}}{((\alpha-1)a_1+\beta)^2(1+a_1)^2}(-(\alpha\mu(\alpha-1)+(\alpha-1)+\beta)a_1^2$$
$$+(\alpha(-2+\mu-2\beta\mu)+(-1+\beta)(-2+\mu))a_1$$
$$+(-\alpha-(-1+\beta)(1+\beta\mu))).$$

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 by 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 4.1, the result follows. ■

Lemma 4.2 is illustrated in Figure 4, where a zoom on the first extremum of the function is provided for the sake of readability.

Remark 4.2: Note that Lemma 4.2 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 (25) 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 4.2 into account, a theorem is now stated which gives necessary and sufficient conditions for the multiplicity of equilibrium profiles for distinct Peclet numbers.

Theorem 4.1: 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 (22) 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.

Proof: Based on Remark 4.2, 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 (28), this leads to

$$v\left(a_1,\frac{1}{\delta}a_1,0,0\right)=\frac{(1-\delta)k_0L\left(1-0-\frac{1}{\delta}a_1\right)e^{\frac{-\mu}{1+a_1}}}{\left(\frac{1}{\delta}-1\right)a_1+0}$$
$$=\frac{(1-\delta)k_0L\left(\frac{\delta-a_1}{\delta}\right)e^{\frac{-\mu}{1+a_1}}}{\left(\frac{1-\delta}{\delta}\right)a_1}$$
$$=\frac{k_0L(\delta-a_1)e^{\frac{-\mu}{1+a_1}}}{a_1}.$$

The conclusion follows by Lemma 4.2 and by noting that function v has the same expression as in Lemma 4.1 (see equation (12)). ■

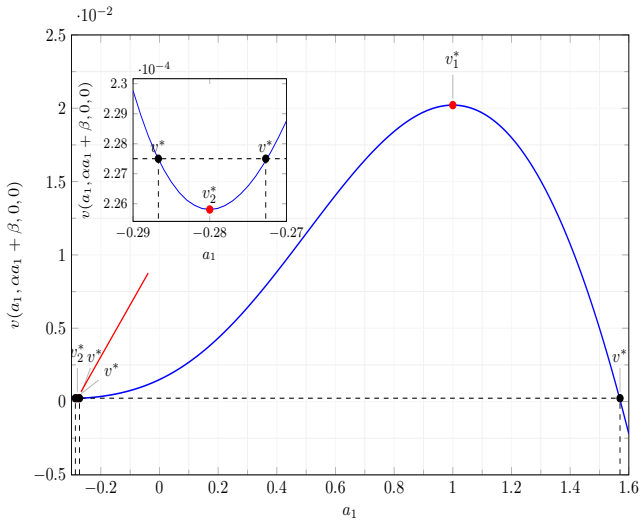

Fig. 4. Illustration of Lemma 4.2 with $\mu=10,\delta=4,\alpha=0.7$ and $\beta=-0.1$.

Similarly as in Case 1, approximated solutions of equations (23) are given in the following corollary.

Corollary 4.2: Taking into account the existence of equilibrium profiles under the conditions of Theorem 4.1, approximated solutions of equations (23) are given by

$$u_{\varepsilon_1}(z)=a_1-\frac{\varepsilon_1k_p\delta g\left(a_1,\frac{1}{\delta}a_1\right)}{2}z^2,$$
$$u_{\varepsilon_2}(z)=\frac{1}{\delta}a_1-\frac{\varepsilon_2 g\left(a_1,\frac{1}{\delta}a_1\right)}{2}z^2,$$
$$w_{\varepsilon_1}(z)=k_p\delta g\left(a_1,\frac{1}{\delta}a_1\right)z-\frac{\varepsilon_1k_p^2v_{\varepsilon_1,\varepsilon_2}\delta g\left(a_1,\frac{1}{\delta}a_1\right)}{2}z^2,$$
$$w_{\varepsilon_2}(z)=g\left(a_1,\frac{1}{\delta}a_1\right)z-\frac{\varepsilon_2v_{\varepsilon_1,\varepsilon_2}g\left(a_1,\frac{1}{\delta}a_1\right)}{2}z^2,$$

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

$$v_{\varepsilon_1,\varepsilon_2}=\frac{k_0L(\delta-a_1)e^{\frac{-\mu}{1+a_1}}}{a_1}.$$

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 $g(u_{0_1}+u_{1_1}\varepsilon_1,u_{0_2}+u_{1_2}\varepsilon_2)$ is approximated by $g(u_{0_1},u_{0_2})$ for $\varepsilon_1,\varepsilon_2$ small enough. ■

As in Case 1, approximated solutions of equilibrium equations (21) are obtained by applying Corollary 4.2. These are expressed as

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

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

C. 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 (6) 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 $Pe_m = \frac{v}{D}$, 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. $k_\eta = 1 + \frac{\eta}{Pe_m}$. Then the equilibrium equations take the form

$$\begin{cases} D\frac{d^2x_1}{dz^2} - vk_\eta\frac{dx_1}{dz} + k_\eta\delta g(x_1,x_2) = 0, \\ D\frac{d^2x_2}{dz^2} - v\frac{dx_2}{dz} + g(x_1,x_2) = 0, \\ \\ D\frac{dx_1}{dz}(0) - vk_\eta x_1(0) = \frac{dx_1}{dz}(1) = 0, \\ D\frac{dx_2}{dz}(0) - vx_2(0) = \frac{dx_2}{dz}(1) = 0. \end{cases} \tag{29}$$

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 (29) have the same form as the equations (21). Hence, the analysis is the same as in Section IV-B. Note also that if one lets $\eta \to 0$, then one recovers the case $Pe_m = Pe_h$.

V. Perspectives

This section is essentialy dedicated to an overview of the stability analysis for nonisothermal axial dispersion tubular reactors. This question is discussed notably on the basis of the relation between the thermal and the mass Peclet numbers. Addressing stability for infinite-dimensional systems is quite challenging when one deals with nonlinear operators. Here, some results are highlighted, that can be derived for an appropriate linearization of the system around an equilibrium profile.

As pointed out in [5, Section 2.5.2.1.] and in [24, Lemma 15, Corollary A, Corollary B] for equal Peclet numbers, in the case of only one equilibrium profile, the latter is always asymptotically stable and, when three equilibria are exhibited, they are alternatively asymptotically stable and unstable with the pattern *stable – unstable – stable*. Moreover, a result first shown in [25, Theorem p. 52] and then recalled in [5, Section 2.5.2.1.] provides us with necessary and sufficient conditions for an equilibrium profile to be asymptotically stable or unstable.

The case of different Peclet numbers is much less understood and less studied in the literature. To the best of our knowledge, no systematic pattern as the one described above has been established. However, a similar theorem as [25, Theorem p. 52] can be found in [26, Theorem 3], that presents some sufficient conditions to adress stability for different Peclet numbers.

Another method has been developed in [27], which is called the *Galerkin Residuals Method*. It is based on the parabolicity of the PDEs. This property allows one to write the solution as an infinite serie of product of functions that are only depending on time and on the spatial variable. The key point of the method consists in truncating the solution up to a finite order N and then to write the system as $\dot{x} = \mathfrak{A}x$ where the $N-$th order vector x contains the functions that depend on time only. Hence, (local) stability is deduced by evaluating the dominant eigenvalue of matrix $\mathfrak{A}$, i.e. the eigenvalue with the largest real part.

Further analysis could lead to the consolidation and/or the extension of the either theoretical or numerical results above to different or close Peclet numbers. Tools like Lyapunov indirect method or LaSalle's invariance principle could be used to achieve these goals. An extension of the *Galerkin Residuals Method* to different Peclet numbers can be found in [28, Chapter 5] where the results of some numerical simulations are given and commented.

VI. Conclusions and future works

In this paper an analysis of multiple equilibrium for non-isothermal tubular reactors is performed. It was shown that, beyond a certain value for the diffusion coefficient D, tubular reactors can have at least three different equilibria. A similar result on the multiplicity was exhibited for $Pe_h \neq Pe_m$ by considering a specific direction for the analysis. Moreover, for close enough Peclet numbers, i.e. $Pe_h = Pe_m + \eta$, it was proved that by letting η tend to 0, the equality case is recovered.

It is worth noting that, in this analysis, the equilibrium profiles of the plug-flow and continuous stirred tank reactor (CSTR) models are retrieved as expected.

As already mentioned, a large part of the contributions concerns the analysis of the dynamics of tubular reactors. While many references concerning control problem considerations are on lumped parameters systems CSTR, see [8] and references therein, few literature consider PDEs model for tubular reactors, see for instance [10]. Future works may be to study the linearised system around a well-chosen equilibrium. Aspects like the well-posedness of this system or the exponential stability anaysis of the operator describing this system for each equilibrium profile can then be considered. It is expected that

this preliminary analysis is a first important step towards the solution of the LQ-optimal control problem for nonisothermal tubular reactors.

APPENDIX

In this section, more detailed arguments are provided to the reader for the derivation of the main results in Section IV.

A. Case 1 : $Pe_h = Pe_m$

First at all, we will develop only once the transition from Equations (6) to Equations (9). Note that we denoted Pe_h and Pe_m by Pe for simplicity of notation. The first change of variables is

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

Then the first equation of (6) 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[4],

$$\frac{1}{Pe}\frac{d^2y_1}{dz^2} - \frac{dy_1}{dz} + \alpha(\delta - y_1)e^{\frac{\mu y_1}{1+y_1}} = 0. \tag{30}$$

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 (30) 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

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

[4]Since $y_2 \equiv 0$, the variables x_1 and x_2 are related by $x_1 = \delta x_2$. Hence, we have to deal with only one second order differential equation instead of two. Obviously this makes the analysis simpler.

In addition, the boundary conditions are derived as follows:

$$\begin{aligned}u(0) &= y_1(1) := a, \\ w(0) &= \frac{dy_1}{dz}(1) = 0, \\ w(1) &= \frac{dy_1}{dz}(0) = Pey_1(0) = \frac{v}{D}u(1).\end{aligned}$$

Note that the role of y_2 is paramount and the key of the study of the existence of equilibrium profiles for equal Peclet numbers. Actually, as mentioned above, the introduction of y_2 allows us to cancel one of the two second order ordinary differential equations (Equations (6)). Furthermore, y_2 corresponds to the concept of reaction invariant which is fundamental in the dynamics of reaction systems, see e.g. [22].

In the proof of Lemma 4.1, we first give some details about the calculation of the first order derivative of the function $v(a,0)$. Since $v(a,0)$ is given by $\frac{k_0L(\delta-a)e^{\frac{-\mu}{1+a}}}{a}$, it holds

$$\begin{aligned}&\frac{d}{da}v(a,0) \\ &= k_0L\frac{d}{da}\left[\frac{(\delta-a)e^{\frac{-\mu}{1+a}}}{a}\right] \\ &= k_0L\frac{\frac{d}{da}\left[(\delta-a)e^{\frac{-\mu}{1+a}}\right]a - (\delta-a)e^{\frac{-\mu}{1+a}}}{a^2} \\ &= k_0L\frac{\left(-e^{\frac{-\mu}{1+a}} + (\delta-a)\frac{\mu}{(1+a)^2}e^{\frac{-\mu}{1+a}}\right)a - (\delta-a)e^{\frac{-\mu}{1+a}}}{a^2} \\ &= k_0Le^{\frac{-\mu}{1+a}}\frac{\left(\frac{-(1+a)^2+\mu(\delta-a)}{(1+a)^2}\right)a - \frac{(\delta-a)(1+a)^2}{(1+a)^2}}{a^2} \\ &= k_0Le^{\frac{-\mu}{1+a}}\frac{-(1+a)^2a + \mu(\delta-a)a - \delta(1+a)^2 + a(1+a)^2}{a^2(1+a)^2} \\ &= k_0Le^{\frac{-\mu}{1+a}}\frac{\left[-(\mu+\delta)a^2 + \delta(\mu-2)a - \delta\right]}{a^2(1+a)^2}.\end{aligned}$$

Hence (13) holds. In the sequel of the same proof, in the case 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. This 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 Section II) and δ have to satisfy either

$$\delta > 0, \mu > 4, \delta(\mu - 4) > 4 \tag{31}$$

or

$$\delta < -2, \mu > 2, \mu + \delta < 0, \delta(\mu - 4) < 4. \tag{32}$$

Noting that the coefficient of a^2 in the first order derivative of v is $-(\mu+\delta)$, it is obvious that, in the case (31), a_1^* corresponds to a minimum and a_2^* to a maximum and vice-versa for the case (32).

Now we take a look at the last part of the proof of Lemma 4.1 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

$$\delta = \frac{4}{\mu - 4}. \tag{33}$$

Putting the identity (33) into the polynomial factor in the second order derivative of v yields the following expression:

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

B. 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

$$u_{\varepsilon_1}(z) = a_1, \qquad w_{\varepsilon_1}(z) = k_p\delta g(a_1,a_2)z,$$
$$u_{\varepsilon_2}(z) = a_2, \qquad w_{\varepsilon_2}(z) = g(a_1,a_2)z$$

and we used the boundary conditions

$$w_{\varepsilon_1}(1) = vk_p u_{\varepsilon_1}(1),$$
$$w_{\varepsilon_2}(1) = vu_{\varepsilon_2}(1).$$

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, therefore its eigenvalues are real and its determinant satisfies

$$\det\mathcal{H} = \prod_{i=1}^{2}\lambda_i, \tag{34}$$

where $\{\lambda_i\}_{i=1}^2$ denotes the set of eigenvalues of $\mathcal{H}$. Since the matrix $\mathcal{H}$ evaluated at (a_1^*, a_2^*) is given by

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

we deduce that

$$\det\mathcal{H}\left(1, \frac{\mu-4}{\mu}\right) = -k_0^2 L^2 (1-\delta)^2 e^{-\mu}\left(\frac{\mu^2}{16}\right)^2 < 0.$$

Using (34), we find that $\lambda_1\lambda_2 < 0$, which means that $\mathcal{H}$ is indefinite. The point (a_1^*, a_2^*) is therefore a saddle point.

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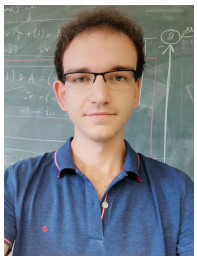

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