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Analysis of equilibrium profiles in nonisothermal axial dispersion tubular reactors

Anthony Hastir, François Lamoline, Joseph J. Winkin* and Denis Dochain†
* Namur Institute for Complex Systems (naXys) and Department of Mathematics,
University of Namur, Rempart de la vierge 8, B-5000 Namur, Belgium
† Institute of Information and Communication Technologies, Electronics and Applied Mathematics (ICTEAM),
Université Catholique de Louvain, Avenue Georges Lemaitre 4-6, B-1348 Louvain-La-Neuve, Belgium
`anthony.hastir@unamur.be`, `francois.lamoline@unamur.be`, `joseph.winkin@unamur.be`, `denis.dochain@uclouvain.be`

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 for which convection and/or diffusion are of interest. Nonlinearities in the dynamics are typically located in the kinetic terms and are based notably on the Arrhenius law for nonisothermal reactors, see [1].

Here, we are interested in tubular reactors involving a chemical reaction of the form $A \to B$ 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. They are given by

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

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 convection – diffusion – reaction equations. See [1], [4] for the description of the parameters. To the PDEs (1), we associate specific boundary conditions, known as Danckwerts'conditions, which are given by $\frac{\lambda_{ea}}{\rho C_p}\frac{\partial T}{\partial z}(t,0) = v(T(t,0) - T_{in}), D_{ma}\frac{\partial C}{\partial z}(t,0) = v(C(t,0) - C_{in}), \frac{\partial T}{\partial z}(t,L) = 0$ and $\frac{\partial C}{\partial z}(t,L) = 0$. The variable T_w is due to a heat exchanger that acts along the whole spatial domain. Furthermore, the boundary variables $T_{in}(t)$ and $C_{in}(t)$ can be fixed at the inlet of the reactor.

From [2], tubular reactors are known to be well-posed, i.e. there exist unique state trajectories describing the temperature and the evolution of reactant concentration. Such considerations are based on state space and semigroup approaches.

The existence, the multiplicity and the stability of equilibrium profiles have been widely studied over the years, either on the nonlinear model with only the convection phenomenon or on the linear one involving mass axial dispersion.

More recently, in [3], 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, $\frac{vL\rho C_p}{\lambda_{ea}}$) or the ratio between the convection transfer and the diffusion transfer (mass Peclet number, $\frac{vL}{D_{ma}}$). Here, the main contributions are the extension of this study to the case of different or close Peclet numbers, see [4], and the statement of sufficient conditions for the equilibria to be exponentially stable in the case of equal Peclet numbers.

The aim of this research is to study the existence of equilibrium profiles for nonisothermal tubular reactors, to derive multiplicity criteria for these equilibrium profiles and to study their stability properties. It is shown that such reactors can exhibit different numbers of equilibrium profiles depending on parameters of the system, particularly on the diffusion coefficient, see [4]. Furthermore, it is shown that in the case of only one equilibrium profile, the latter is always exponentially stable and if three equilibria are exhibited, the pattern ”exponentially stable – unstable – exponentially stable” is highlighted.

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