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Optimal LQ-Feedback Regulation of a Nonisothermal Plug Flow Reactor Model by Spectral Factorization

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***Abstract*—The linear-quadratic (LQ) optimal temperature and reactant concentration regulation problem is studied for a partial differential equation model of a nonisothermal plug flow tubular reactor by using a nonlinear infinite dimensional Hilbert state space description. First the dynamical properties of the linearized model around a constant temperature equilibrium profile along the reactor are studied: it is shown that it is exponentially stable and (approximately) reachable. Next the general concept of LQ-feedback is introduced. It turns out that any LQ-feedback is optimal from the input-output viewpoint and stabilizing. For the plug flow reactor linearized model, a state LQ-feedback operator is computed via the solution of a matrix Riccati differential equation (MRDE) in the space variable. Thanks to the reachability property, the computed LQ-feedback is actually the optimal one. Then the latter is applied to the nonlinear model, and the resulting closed-loop system dynamical performances are analyzed. A criterion is given which guarantees that the constant temperature equilibrium profile is an asymptotically stable equilibrium of the closed-loop system. Moreover, under the same criterion, it is shown that the control law designed previously is optimal along the nonlinear closed-loop model with respect to some cost criterion. The results are illustrated by some numerical simulations.**

***Index Terms*—Linear-quadratic (LQ) optimal control, nonisothermal plug flow reactor, nonlinear infinite dimensional systems, regulation, spectral factorization.**

I. Introduction

TUBULAR reactors play a very important role in chemical and biochemical engineering (see, e.g., [20], [13], [9], [17]). Typically in such reactors the medium is not homogeneous (e.g., fixed-bed reactors, packed-bed reactors, fluidized-bed reactors,…) and possibly involve different phases (liquid/solid/gas). The dynamics of nonisothermal plug flow reactors are described by nonlinear partial differential equations (PDEs) derived from mass and energy balances (see e.g., [4], [16], [27], and the references therein). The main source of nonlinearities in the dynamics of a (bio)chemical process is usually concentrated in the kinetics terms of the model equations. In this paper, we are interested in a nonisothermal chemical reaction occurring in a plug flow reactor with one reactant A and one product B. The kinetic term is modeled by first-order kinetics with respect to the reactant concentration and by the most often used Arrhenius law with respect to the temperature. The choice of a first-order dependence with respect to the reactant concentration corresponds to the situation found, e.g., in thermal cracking processes [14].

In the control literature, linear quadratic (LQ) optimal control plays a paramount role. It is known that the solution of the LQ-optimal control problem for infinite-dimensional state space systems with bounded measurement and control can be obtained by solving an algebraic operator Riccati equation (see, e.g., [11]). On the other hand, it is known that the LQ-optimal feedback operator can be alternatively derived by solving a spectral factorization problem and by obtaining the solution of an operator Diophantine equation: see [6] and [7]. These two papers deal with the case of stabilizable/detectable systems with finite-dimensional input and output spaces and with bounded measurement and control. In [25], the general case of stable weakly regular linear systems with admissible unbounded input and output operators, was studied.

The objective of this paper is basically twofold. From a theoretical viewpoint the spectral factorization approach is extended to the more specific case of exponentially stable linear systems with bounded measurement and control and infinite-dimensional output and input spaces. Second, an LQ-optimal feedback is computed for the linearized model of a nonisothermal plug flow reactor around a constant temperature equilibrium profile by using this approach. Next, this feedback is applied to the nonlinear model and the closed-loop system performances are analyzed.

The contributions of this paper can be summarized as follows. Section II deals with the infinite-dimensional state space description of a nonisothermal plug flow reactor model with a specific equilibrium profile. Here, a constant temperature profile is chosen. The choice of such a profile is motivated by the fact that it minimizes the energy consumption along the reactor (see [23]). Section III is concerned with the linearized model around the chosen profile, its equivalent triangularized model and its properties: its exponential stability and reacha-

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bility are established. In Section IV we are interested in the design of a LQ-feedback control by spectral factorization for a specific class of infinite-dimensional systems, that includes the linearized plug flow reactor model. In this section the general concept of LQ-feedback is introduced as a solution of a partial realization problem for the standard spectral factor of the LQ-problem Popov function. It turns out that any LQ-feedback is optimal from the input-output viewpoint and stabilizing. Section V deals with the computation of a particular LQ-feedback for the linearized plug flow reactor model by using the approach developed in the previous section. This LQ-feedback is computed via a matrix Riccati differential equation (MRDE) in the space variable. Thanks to the reachability property of the linearized model, the computed LQ-feedback turns out to be the optimal one. The resulting nonlinear closed-loop system performances are analyzed in Section VI. More precisely it is shown, under suitable conditions on the systems parameters, that any constant temperature equilibrium profile is an asymptotically stable equilibrium of the closed-loop system. This result follows by the analysis developed in [2] and [4], that is based on the concepts of m-dissipativity and nonlinear contraction semigroup, see, e.g., [18]. Moreover, under the same conditions, it is shown that the control law designed previously is optimal along the nonlinear closed-loop model with respect to a modified cost criterion, which takes care of the nonlinearity. The theoretical results are illustrated by some numerical simulations. Section VII contains some concluding remarks and perspectives for further research.

II. Nonlinear Plug-Flow Reactor Model

A. Nonlinear PDE Model

Let us consider a nonisothermal plug flow reactor with the following chemical reaction:

$$A \longrightarrow bB,$$

where $b > 0$ denotes the stoichiometric coefficient of the reaction. In general the dynamics of tubular reactors are typically described by nonlinear PDEs derived from mass and energy balance principles. Here, if the kinetics of the above reaction are characterized by first-order kinetics with respect to the reactant concentration C_A (mol/L) and by an Arrhenius-type dependence with respect to the temperature $T\ (K)$, the dynamics of the process are given by the following energy and mass balance PDEs, where C_B (mol/L) and $T_c\ (K)$ denote the product concentration and the coolant temperature, respectively. The latter will be used as control variable of this process.

$$\frac{\partial T}{\partial \tau} = -v\frac{\partial T}{\partial \zeta} - \frac{\Delta H}{\rho C_p}k_0 C_A \exp\left(-\frac{E}{RT}\right) - \frac{4h}{\rho C_p d}(T-T_c) \quad (1)$$

$$\frac{\partial C_A}{\partial \tau} = -v\frac{\partial C_A}{\partial \zeta} - k_0 C_A \exp\left(-\frac{E}{RT}\right) \quad (2)$$

$$\frac{\partial C_B}{\partial \tau} = -v\frac{\partial C_B}{\partial \zeta} + bk_0 C_A \exp\left(-\frac{E}{RT}\right) \quad (3)$$

with the boundary conditions given, for $\tau \geq 0$, by

$$T(0,\tau) = T_{\text{in}},\ C_A(0,\tau) = C_{A,\text{in}},\ C_B(0,\tau) = 0. \quad (4)$$

The initial conditions are given, for $0 \leq \zeta \leq L$, by

$$T(\zeta,0) = T_0(\zeta),\ C_A(\zeta,0) = C_{A,0}(\zeta),\ C_B(\zeta,0) = 0. \quad (5)$$

In these equations, $v, \Delta H, \rho, C_p, k_0, E, R, h, d, T_{\text{in}}$, and $C_{A,\text{in}}$ hold for the superficial fluid velocity, the heat of reaction, the density, the specific heat, the kinetic constant, the activation energy, the ideal gas constant, the wall heat transfer coefficient, the reactor diameter, the inlet temperature, and the inlet reactant concentration, respectively. In addition τ, ζ and L denote the time and space independent variables, and the length of the reactor, respectively. Finally T_0 and $C_{A,0}$ denote the initial temperature and reactant concentration profiles, respectively, such that $T_0(0) = T_{\text{in}}$ and $C_{A,0}(0) = C_{A,\text{in}}$.

Comment 2.1: From a physical point of view it is expected that for all $\zeta \in [0,L]$, and for all $\tau \geq 0$, $0 \leq T(\zeta,\tau) \leq T_{\max}$ and $0 \leq C(\zeta,\tau) \leq C_{A,\text{in}}$ where the upper bound $T_{\max}$ could possibly be equal to ∞. It turns out that the case $T_{\max} < +\infty$ is the most interesting one in the stability analysis for the open-loop model (see [2] and [4]) and also for the closed-loop model (see below). Moreover, this case is physically feasible: see [13, Th. 4.1].

B. Constant Temperature Equilibrium Profile

In this paper, we are interested in equilibrium profiles for the model (1)–(5) of the form

$$\mathbf{X_e} = [\,T_e(.) \quad C_{A,e}(.) \quad C_{B,e}(.)\,]^T \quad (6)$$

in the state-space $L^2(0,L)^3$ where the temperature equilibrium profile is assumed to be constant, i.e.

$$T_e(\zeta) = T_e > 0 \quad \text{a.e. in } [0,L]\,. \quad (7)$$

Comment 2.2:

a) An equilibrium profile X_e must satisfy the boundary conditions (4). Hence, by continuity of the function T_e, in view of identity (7), one should have $T_e(\zeta) = T_{\text{in}}$ for all $\zeta \in [0,L]$, i.e., the inlet temperature dictates that of the constant temperature equilibrium profile.
b) In [23] temperature equilibrium profiles are studied that minimize different kinds of performance criteria for the (finite-dimensional) steady-state model: the specific temperature equilibrium profile (7) corresponds to a minimum for the energy consumption along the reactor.

By integrating the equilibrium ordinary differential equations corresponding to (1)–(3), it can easily be shown that in this case the reactant and product concentration equilibrium profiles are given by

$$C_{A,e}(\zeta) = C_{A,\text{in}}\exp(-\alpha_e\zeta),\quad 0 \leq \zeta \leq L \quad (8)$$

$$C_{B,e}(\zeta) = bC_{A,\text{in}}(1-\exp(-\alpha_e\zeta)),\quad 0 \leq \zeta \leq L \quad (9)$$

respectively, where α_e is the positive constant given by $\alpha_e := (k_0/v)\exp(-E/RT_e) > 0$, and the corresponding coolant temperature equilibrium profile reads for $0 \leq \zeta \leq L$ as follows:

$$T_{c,e}(\zeta) = T_e + \frac{\Delta H dv}{4h}\alpha_e C_{A,\mathrm{in}} \exp(-\alpha_e \zeta). \qquad (10)$$

The latter can be interpreted as an open-loop infinite-dimensional control profile distributed along the whole reactor.

C. *Infinite Dimensional System Description*

Observe that in (1)–(5), the product concentration C_B is known if the reactant concentration C_A and the temperature T are known. Therefore, we shall only consider the two first state components, *viz.* the reactor temperature and the reactant concentration. Let us consider the following dimensionless state variables $\theta_1(t)$ and $\theta_2(t),\ \ t \geq 0$ defined as follows:

$$\theta_1 = \frac{T - T_{\mathrm{in}}}{T_{\mathrm{in}}}, \quad \theta_2 = \frac{C_{A,\mathrm{in}} - C_A}{C_{A,\mathrm{in}}}. \qquad (11)$$

Let us consider also dimensionless time $t := \tau v/L$ and space $z := \zeta/L$. Then the equivalent state space description of the model (1)–(2) (without considering the product concentration dynamics (3)) is given by the following abstract differential equation on the space $H := L^2(0,1)^2$:

$$\begin{cases} \dot{\theta}(t) &= A_0\theta(t) + N(\theta(t)) + B\theta_c \\ \theta(0) &= \theta_0 \in D(A_0) \cap F \end{cases} \qquad (12)$$

where A_0 is the linear operator defined on its domain

$$D(A_0) := \left\{\theta \in H : \theta \text{ is a.c., } \frac{d\theta}{dz} \in H \text{ and } \theta(0) = 0\right\} \quad (13)$$

(where a.c. means absolutely continuous) by

$$A_0\,\theta := \begin{bmatrix} -\frac{d.}{dz} - \beta I & 0 \\ 0 & -\frac{d.}{dz} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \qquad (14)$$

and the nonlinear operator N is defined on

$$F := \{\theta \in H : \theta_1 \geq -1,\ 0 \leq \theta_2 \leq 1,\ \text{a.e. in } [0,1]\}$$

by

$$N(\theta) := \begin{bmatrix} \alpha\delta(1-\theta_2)\exp\left(\frac{\mu\theta_1}{\theta_1+1}\right) \\ \alpha(1-\theta_2)\exp\left(\frac{\mu\theta_1}{\theta_1+1}\right) \end{bmatrix}. \qquad (15)$$

The operator $B \in \mathcal{L}(L^2(0,1), H)$ is the bounded linear operator defined by

$$B = \beta\,[I \quad 0]^T \qquad (16)$$

where θ_c is the dimensionless coolant temperature $\theta_c = (T_c - T_{\mathrm{in}})/T_{\mathrm{in}}$ and the parameters α, β, δ, and μ are related to the original parameters as follows:

$$\mu = \frac{E}{RT_{\mathrm{in}}},\ \alpha = \frac{k_0 L}{v}\exp(-\mu)$$
$$\beta = \frac{4hL}{\rho C_p dv},\ \delta = -\frac{\Delta H}{\rho C_p}\frac{C_{A,\mathrm{in}}}{T_{\mathrm{in}}}.$$

Denote by θ_e and θ_{ce} the dimensionless equilibrium profile and the corresponding coolant temperature, which satisfy the equation $A_0\theta_e + N(\theta_e) + B\theta_{c,e} = 0$.

III. Linearized Model Analysis

Our objective is to synthesize a robust closed-loop infinite-dimensional control by state (trajectories) feedback. Let us consider the state transformation

$$x(t) := [\,x_1(t) \quad x_2(t)\,]^T := \theta(t) - \theta_e \qquad (17)$$

and the new input vector by $u(t) := \theta_c(t) - \theta_{c,e}$. Then (12) can be rewritten as the following abstract differential equation on the Hilbert space $H = L^2(0,1) \times L^2(0,1)$

$$\begin{cases} \dot{x}(t) &= A_0 x(t) + N_0(x(t)) + Bu(t) \\ x(0) &= x_0 \in D(A_0) \cap F_0 \end{cases} \qquad (18)$$

where the operator A_0 is given by (13)–(14) and the nonlinear operator N_0 is given on the closed subset $F_0 := \{x \in H : x + \theta_e \in F\}$ by

$$N_0(x) := N(x + \theta_e) - N(\theta_e) \qquad (19)$$

where the operator N is given by (15).

A. *Linearization and Triangularization*

The linearization of the system (18) around its zero equilibrium leads to the following linear infinite-dimensional system on the Hilbert space H:

$$\begin{cases} \dot{x}(t) &= Ax(t) + Bu(t) \\ x(0) &= x_0 \in H\,. \end{cases}. \qquad (20)$$

Here A is the linear operator defined on its domain

$$D(A) = \left\{x \in H : x \text{ is a.c. , } \frac{dx}{dz} \in H \text{ and } x(0) = 0\right\} \quad (21)$$

by

$$Ax = \begin{bmatrix} -\frac{d.}{dz} - \alpha_1 I & -\alpha_2 I \\ -\alpha_3 I & -\frac{d.}{dz} - \alpha_4 I \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad (22)$$

where the functions α_i are given by

$$\alpha_1(z) = \beta - \alpha\delta\mu\ \exp(-\alpha_e z), \quad \alpha_2(z) = \alpha\delta$$
$$\alpha_3(z) = -\alpha\mu\ \exp(-\alpha_e z) \quad \text{and} \quad \alpha_4(z) = \alpha.$$

For the analysis of the system (20)–(22), and in particular of its stability properties, we first perform a similarity transformation (i.e., Banach isomorphism) in order to get an equivalent state-space description whose generator is triangular.

Consider the state transformation defined by the following linear operator $J \in \mathcal{L}(H)$ given by

$$J := \begin{bmatrix} I & \gamma I \\ 0 & I \end{bmatrix} \tag{23}$$

where the function γ is a bounded C^1-solution of the following Riccati differential equation (RDE), whose existence is established below (see Theorem 3.1):

$$-\frac{d\gamma}{dz} = \alpha_3\gamma^2 + (\alpha_1 - \alpha_4)\gamma - \alpha_2 \, . \tag{24}$$

Observe that J defines a similarity transformation. Applying this similarity transformation to the operator A yields the triangular operator $\tilde{A} := JAJ^{-1}$ given on its domain $D(\tilde{A}) = D(A)$ by

$$\tilde{A} = \begin{bmatrix} -\frac{d.}{dz} - (\alpha_1 + \alpha_3\gamma)I & 0 \\ -\alpha_3 I & -\frac{d.}{dz} - (\alpha_4 - \alpha_3\gamma)I \end{bmatrix}. \tag{25}$$

Theorem 3.1: The RDE (24) has a bounded C^1-solution in [0, 1]. Consequently, the operator J given by (23) is a similarity transformation which triangularizes the operator A.

The proof of this theorem is given in the Appendix .

B. Stability Analysis

This section deals with the exponential stability of the linearized plug flow reactor model (20)–(22). With the similarity transformation (23) and by using the invariance of stability under system equivalence, it is sufficient to concentrate on the analysis of the triangular operator $\tilde{A}$, i.e., more specifically on its diagonal entries. In order to do so, let us consider the following closed densely defined linear operator on the Hilbert space $H_1 := L^2(0,1)$:

$$A_1 := -\frac{d.}{dz} + \psi I$$

on the domain $D(A_1) := \{x \in H_1 : x \text{ is a.c.}, dx/dz \in H_1 \text{ and } x(0) = 0\}$, where I denotes the identity operator and ψ is an essentially bounded measurable function, i.e. $\psi \in L^\infty(0,1)$.

Lemma 3.1: The operator A_1 is the infinitesimal generator of an exponentially stable C_0-semigroup on $L^2(0,1)$ whose growth bound is equal to $-\infty$, i.e., $(1/t)log\|e^{A_1 t}\| \to -\infty$ as $t \to \infty$.

Proof: Since ψI is a bounded linear operator on H and since $A_1 - \psi I$, with $D(A_1 - \psi I) = D(A_1)$, is the infinitesimal generator of a C_0-semigroup on $L^2(0,1)$ (see [27]), then by [11, Theorem 3.2.1, p. 110], the operator A_1 is the infinitesimal generator of a C_0-semigroup. It can be shown that the C_0-semigroup $(e^{A_1 t})_{t\geq 0}$ generated by A_1 is given for any $x \in L^2(0,1)$ by

$$(e^{A_1 t}x)(z) = \begin{cases} e^{\int_{z-t}^{z} \psi(\nu)d\nu}.x(z-t), & \text{if } t \in [0,\ z] \\ 0 & \text{otherwise} \end{cases} \tag{26}$$

for all $z \in [0,1]$ and $t \geq 0$.

Since the function ψ is in $L^\infty(0,1)$, there exists a constant $M > 0$ such that $|\psi(\nu)| \leq M$ for almost all $\nu \in [0,1]$. Now consider an arbitrary function $x \in L^2(0,1)$. By using (26), it can be shown that

$$\int_0^\infty \|e^{A_1 t}x\|^2 dt \leq \frac{\exp(2M) - 1}{2M}.\|x\|_2^2.$$

It follows by [11, Lemma 5.2.1, p. 215] that the C_0-semigroup $(e^{A_1 t})_{t\geq 0}$ is exponentially stable. □

Comment 3.1: It follows from Lemma 3.1 that the homogeneous Cauchy problem

$$\dot{x}_1(t) = A_1 x_1(t), \quad t \geq 0, \quad x_1(0) = x_{10} \in D(A_1) \tag{27}$$

has a unique (strong) solution, which is given by

$$x_1(.,t) = e^{A_1 t}x_{10}(.) \, . \tag{28}$$

Now let us consider the Laplace transform of (28) with respect to t. Then

$$\frac{d\hat{x}_1}{dz} = -(s - \psi)\hat{x}_1 + x_{10} \tag{29}$$

where $\hat{x}_1(z,s)$ is the Laplace transform of $x_1(z,\ t)$. The integration of the differential (29) with respect to the spatial coordinate z gives

$$\begin{aligned} \hat{x}_1(z,s) &= (sI - A_1)^{-1}x_{10} \\ &= \int_0^z \frac{E_{\psi,s}(\eta)}{E_{\psi,s}(z)} x_{10}(\eta)d\eta \end{aligned} \tag{30}$$

$$\text{where } E_{\psi,s}(z) = \exp(sz)\exp\left(-\int_0^z \psi(\nu)d\nu\right). \tag{31}$$

We can now state the following theorem, which follows from the similarity of the operators A and $\tilde{A}$, under the state transformation J (see (22)–(25)).

Theorem 3.2: The operator A defined by (21)–(22) is the infinitesimal generator of an exponentially stable C_0-semigroup on the Hilbert state space H.

Proof: By [22, Lemma 4.5, p. 84], the operator $\tilde{A}$ defined by (25) is the infinitesimal generator of a C_0-semigroup $(\tilde{S}(t))_{t\geq 0}$ on H whose growth constant is equal to that of the C_0-semigroup $(S(t))_{t\geq 0}$ generated by A. In particular $(S(t))_{t\geq 0}$ is exponentially stable if and only if so is $(\tilde{S}(t))_{t\geq 0}$.

Now in view of Lemma 3.1, each diagonal entry operator of $\tilde{A}$ is the infinitesimal generator of an exponentially stable C_0-semigroup on $L^2[0,\ 1]$. Hence, by [11, Lemma 3.2.2, p.114], $(\tilde{S}(t))_{t\geq 0}$ is exponentially stable. □

It follows from Lemma 3.1 and the proof of Theorem 3.2 that the growth bound of the C_0-semigroup $S(t)$ generated by the operator A is equal to $-\infty$. Intuitively this result could follow from the fact that A can be written as the sum of a bounded linear operator and a (e.g., lower triangular) infinitesimal generator of a C_0-semigroup whose growth bound equals $-\infty$ (see (22)). However this line of reasoning does not hold in general as it is explained in [2, Example 2.2.2, p. 20] and [3, Comment 5.1, p. 2420].

C. Reachability Analysis

Here we are interested in the reachability in the sense of [7] (or equivalently the approximate controllability in the sense of [11, Definition 4.1.17]) of the linearized plug flow reactor, i.e the operator pair (A, B), where A and B are given by (21)–(22) and (16), respectively. This property plays a crucial role in the LQ-feedback design problem: see Sections IV and V.

The reachability of the (infinite-dimensional) linearized plug flow reactor model follows from the total controllability of a related finite-dimensional space-varying system.

Lemma 3.2: Let us consider the matrix pair $(\mathcal{A}(z), \mathcal{B}(z))$ where $\mathcal{A}$ and $\mathcal{B}$ are given by

$$\mathcal{A} := -\begin{bmatrix} \alpha_1 & \alpha_2 \\ \alpha_3 & \alpha_4 \end{bmatrix} \quad \text{and} \quad \mathcal{B} := \begin{bmatrix} \beta \\ 0 \end{bmatrix}. \tag{32}$$

Then $(\mathcal{A}(\cdot), \mathcal{B}(\cdot))$ is totally controllable on [0, 1]. Hence, the reachability gramian, which is the unique solution of the following matrix Lyapunov differential equation:

$$\frac{d\Theta}{dz} = \mathcal{A}\Theta + \Theta\mathcal{A}^T + \mathcal{B}\mathcal{B}^T, \ \Theta(0) = 0 \tag{33}$$

is positive definite.

Proof: Recall that for any matrix pair $(\mathcal{A}(z), \mathcal{B}(z))$, the controllability matrix is defined as follows: (see [24, p. 66])

$$Q_c(z) = [P_0(z)\ P_1(z)\ \ldots\ P_{n-1}(z)] \tag{34}$$

where $P_{k+1}(z) = -\mathcal{A}(z)P_k(z) + dP_k/dz(z),\ P_0(z) = \mathcal{B}(z)$. Here in view of (32), the controllability matrix is given by

$$Q_c(z) = \beta \begin{bmatrix} 1 & \alpha_1(z) \\ 0 & \alpha_3(z) \end{bmatrix}. \tag{35}$$

By [24, Th. 4, p.69], $(\mathcal{A}(\cdot), \mathcal{B}(\cdot))$ is totally controllable on [0, 1] since $\mathrm{rank}(Q_c(z)) = 2$, for all $z \in [0, 1]$. Hence by [5, Th. 12, p.227] and [5, Comments 18, pp. 227 and 228] (β), the gramian $\Theta(z)$ is positive definite for all $z \in [0, 1]$. □

Now we can state the following theorem.

Theorem 3.3: Let A and B be the operators defined by (21)–(22) and (16), respectively. Then the operator pair (A, B) is reachable.

Proof: First recall that the operator A generates an exponentially stable C_0-semigroup (see Theorem 3.2), then by [11, Th. 4.1.23, p. 160] the extended reachability gramian, denoted by L_B, is the unique self-adjoint solution to the Lyapunov equation: $L_B D(A^*) \subset D(A)$ and

$$[AL_B + L_B A^* + BB^*]x = 0, \text{ for } x \in D(A^*). \tag{36}$$

In order to prove the reachability of (A, B), it is sufficient to prove that L_B is positive definite: see [11, Th. 4.1.22 (a), p. 160]. A straightforward calculation reveals that if the matrix

$$\Theta =: \begin{bmatrix} \theta_1 & \theta_2 \\ \theta_2 & \theta_3 \end{bmatrix}$$

is the solution of the matrix Lyapunov differential (33), then the solution of the operator Lyapunov algebraic (36) is given by $L_B := \Theta I$, where I is the identity operator. Observe that for any x in H, $\langle L_B x, x\rangle_H = \int_0^1 (x(z)^T \Theta(z) x(z)) dz$. Then one can conclude that the operator L_B is positive definite since, by Lemma 3.2, $\Theta(z)$ is positive definite for all $z \in [0, 1]$. □

IV. LQ-Feedback Control and Spectral Factorization

In this section we are interested in the standard linear quadratic optimal (LQ-)problem (see e.g., [11] and references therein), with a view to synthesize a state LQ-feedback operator for the linearized plug flow reactor model studied in the previous section and to apply it to the corresponding nonlinear model introduced in Section II.

It is known that the LQ-problem can be solved by spectral factorization: see, e.g [6], [7] for the case of finite rank bounded observation and control operators, and, e.g., [25] for the general case of stable weakly regular linear systems with admissible unbounded observation and control operators. Here we consider the spectral factorization approach for the more specific case of exponentially stable linear systems with bounded observation and control operators and infinite-dimensional output and input spaces. This is motivated in particular by the structure of the control operator B of the plug flow reactor model given by (16).

The spectral factorization problem, especially the one related to the LQ-problem, has been extensively studied in the system and control literature. In particular computational techniques, like the symmetric extraction method, have been analyzed in detail. For example this method has been successfully implemented for a heat diffusion model in [7] and for a larger class of semigroup Hilbert state-space systems with a Riesz-spectral generator, including also damped vibrating string models, in [26] (see also the references cited therein).

Let us consider the following class of infinite-dimensional state space systems:

$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t)\ , \quad x(0) = x_0 \in D(A)\ , \\ y(t) = Cx(t)\ , \end{cases} \tag{37}$$

where the following assumptions hold : (A1) the state $x(t) \in H$, a real separable Hilbert space with inner product $\langle \cdot, \cdot \rangle$, the input $u(t) \in U$ and the output $y(t) \in Y$, where U and Y are real separable Hilbert spaces, (A2) $A : D(A) \subset H \to H$ is the infinitesimal generator of a C_0-semigroup $(e^{At})_{t\geq 0}$ on H, where $e^{At} \in \mathcal{L}(H)$ for all $t \geq 0$, (A3) B and C are bounded linear operators, i.e., $B \in \mathcal{L}(U, H)$ and $C \in \mathcal{L}(H, Y)$ and (A4) $(e^{At})_{t\geq 0}$ is an exponentially stable C_0-semigroup.

The transfer function $\hat{G}$ of such a system is given by $\hat{G}(s) = C(sI - A)^{-1}B \in H^\infty(\mathcal{L}(U, Y))$ as a bounded and analytic

$\mathcal{L}(U,Y)$-valued function on the open right-half plane $\mathbb{C}^o_+$, where I is the identity operator, $(sI-A)^{-1}$ denotes the resolvent of A and $H^\infty(\mathcal{B})$ denotes the space of bounded analytic $\mathcal{B}$-valued functions on $\mathbb{C}^o_+$ (see [25, p. 291]) for any Banach space $\mathcal{B}$.

For any system given by (37) let us consider the *LQ-(optimal) control problem*: for any initial state $x_0 \in H$, find a square integrable control $u_0 \in L^2[0,\infty;U]$ that minimizes the cost functional

$$\Lambda(x_0,u) = \int_0^\infty (\|Cx(t)\|^2 + \|u(t)\|^2)\, dt\,. \tag{38}$$

The solution of this problem can be obtained by finding the nonnegative self-adjoint operator $Q_o \in \mathcal{L}(H)$ that solves the Operator Riccati Equation (ORE), *viz.*

$$[A^*Q_o + Q_oA + C^*C - Q_oBB^*Q_o]x = 0 \tag{39}$$

for all $x \in D(A)$ where $Q_o(D(A)) \subset D(A^*)$.

Theorem 4.1: Consider an infinite-dimensional state-space system of the form (37). Assume that conditions (A1)–(A4) hold. Then the ORE (39) has a unique nonnegative self-adjoint solution $Q_o \in \mathcal{L}(H)$ and for any initial state $x_0 \in H$, the quadratic cost (38) is minimized by the unique control u_{opt} given on $t \geq 0$ by

$$u_{opt}(t) = K_ox(t)\,, \quad x(t) = e^{(A+BK_o)t}x_0 \tag{40}$$

where the optimal feedback

$$K_o = -B^*Q_o \in \mathcal{L}(H,U) \tag{41}$$

is *stabilizing*, i.e., the feedback semigroup $(e^{(A+BK_o)t})_{t\geq 0}$ is exponentially stable. In addition, the optimal cost is given by $\Lambda(x_0,u_{opt}) = \langle x_0, Q_ox_0\rangle$. Finally, with $\mathcal{N}[P]$ denoting the null space of an operator P and $NO(C,A)$ denoting the unobservable subspace of system (37), $\mathcal{N}[Q_o] = NO(C,A)$, where the optimal cost is zero iff the initial state x_0 is unobservable.

Comment 4.1: The latter result is well known: see, e.g., [11, Section 6.2] and references therein. The proof of the last assertion about the null space of Q_o is the same as the one of [7, Theorem 2, p. 761] (where the output and input spaces are assumed to be finite-dimensional).

In [7, Theorem 3, p. 761] relates the solution of the LQ-control problem to a spectral factorization problem when (A,B) is exponentially stabilizable and (C,A) is exponentially detectable and when U and Y are finite-dimensional spaces. This result is extended in Theorem 4.2, to the more general case of infinite-dimensional separable Hilbert input and output spaces U and Y when A generates an exponentially stable C_0-semigroup. The proof of this result is similar to that of [7, Theorem 3] and can be found in [2, pp. 39, 40].

Theorem 4.2: Consider any system (37) and assume that conditions (A1)–(A4) hold. Let $\hat{G} \in H^\infty(\mathcal{L}(U,Y))$ denote its transfer function. Let K_o denote the LQ-optimal state feedback operator for the LQ-control problem associated with the cost (38). Under these conditions, the LQ-optimal feedback operator K_o is a solution of the following equation:

$$K_o(sI-A)^{-1}B = I - \hat{R}(s) \tag{42}$$

where the invertible standard spectral factor $\hat{R}(s) \in H^\infty(\mathcal{L}(U))$ (such that $\hat{R}(s)^{-1}$ is in $H^\infty(\mathcal{L}(U))$ and $\hat{R}(\infty) = I$ where the (strong) limit is to be taken along the positive axis) is a solution of the following spectral factorization problem

$$\hat{G}_*(s)\hat{G}(s) + I = \hat{R}_*(s)\hat{R}(s) \tag{43}$$

where $\hat{G}_*(s) := \hat{G}(-\overline{s})^*$.

Comment 4.2:

(a) The spectral factorization problem (43) admits a solution, i.e., there exists an operator valued function $\hat{R}$ in $H^\infty(\mathcal{L}(U))$ together with its inverse such that (43) holds, if and only if the Popov (spectral density) function $\hat{G}_*\hat{G} + I$ is coercive, i.e., there exists $\eta > 0$ such that, for all $\omega \in \mathbb{R}$, $\hat{G}_*(j\omega)\hat{G}(j\omega) + I \geq \eta I$: see [25, p. 316]. Such a spectral factor can be computed by using the solution of the operator Riccati equation: see (42), from which it can also be shown that $\hat{R}(s)^{-1} = I + K_o(sI-A-BK_o)^{-1}B$.

(b) Since the operators A and B are known, (42) can be seen as a partial realization problem for the strictly proper transfer function $I - \hat{R}(s)$. This equation corresponds to the Diophantine (19) in [7], where the stabilizing feedback K has been chosen equal to zero.

By Theorem 4.2, K_o is a solution of (42). However it turns out that in general it is not the only one. This motivates the following definition.

Definition 4.1: Consider any system (37) satisfying (A1)–(A4), with its transfer function $\hat{G} \in H^\infty(\mathcal{L}(U,Y))$. A state feedback operator $\mathcal{K} \in \mathcal{L}(H,U)$ is called an *LQ-feedback* if it is a solution to

$$\mathcal{K}(sI-A)^{-1}B = I - \hat{R}(s) \tag{44}$$

where $\hat{R} \in H^\infty(\mathcal{L}(U))$ is the unique invertible standard spectral factor of the Popov function $\hat{G}_*\hat{G} + I$.

Theorem 4.3: Consider any system (37) satisfying (A1)–(A4). Let $K_o\Pi$ denote the reachable restriction of the optimal feedback K_o, where $\Pi \in \mathcal{L}(H)$ denotes the orthogonal projection onto the reachable subspace $\mathcal{R}(A,B)$. Then any LQ-feedback $\mathcal{K}$ is given by

$$\mathcal{K} = K_o\Pi + \mathcal{V} \tag{45}$$

where $\mathcal{V} \in \mathcal{L}(H,U)$ is any solution of

$$\mathcal{V}(sI-A)^{-1}B = 0\,. \tag{46}$$

Moreover, there exists a unique LQ-feedback, *viz.* K_o, whenever (A,B) is reachable.

Proof: Obviously, in view of Theorem 4.2, i.e., (42), and since $\Pi(sI-A)^{-1}B = (sI-A)^{-1}B$, any operator $\mathcal{K}$ given by (45)–(46) is an LQ-feedback. Conversely assume that $\mathcal{K} \in \mathcal{L}(H,U)$ is an LQ-feedback. Define the operator $\mathcal{V} \in \mathcal{L}(H,U)$ by $\mathcal{V} := \mathcal{K} - K_o\Pi$. Then, by identities (42) and (44), it follows that (46) holds. Now assume that (A,B) is reachable, i.e., $\mathcal{R}(A,B) = H$. By (46)

$$\mathcal{R}(A,B) \subset \mathcal{N}(\mathcal{V}). \tag{47}$$

Indeed, let x be in $\mathcal{R}(A,B)$, hence, there exists a sequence (x_n) in H such that

$$x_n = \int_0^{\tau_n} e^{A(\tau_n - s)} B u_n(s) ds, u_n \in L^2([0,\tau_n];U)$$

where $\tau_n > 0$ and x_n converges to x. Observe also that taking the inverse Laplace transform of (46) leads to the identity $\mathcal{V}e^{At}B = 0$, for all $t \geq 0$. Hence

$$\mathcal{V}x = \lim_{n\to\infty} \int_0^{\tau_n} \mathcal{V}e^{A(\tau_n - s)} B u_n(s) ds = 0.$$

In view of (47), the reachability of (A,B) implies that $\mathcal{V} = 0$ and obviously $\Pi = I$. Consequently $\mathcal{K} = K_0$ is the unique LQ-feedback. □

In [7, Theorem 4], it is shown that, for any exponentially stabilizable and detectable SGB system, the reachable restriction $K_o\Pi$ of the optimal feedback K_o is stabilizing and optimal from the input-output viewpoint. It turns out that these properties still hold for any LQ-feedback associated with any system (37) satisfying (A1)–(A4).

Theorem 4.4: Consider any system (37) such that (A1)–(A4) hold. Let $\mathcal{K} \in \mathcal{L}(H,U)$ be any LQ-feedback associated with this system, i.e., such that (44) holds, or equivalently (45)–(46) hold. Then (a) the feedback $\mathcal{K}$ is optimal from the input/output viewpoint. More precisely, the closed-loop transfer function due to $\mathcal{K}$, i.e $\hat{G}_{cl}(s) = C(sI - A - B\mathcal{K})^{-1}B \in H^\infty(\mathcal{L}(U,Y))$, is the optimal one, i.e.,

$$\hat{G}_{cl}(s) = C(sI - A - BK_o)^{-1}B$$

and (b) the feedback C_0-semigroup $(e^{(A+B\mathcal{K})t})_{t\geq 0}$ generated by the closed-loop operator $A + B\mathcal{K}$ is exponentially stable.

Proof:

a) Let us consider any LQ-feedback $\mathcal{K} = K_o\Pi + \mathcal{V}$ with $\mathcal{V}(sI - A)^{-1}B = 0$. Then the spectral factor of Theorem 4.2 is given by

$$\hat{R}(s) = I - \mathcal{K}(sI - A)^{-1}B = I - K_o(sI - A)^{-1}B\ .$$

Using the fact that the optimal closed-loop transfer function is given by $C(sI - A - BK_o)^{-1}B = \hat{G}(s).\hat{R}(s)^{-1}$, one can easily see that the transfer function $C(sI - A - B\mathcal{K})^{-1}B \in H^\infty(\mathcal{L}(U,Y))$ is the optimal closed-loop one.

b) By (45), for any initial state $x_0 \in H$

$$e^{(A+B\mathcal{K})t}x_0 = e^{(A+BK_o\Pi)t}x_0 + \int_0^t e^{(A+BK_o\Pi)(t-s)} B\mathcal{V}e^{(A+B\mathcal{K})s}x_0 ds. \quad (48)$$

By the proof of [7, Th. 4], $(e^{(A+BK_o\Pi)t})_{t\geq 0}$ is exponentially stable. Now observe that

$$\int_0^t e^{(A+BK_o\Pi)(t-s)} B\mathcal{V}e^{(A+B\mathcal{K})s}x_0 ds \in \mathcal{R}(A,B)$$

since $\mathcal{R}(A,B)$ is invariant under state feedback (see e.g [10]), where $\mathcal{R}(A + BK_0\Pi, B) = \mathcal{R}(A,B)$. Then by applying the operator $\mathcal{V}$ to both sides of (48) and using (47), the following identity holds: $\mathcal{V}e^{(A+B\mathcal{K})t}x_0 = \mathcal{V}e^{(A+BK_o\Pi)t}x_0$. Consequently, in view of (48), the C_0-semigroup $(e^{(A+B\mathcal{K})t})_{t\geq 0}$ is exponentially stable. □

Comment 4.3: In this section, we have extended the fact that the optimal LQ-feedback can be computed via a spectral factorization problem coupled with some Diophantine equation. Generally speaking, the spectral factorization method is an interesting alternative to the ORE approach for solving the LQ-problem. It turns out a posteriori that, for the specific problem handled here, the computational load is the same for both methods. Yet, as an educated guess based on the observations reported in [26], the symmetric extraction method of spectral factorization should be efficient for axial dispersion reactor models. Indeed such models can be seen as perturbed diffusion equations (see, e.g., [2, Sec. 5.1] and [16]), that involve operators whose spectrum is known to be numerically well-conditioned for spectral factorization by symmetric extraction: see [26, Remark 4.1 and Sec. 4.2] and [27, Sec. 5].

V. LQ-Optimal Feedback Operator Design

This section deals with the computation of an LQ-optimal feedback operator for the linearized plug flow reactor model (20)–(22), (16) by using the spectral factorization method described in the previous section. First let us define an output function $y(.)$ by

$$y(t) = Cx(t) := [\, w_1 I \quad w_2 I \,]\, x(t), \quad t \geq 0 \qquad (49)$$

where $w_1, w_2 : [0,\ 1] \to \mathbb{R}$ are continuous functions. In view of (38) of the corresponding quadratic cost and the linearized model state definition (17), these functions can be interpreted as weighting factors for estimates of the distance between the initial model state and the chosen equilibrium profile.

Comment 5.1: By using duality and arguments similar to those used in Section III.C, the functions w_1 and w_2 can be chosen such that the operator pair (C,A) is observable. In order to compute an LQ-feedback in the sense of Definition 4.1, the standard spectral factor $\hat{R}(s) \in H^\infty(\mathcal{L}(L^2(0,1)))$ of the Popov function $\hat{G}_*(s)\hat{G}(s) + I$ is needed. The idea is to observe that by (44) this spectral factor has the form

$$\hat{R}(s) = I - \mathcal{K}(sI - A)^{-1}B. \qquad (50)$$

In other words, $[A, B, -\mathcal{K}, I]$ is a realization of $\hat{R}$, where the operator $\mathcal{K}$ plays the role of an observation operator. In view of the structure of the observation operator C, given by (49), in the open-loop transfer function $\hat{G}$, it seems natural to look for an operator $\mathcal{K}$ of the same form, i.e.

$$\mathcal{K} = [\, \psi_1 I \quad \psi_2 I \,] \qquad (51)$$

where ψ_1 and ψ_2 are continuous functions. Working out this idea leads to Theorem 5.1 whose proof is based on several auxiliary results.

Lemma 5.1: Let us consider arbitrary functions u, v in $L^2(0,1)$. Let us define the following auxiliary functions $x := (x_1, x_2)^T = (sI - \tilde{A})^{-1}u$ and $y := (y_1, y_2)^T = (-\overline{s}I - \tilde{A})^{-1}v$

in $L^2(0,1) \times L^2(0,1)$. Then the following identities hold:

$$f_1(x,s) := \alpha_3 x_1 + s x_2 + \frac{dx_2}{dz} + \alpha_4 x_2 = 0, \tag{52}$$

$$u = f_2(x,s) := s x_1 + \frac{dx_1}{dz} + \alpha_1 x_1 + \alpha_2 x_2, \tag{53}$$

$$f_1(y,-\overline{s}) = 0 \text{ and } v = f_2(y,-\overline{s}). \tag{54}$$

The proof of this lemma is given in the Appendix .

We now consider the open-loop transfer function, i.e., the linearized model transfer function $\hat{G}(s)$. By a straightforward computation based on

$$\hat{G}(s) = C(sI-A)^{-1}B = CJ^{-1}(sI-\tilde{A})^{-1}JB$$

where the operator J is defined by (23), it can be shown that this transfer function can be expressed as follows.

Lemma 5.2: **[Open-loop Transfer Function]** Let us consider the linearized plug flow reactor model (20)–(22), with control operator B given by (16) and observation operator C given by (49). Then its transfer function is given by

$$\hat{G}(s) = \beta\left(w_1 I + [w_1\gamma - w_2]\,\tilde{\mathcal{R}}_2(s)\alpha_3 I\right)\tilde{\mathcal{R}}_1(s) \tag{55}$$

where $\tilde{\mathcal{R}}_1$ and $\tilde{\mathcal{R}}_2$ are the resolvent operators of the diagonal entries of the operator $\tilde{A}$. See Comment 3.1 for the explicit form of such operators.

An important observation for the proof of Theorem 5.1 is the fact that any feedback operator of the form (51) is stabilizing.

Lemma 5.3: **[Stabilizing State Feedback]** Let us consider the operators A and B as in Lemma 5.2. For any continuous functions ψ_1 and ψ_2 on [0, 1], the feedback operator $\mathcal{K} := [\,\psi_1 I \quad \psi_2 I\,]$ is stabilizing, i.e., the C_0-semigroup $e^{(A+B\mathcal{K})t}$ is exponentially stable.

Proof: The operator $A + B\mathcal{K}$ is given by

$$A + B\mathcal{K} = -\begin{bmatrix} \frac{d.}{dz} + (\alpha_1 - \beta\psi_1)I & (\alpha_2 - \beta\psi_2)I \\ \alpha_3 I & \frac{d.}{dz} + \alpha_4 I \end{bmatrix}.$$

Observe that $A + B\mathcal{K}$ has the same form than the operator A. Therefore one can use the arguments of Section III. The crucial difficulty in this analysis is to prove that the corresponding scalar RDE (similar to (24)) has a solution in [0, 1]. Here this equation takes the following form:

$$-\frac{d\varrho}{dz} = \alpha_3\varrho^2 + (\alpha_1 - \beta\psi_1 - \alpha_4)\varrho - (\alpha_2 - \beta\psi_2). \tag{56}$$

Observe that the independent term $\alpha_2 - \beta\psi_2$ is not constant. However, the fact that the latter is a bounded function, i.e there exist constants ψ_m, ψ_M such that $\psi_m \le \alpha_2 - \beta\psi_2 \le \psi_M$, implies that (56) has a solution if the following lower and upper RDEs

$$-\frac{d\varrho_l}{dz} = \alpha_3\varrho_l^2 + (\alpha_1 - \beta\psi_1 - \alpha_4)\varrho_l - \psi_M, \tag{57}$$

$$-\frac{d\varrho_u}{dz} = \alpha_3\varrho_u^2 + (\alpha_1 - \beta\psi_1 - \alpha_4)\varrho_u - \psi_m \tag{58}$$

have solutions with $\varrho_l(1) \le \varrho(1) \le \varrho_u(1)$ (see [1, Corollary 6.7.35, p.363]). Observe that (57) and (58) have the same form than (24). Hence, by using the arguments of the proof of Theorem 3.1, it follows that each equation admits a (bounded) solution. Indeed, such a proof is based on the signs of the quadratic and the independent terms. Here, only the independant term α_2 in (24) has been changed and replaced by ψ_M and ψ_m, respectively, and both cases can be studied relatively to the sign of ψ_M and ψ_m as for (24). Consequently, by the analysis developed in Sections III-A and B, $A + B\mathcal{K}$ generates an exponentially stable C_0-semigroup. $\square$

It turns out that the computation of a spectral factor of the form (50)–(51) is based on the solution of a matrix Riccati differential equation (MRDE). The need for such an equation appears when plugging the expression of $\hat{R}$ in the spectral factorization identity (43).

Lemma 5.4: **[MRDE]** Let us consider the following matrix functions on [0, 1]:

$$F := -\begin{bmatrix} \alpha_1 & \alpha_2 \\ \alpha_3 & \alpha_4 \end{bmatrix},\; Q := \beta^2\begin{bmatrix} w_1^2 & w_1 w_2 \\ w_1 w_2 & w_2^2 \end{bmatrix}$$

and $S := diag(1,0)$ and let us consider the following MRDE:

$$-\frac{d\Phi}{dz} = F^*\Phi + \Phi F + Q - \Phi S \Phi,\;\; \Phi(1) = 0. \tag{59}$$

Then the latter has a unique positive semidefinite solution $\Phi =: \begin{bmatrix} \phi_1 & \phi_2 \\ \phi_2 & \phi_3 \end{bmatrix}$ on [0, 1].

Proof: Observe that the entries of the matrices F, Q and S are continuous functions and that Q and S are positive semidefinite. Then this lemma is an immediate consequence of [1, Theorem 4.1.6]. $\square$

Now we are in a position to state the following theorem, whose proof is given in the Appendix .

Theorem 5.1: **[Spectral Factor and LQ-Feedback]** Let us consider the linearized plug flow reactor model as in Lemma 5.2, with transfer function $\hat{G}(s)$ given by (55). Let $\hat{R}(s) \in H^\infty(\mathcal{L}(L^2(0,1)))$ be the unique invertible standard spectral factor of the Popov function $\hat{G}_*\hat{G} + I$. Let

$$\Phi(z) =: -\beta\begin{bmatrix} \psi_1(z) & \psi_2(z) \\ \psi_2(z) & \psi_3(z) \end{bmatrix} = \Phi^*(z) \ge 0 \tag{60}$$

be the solution of the MRDE (59). Then $\hat{R}$ is given by

$$\hat{R} = I - \beta\left(\psi_1 I + [\psi_1\gamma - \psi_2]\,\tilde{\mathcal{R}}_2\alpha_3 I\right)\tilde{\mathcal{R}}_1\,. \tag{61}$$

Hence, the operator $\mathcal{K}$ given for all $x \in H$ by

$$\mathcal{K}x = \psi_1 x_1 + \psi_2 x_2 \tag{62}$$

is an LQ-feedback (in the sense of Definition 4.1).

Comment 5.2: Note that formula (61) is based on the *a priori* knowledge of the solution γ of the triangularization RDE (24). Another expression of $\hat{R}$, in terms of the system parameters only, could also be used. However, (61) turns out to be easier to handle, especially when checking the spectral factorization identity: see the proof in the Appendix .

Since the pair (A,B) is reachable (see Theorem 3.3), the following corollary is immediate in view of Theorem 4.3.

Corollary 5.1: The LQ-feedback operator $\mathcal{K}$ given by (62) is unique, where it is the LQ-optimal state feedback operator K_0. Moreover, the optimal control is given on $t \geq 0$ by

$$u_{opt}(t) = K_0 x(t) = \psi_1 x_1(t) + \psi_2 x_2(t) \qquad (63)$$

where the functions ψ_1 and ψ_2 can be computed by finding the matrix Φ, given by (60), that is the solution of the MRDE (59).

VI. Nonlinear Closed-Loop System Analysis

A. Stability Analysis

This section deals with the stability of any constant temperature equilibrium profile for the nonlinear closed-loop system by applying the LQ-optimal feedback, computed in the previous section, to the plug flow reactor nonlinear model. The analysis is based on an asymptotic stability criterion for a class of infinite-dimensional semilinear systems. This criterion is based on the theory of nonlinear contraction semigroups (see [18], [2] and [4]). Due to the lack of space, we refer the reader to those references for detailed definitions of the basic mathematical concepts used in this section.

Definition 6.1: Let A be a dissipative operator on a reflexive Banach space X. Let X_0 be a subset of X. $\mathcal{A}$ is said to be in $Q(X_0)$ if $\overline{D(\mathcal{A})} \subset X_0$ and $X_0 \subset \mathcal{R}(I - \lambda\mathcal{A})$ for all $\lambda > 0$.

Now we state an important result with a view to show the stability of the closed-loop nonlinear plug flow reactor. The proof of this result can be found in [2, Section 4.3.3] and [4, Theorem 16].

Theorem 6.1: Let F be a closed convex subset of X. Consider a linear closed dissipative operator $\widetilde{\mathbf{A}}$ such that $(I - \lambda A_{cl})^{-1}$ is compact for some $\lambda > 0$. Consider a Lipshitz continuous nonlinear operator $\widetilde{\mathbf{N}}$ on F. Assume that $\mathcal{A} = \widetilde{\mathbf{A}} + \widetilde{\mathbf{N}}$ is strictly dissipative and the restriction of $\widetilde{\mathbf{A}}$ to $D(\widetilde{\mathbf{A}}) \cap F$ is in $Q(F)$ and that

$$\liminf_{\lambda \to 0^+} \lambda^{-1} d(F, x + \lambda \widetilde{\mathbf{N}}(x)) = 0, \text{ for } x \in \overline{D(\mathcal{A})}$$

holds, where $d(F, p)$ denotes the distance from $p \in X$ to F. Let $\Gamma(t)$ be the contraction semigroup generated by $\mathcal{A}$. Assume that $\overline{x}$ is an equilibrium point of $\mathcal{A}$. Then for any $x_0 \in \overline{D(\mathcal{A})}$, $x(t, x_0) := \Gamma(t)x_0 \to \overline{x}$ as $t \to \infty$.

Applying the LQ-optimal state feedback K_0, given by (63), to the nonlinear plug flow reactor model (12) yields the following nonlinear closed-loop system:

$$\begin{cases} \dot{\theta}(t) &= A_{cl}\theta(t) + N(\theta(t)) \\ x(0) &= x_0 \in D(A_{cl}) \cap F \end{cases} \qquad (64)$$

where A_{cl} is the linear operator defined on its domain $D(A_{cl}) = D(A_\psi) = D(A_0)$ by $A_{cl}\theta :=$

$$A_\psi \theta + q := \begin{bmatrix} -\frac{d.}{dz} - \psi_\beta I & \beta\psi_2 I \\ 0 & -\frac{d.}{dz} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} + \begin{bmatrix} q_1 \\ 0 \end{bmatrix} \qquad (65)$$

with $\psi_\beta := \beta(1 - \psi_1)$ and $q_1 := \beta\theta_{ce} - \beta\psi_2\theta_{2e}$, and N is the nonlinear operator given by (15).

In order to apply Theorem 6.1, the following lemmas are useful.

Lemma 6.1: If $\beta_0 := \int_0^1 |\psi_2(z)|^2 dz \leq 1$, then the operator A_ψ is m-dissipative. Moreover

$$\|e^{A_\psi t}\| \leq 1, \ \forall t \geq 0.$$

Hence, A_{cl} is a closed dissipative operator.

Proof: Denote by $A_{\psi 1}$ and $A_{\psi 2}$ the diagonal entries of A_ψ, respectively. Let $x = (x_1, x_2) \in D(A_0)$, one has

$$e^{A_\psi t} x = \begin{bmatrix} e^{A_{\psi 1} t} x_1 + \int_0^t e^{A_{\psi 1}(t-s)} \beta\psi_2 e^{A_{\psi 2} s} x_2 ds \\ e^{A_{\psi 2} t} x_2 \end{bmatrix}.$$

Hence, the following inequality $\|e^{A_\psi t} x\| \leq$:

$$\max\left(e^{-\beta t}\|x_1\| + \sqrt{\beta_0}(1 - e^{-\beta t})\|x_2\|, \|x_2\|\right)$$

holds. Then under the condition $\beta_0 \leq 1$, we have $\|e^{A_\psi t}\| \leq 1$ and consequently A_ψ is m-dissipative. □

Lemma 6.2: If $\beta_0 \leq 1$, there exists $\lambda > 0$ such that $(I - \lambda A_{cl})^{-1}$ is compact.

Proof: The compactness of $(I - \lambda A_{cl})^{-1}$ can be proved by using the one of $(I - \lambda A_0)^{-1}$ (see [2, Lemma 6.2] and [4, Lemma 20]) and the dissipativity of A_{cl} (see Lemma 6.1). □

Lemma 6.3: If $\beta_0 \leq 1$ and

$$\lim_{h \to 0^+} h^{-1} d\left(F, \theta + h \begin{bmatrix} q_1 + \beta\psi_2\theta_2 \\ 0 \end{bmatrix}\right) = 0, \qquad (66)$$

holds, where $\forall x \in F$, then the restriction of A_{cl} on $D(A_0) \cap F$ is in $Q(F)$.

Proof: This result can be proved in the same way than [2, Lemma 6.3] and [4, Lemma 22]. □

Concerning the nonlinear operator, many of its properties are studied in [16, Lemmas 3.1 and 3.2] in the framework of the trajectory analysis of the same model. The following result gives a condition that guarantees the strict dissipativity of $A_{cl} + N$, whose proof can be seen as an extension of the one of [2, Lemma 6.5] and [4, Lemma 25], and therefore omitted.

Lemma 6.4: If

$$l = \max(l_1, l_2) < \beta \qquad (67)$$

holds, where l_1 and l_2 are given by

$$\begin{aligned} l_1 &= |\delta| \frac{K_o L}{v} \left[F_{\psi_2/\delta} + \frac{4RT_{\text{in}}}{Ee^2}\right] \quad \text{if } \frac{E}{2R} \leq T_{\max} \\ &= |\delta| \frac{K_o L}{v} \left[F_{\psi_2/\delta} + \frac{ET_{\text{in}}\mu_m}{RT_{\max}^2}\right] \quad \text{if } \frac{E}{2R} > T_{\max} \end{aligned} \qquad (68)$$

and

$$\begin{aligned} l_2 &= \frac{K_o L}{v} \left[F_1 + \frac{4RT_{\text{in}}}{Ee^2}\right] \quad \text{if } \frac{E}{2R} \leq T_{\max} \\ &= \frac{K_o L}{v} \left[F_1 + \frac{ET_{\text{in}}\mu_m}{RT_{\max}^2}\right] \quad \text{if } \frac{E}{2R} > T_{\max} \end{aligned} \qquad (69)$$

where $\mu_m := \exp(-E/RT_{\max})$ and for any parameter a,

$$F_a := \max_{0 \leq T \leq T_{\max}} \left| \exp\left(\frac{-E}{RT}\right) - a\frac{4h}{K_o \rho C_p d}\right| \qquad (70)$$

then the operator $A_{cl} + N$ is strictly dissipative.

An immediate and important consequence of the Lemmas above and Theorem 6.1 is the following theorem giving an asymptotic stability criteria.

Theorem 6.2: Consider the nonlinear closed-loop plug flow reactor model (64)–(65) such that conditions (67) and (66) hold. If $\beta_0 \leq 1$, then the operator $A_{cl} + N_0$ is the generator of a unique nonlinear contraction semigroup $\Gamma(t)$ on F. Moreover, for any $x_0 \in F, x(t, x_0) := \Gamma(t)x_0 \to 0$ as $t \to \infty$ i.e., the zero state is an asymptotically stable equilibrium point of (64)–(65) on F.

1) Comment 6.1: Typically, in most cases, the condition $E > 2RT_{\max}$ is satisfied, since the activation energy E is very large. In this case, the asymptotic stability criterion of Theorem 6.2 reads as follows:

$$k_0 \exp\left(-\frac{E}{RT_{\max}}\right) \cdot K < \frac{4h}{\rho C_p d}$$

where the constant K depends on the system parameters. From a physical point of view, the condition above means that the heat transfer coefficient must be large enough in order to dominate a weighted value of the kinetic constant $k_0 \exp(-E/RT_{\max})$.

B. Optimality Analysis

This subsection deals with the optimality of the computed LQ-feedback control along the state trajectories of the nonlinear plug flow reactor. This analysis is inspired from [15], which treats the problem for finite dimensional systems. The (inverse) problem can be reformulated as follows. What type of modification of the cost criterion can restore optimality? Let us consider the controlled plug flow reactor nonlinear model which can be written as follows:

$$\begin{cases} \dot{x}(t) &= A_0 x(t) + N_0(x(t)) + Bu(t) \\ x(0) &= x_0 \in D(A_0) \cap F_0 \end{cases} \tag{71}$$

where the operator A_0 is given by (13)–(14) and the nonlinear operator N_0 is given by (19).

The idea is to write the generator of the latter as the sum of the linearized generator and some nonlinear operator.

$$\begin{cases} \dot{x}(t) &= Ax(t) + Bu(t) + \tilde{N}_0(x(t)) \\ x(0) &= x_0 \in D(A_0) \cap F_0 \end{cases} \tag{72}$$

where the operator $\tilde{N}_0(x) = N_0(x) + A_0 x - Ax$. The LQ-control law u_{opt} given by (63) is not optimal for the nonlinear system (72), but it can be made so with respect to another type of cost criterion which includes the function $\tilde{N}_0$

$$\Lambda_0(x_0, u) = \int_0^\infty \|Cx\|^2 - 2\langle \tilde{N}_0(x), \Phi x\rangle + \|u\|^2 dt \tag{73}$$

where $\Phi(z)$ is given by (60), that is the solution of the MRDE (59). It turns out that the asymptotic stability of the nonlinear closed-loop system (72) leads to the optimality of u_{opt} with respect to the criterion (73).

Theorem 6.3: If zero is an asymptotically stable equilibrium profile for the nonlinear closed-loop system (72), then the LQ-control law u_{opt} given by (63) is optimal for the nonlinear system (72) with respect to the cost criterion (73).

Proof: In view of (72) and by a straightforward calculation, one has

$$\begin{aligned} &\Lambda_0(x_0, u) \\ &\quad = \lim_{t_1 \to \infty} \int_0^{t_1} \left\{\|Cx\|^2 - 2\langle \dot{x} - Ax - Bu, \Phi x\rangle + \|u\|^2\right\} dt. \end{aligned}$$

Now by using the fact that Φ is the unique solution of the MRDE (59),

$$\begin{aligned} \langle Cx, Cx\rangle = \langle Qx, x\rangle = \left\langle -\frac{d\Phi}{dz}x, x\right\rangle - \langle \mathcal{M}^* \Phi x, x\rangle \\ - \langle \Phi \mathcal{M} x, x\rangle + \langle \Phi S \Phi x, x\rangle. \end{aligned}$$

Observe that $\langle Ax, \Phi x\rangle = \langle -(dx/dz), \Phi x\rangle + \langle \mathcal{M}x, \Phi x\rangle$, hence

$$\begin{aligned} &\Lambda_0(x_0, u) \\ &= \lim_{t_1 \to \infty} \int_0^{t_1} \{-2\langle \dot{x}, \Phi x\rangle + \langle \Phi S \Phi x, x\rangle + 2\langle u, B^* \Phi x\rangle + \|u\|^2\} dt \\ &= \langle x_0, \Phi x_0\rangle + \lim_{t_1 \to \infty} \left[-\langle x(t_1), \Phi x(t_1)\rangle + \int_0^{t_1} \{\|u - K_o x\|^2\} dt\right]. \end{aligned}$$

If we replace u by u_{opt} of (63), we obtain

$$\Lambda_0(x_0, u_{opt}) = \langle x_0, \Phi x_0\rangle - \lim_{t_1 \to \infty} \langle x(t_1), \Phi x(t_1)\rangle.$$

Then $\inf \Lambda_0(x_0, u) = \langle x_0, \Phi x_0\rangle$, since $x(t) \to 0$ as $t \to \infty$. □

Corollary 6.1: Under the conditions of Theorem 6.2, the LQ-control law $u_{\rm opt}$ given by (63) is optimal for the nonlinear system (72) with respect to the cost criterion (73).

Comment 6.2: Observe that the new cost criterion (73) might not be positive semi-definite. It would be interesting to analyze whether the controller designed in Section V is, in some sense, close to optimal for the same cost (38), (49), with respect to the nonlinear model, or to study its optimality for another optimal control problem with a positive semi-definite cost.

C. Numerical Simulations

This section is concerned with numerical simulations of the nonlinear closed-loop plug flow reactor model. Our objective is to illustrate the theoretical results related to the asymptotic stability property of this model. This model can be approximated by several methods including polynomial approximations, singular perturbation methods, finite-difference solutions and orthogonal collocation techniques. The two last methods are becoming standardized for many classical chemical engineering problems (see [21]). In the present example, we have considered a finite difference approximation method (with a backward difference for the spatial derivative), which is one of the oldest methods to handle differential equations. On the other hand, the approximation of the controller is based on the numerical solution of the MRDE (59). Numerous research works are concerned with numerical methods for MRDEs. These include carefully redesigned conventional Runge-Kutta method and linear

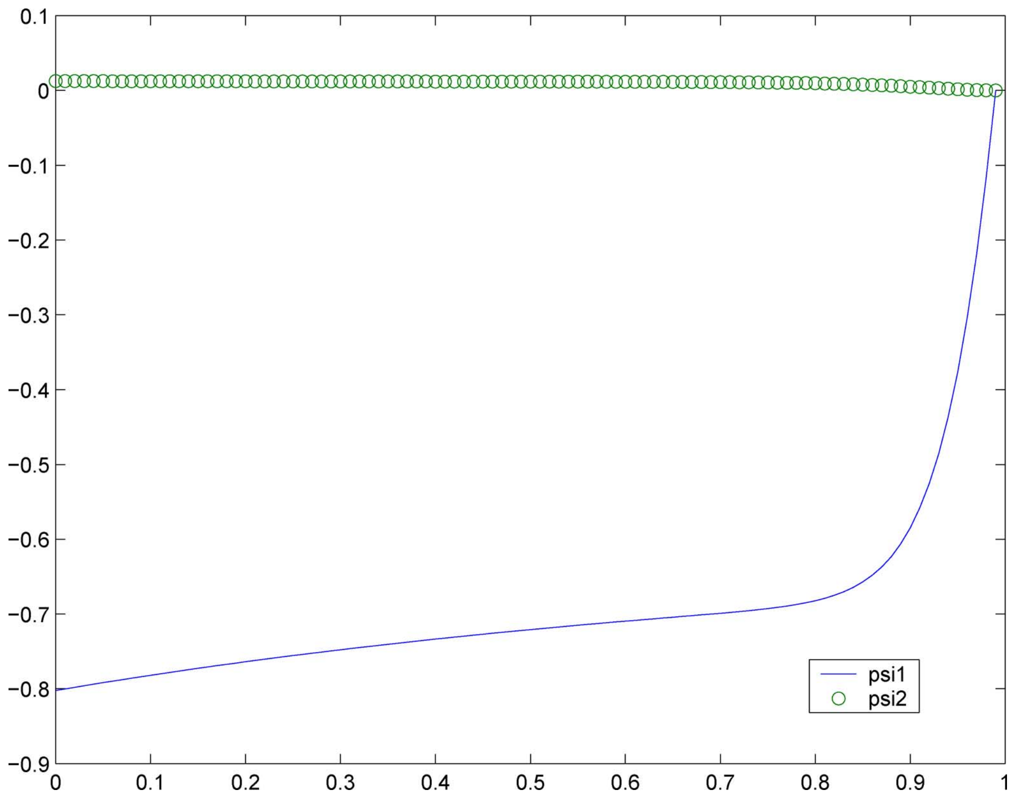


Fig. 1. LQ-feedback functions ψ_i for $w_1 = 10$ and $w_2 = 0$.

TABLE I
PROCESS PARAMETERS USED IN NUMERICAL SIMULATIONS

process parameters	notations	numerical values
superficial fluid velocity	v	0.025 m./s
length of the reactor	L	1 m
activation energy	E	11250 cal/mol
kinetic constant	k_0	10^6 s^{-1}
heat transfer coefficient	$\frac{4h}{\rho C_p d}$	0.2 s^{-1}
inlet reactant concentration	$C_{A,in}$	0.02 mol/L
ideal gas constant	R	1.986 cal/(mol.K)
inlet temperature	T_{in}	340 K
	δ	0.25

multistep methods for ODEs: see [8] and [12]. There are also some unconventional methods which are not suited for time-varying MRDEs. Here, the MRDE is solved by the Runge-Kutta method. Finally, the set of closed-loop ODEs is solved via the Runge-Kutta method as well. The parameter values used here are the same used in [23] (except the value of the superficial fluid velocity v that has been changed from 0.1 m/s to 0.025 m/s) and are depicted in Table I.

It has been theoretically shown in the previous subsection that, under some conditions, any constant temperature equilibrium profile is asymptotically stable for the closed-loop plug flow reactor model. Several initial states and weighted functions have been tested in numerical simulations. The results agree with the theoretical result. In the numerical simulations we have set both initial temperature and reactant concentration profiles to the inlet temperature and concentration, respectively, i.e., for all $z \in [0, L], T_0(z) = T_{\text{in}}$, and $C_{A,0}(z) = C_{A,\text{in}}$. The weighted functions are chosen as follows: for all $z \in [0, L]$, we have set $w_1(z) = 10$ and $w_2(z) = 0$. Fig. 1 shows the resulting LQ-optimal state feedback functions ψ_1 and ψ_2 [see (63)]. Observe that the function ψ_2 is almost identically zero, i.e., there is a very low gain feedback on the reactant concentration relative error; moreover the function ψ_1 induces a negative spatially varying feedback on the temperature relative error (see (17)). These results are not surprising in view of the choice of the weighting functions w_1 and w_2. The coolant temperature, the temperature in the reactor and the reactant concentration, at several points along the reactor and in the 3–D plot, are depicted in Fig. 2. It can be observed that the state numerically converges to the chosen equilibrium profile, as predicted by the theory. In order to illustrate the performances of the LQ-feedback controller, several disturbances have been considered (e.g., the inlet temperature, the inlet reactant concentration, the superficial fluid velocity, …) at some time instant. Here the following case is presented: the inlet temperature T_{in} is disturbed by a step of $\Delta T_{\text{in}} = 10$ K at time $t = 10$ s. The results of the simulations are shown in Fig. 3. It can be observed that in the presence of this disturbance the state converges to the modified equilibrium profile since the latter depends on the inlet temperature.

VII. CONCLUSION

In this paper, the LQ-optimal temperature and reactant concentration regulation problem has been solved by spectral factorization, for a nonisothermal plug flow reactor linearized model. The study of this problem lead to the concept of LQ-feedback control, which was developed for a specific class of exponentially stable linear systems with bounded measurement and control and infinite dimensional input and output spaces. This general approach has been implemented for the

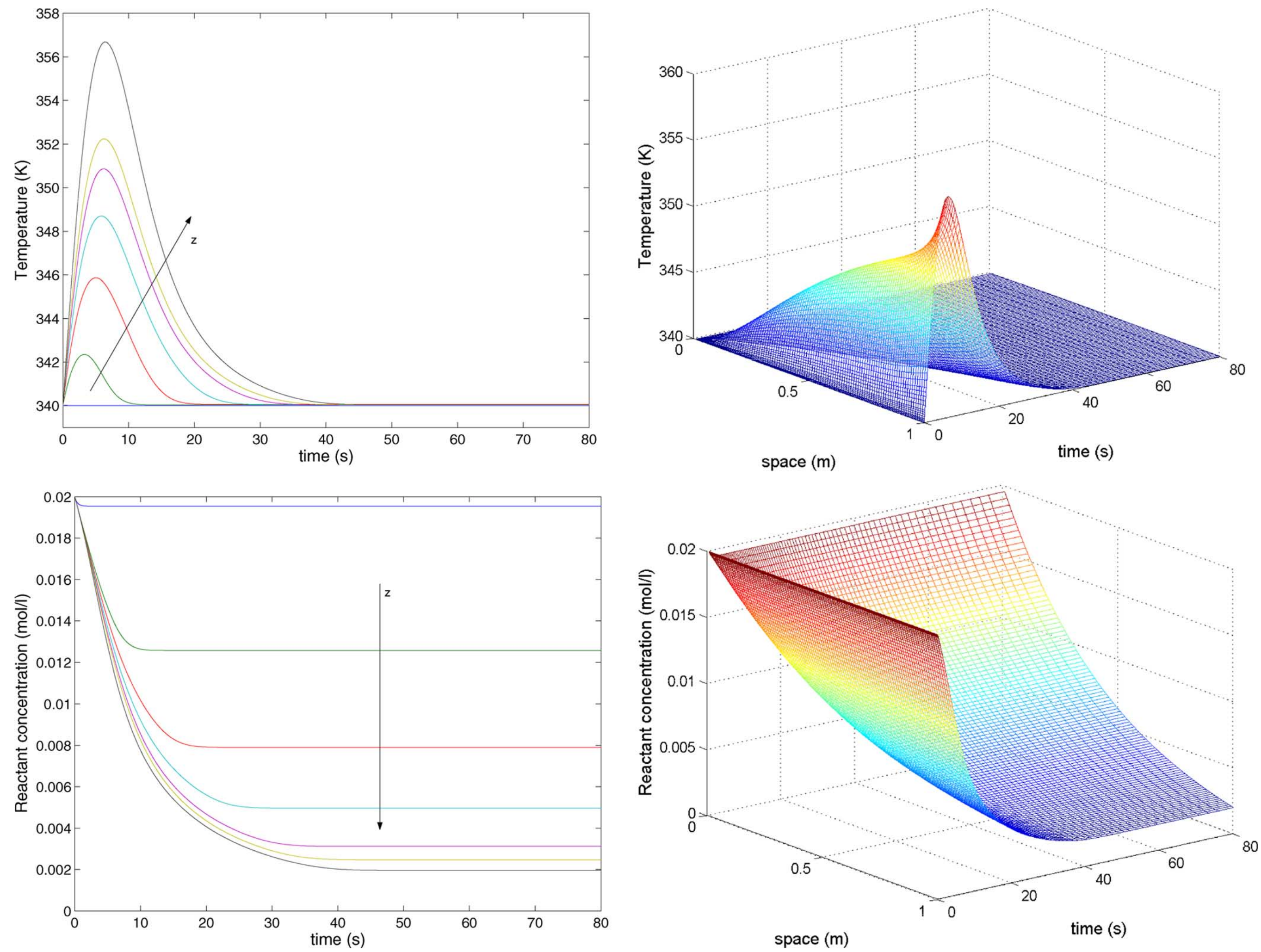


Fig. 2. Closed-loop nonlinear plug flow reactor for $w_1(z) = 10$ and $w_2(z) = 0$. Upper-left plot: temperature T at several points of the reactor; upper-right plot: temperature in 3-D plot; lower-left plot: reactant concentration C at several points of the reactor; lower-right plot: reactant concentration in 3-D plot.

specific reactor model studied here: a state LQ-feedback was computed via an appropriate MRDE. The reachability of the model leads to the uniqueness and therefore to the optimality of the state feedback. By applying the computed optimal LQ-feedback to the nonlinear system it was shown that under some physically feasible condition on the system parameters, the corresponding closed-loop system is asymptotically stable. This result was illustrated by some numerical simulations. In addition it was shown that the designed feedback is optimal along the nonlinear closed-loop system with respect to a modified cost criterion.

The analysis and methodology developed in this paper can be, in principle, extended to any other equilibrium profile, like those obtained in [23] and also to more complex nonlinearities. The main point is to take care of the regularity of the new functions α_i which appear in the linearized model. These functions correspond to the Jacobian of the nonlinear part of the model equations evaluated at the chosen equilibrium profile.

The approach followed here could be extended to the more realistic case where only a finite number of state components are available for measurement along the reactor. This could be done by synthesizing a dynamic output feedback compensator, resulting from the coupling of the static state feedback obtained here with a state observer realized by a static output injection, as in, e.g., [11, Sec. 5.3].

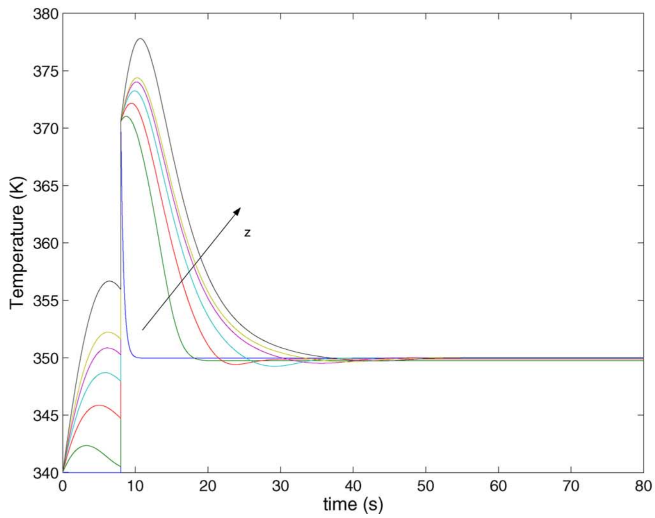
APPENDIX

Proof of Theorem 3.1: We only prove the existence of a solution to the RDE (24). The rest of the theorem follows directly in view of (23)–(25). Two cases are considered.

Case 1: $\boldsymbol{\alpha_2 \leq 0}$ **(endothermic reaction)** Observe that (24) can be identified with [1, eqs. (6.89), (6.75)], with $Q = -\alpha_2$, $L = 0$, $R = 1$, $\Pi \equiv 0$, $A = 2^{-1}(\alpha_1 - \alpha_4)$ and $B = \sqrt{-\alpha_3}$. Since $\alpha_2 \leq 0$, it follows from [1, Corollary 6.7.36, p. 364] that, whenever $\gamma(1) =: \gamma_1 \geq 0$, the solution γ of the latter equation exists on [0, 1].

Case 2: $\boldsymbol{\alpha_2 \geq 0}$ **(exothermic reaction)** First let us define $\mathcal{R}(\gamma) := \alpha_3\gamma^2 + (\alpha_1 - \alpha_4)\gamma - \alpha_2$. Observe that $\gamma_u := 0$ is obviously a solution of the Riccati differential inequation

$$-\frac{d\gamma_u}{dz} \geq \mathcal{R}(\gamma_u)\,. \tag{74}$$



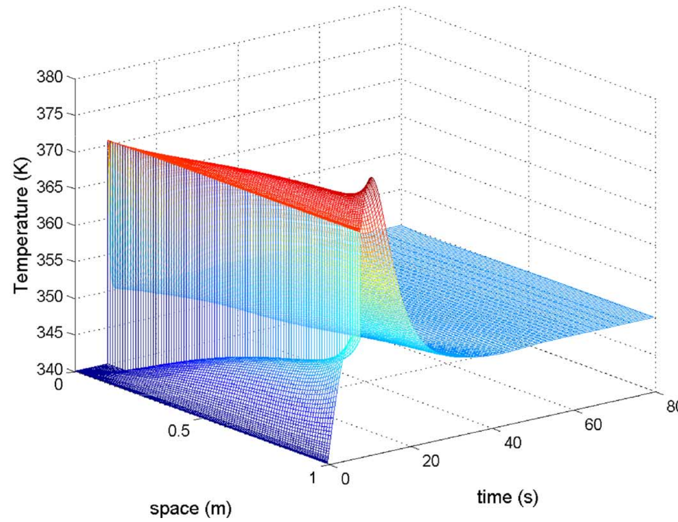


Fig. 3. Closed-loop nonlinear plug flow reactor for $w_1(z) = 10$ and $w_2(z) = 0$, and $\Delta T_{\text{in}} = 10$ K ($T'_{\text{in}} = 350$ K). Left plot: temperature T at several points of the reactor; right plot: temperature in 3-D plot.

Now let us consider the following RDE on the interval [0,1]:

$$-\frac{d\gamma_l}{dz} = \alpha_{3,m}\gamma_l^2 + \alpha_{1,m}\gamma_l - \alpha_2 \tag{75}$$

where $\alpha_{3,m} := -\alpha\mu = \min\{\alpha_3(z) : z \in [0,1]\}$ and $\alpha_{1,m}$ is a (sufficiently large) upper bound of the function $\alpha_1 - \alpha_4$. Let us prove the existence of a solution to the RDE (75). For this purpose let us consider the following transformation:

$$X_l(z) := -\gamma_l(1-z) - \frac{\alpha_{1,m}}{2\alpha_{3,m}}.$$

Therefore, (75) can be rewritten as follows:

$$-\frac{dX_l}{dz} = \alpha_{3,m}X_l^2 - r \tag{76}$$

where $r = \alpha_2 + \alpha_{1,m}^2/4\alpha_{3,m} \leq 0$ for $\alpha_{1,m}$ sufficiently large, i.e., $\alpha_{1,m} \geq 2\sqrt{-\alpha_{3,m}\alpha_2}$. It follows from [1, Corollary 6.7.36, p. 364] that, whenever $X_l(1) \geq 0$, the solution X_l of the latter equation exists on [0, 1]. Indeed one can observe that (76) can be identified with [1, eqs. (6.89), (6.75)], with $Q = -r$, $L = 0$, $R = 1$, $\Pi \equiv 0$, $A = 0$ and $B = \sqrt{-\alpha_{3,m}}$. In addition, by the comparison theorem [1, Theorem 6.7.33, p. 362], if $X_l(1) \geq -\alpha_{1,m}/2\alpha_{3,m} \geq 0$, then for all $z \in [0,1]$, $X_l(z) \geq -\alpha_{1,m}/2\alpha_{3,m}$. It follows that the RDE (75) has a solution

$$\gamma_l(z) = -X_l(1-z) - \frac{\alpha_{1,m}}{2\alpha_{3,m}}$$

on [0, 1] such that, if $\gamma_l(0) \leq 0$, then for all $z \in [0,1]$, $\gamma_l(z) \leq 0$; where γ_l is a solution of the following Riccati differential inequation:

$$-\frac{d\gamma_l}{dz} \leq \mathcal{R}(\gamma_l)\,. \tag{77}$$

By [1, Corollary 6.7.35, p. 363], if we choose $\gamma(1) =: \gamma_1$ such that $\gamma_l(1) \leq \gamma_1 \leq 0$, then the solution of the RDE (24) exists on [0, 1] and fulfills there the inequalities $\gamma_l(z) \leq \gamma(z) \leq 0$. □

Proof of Lemma 5.1: Observe that the variables x_1 and x_2 can be written as

$$x_1 := x_1(s,u) = (I + \gamma\tilde{\mathcal{R}}_2(s)\alpha_3 I)\tilde{\mathcal{R}}_1(s)u$$

and

$$x_2 := x_2(s,u) = -\tilde{\mathcal{R}}_2(s)\alpha_3\tilde{\mathcal{R}}_1(s)u$$

where s is any complex number, γ is the solution of the RDE (24) and where $\tilde{\mathcal{R}}_1$ and $\tilde{\mathcal{R}}_2$ are the resolvent operators of the diagonal entries of the operator $\tilde{A}$.

By a straightforward computation, it follows that

$$\alpha_3 x_1 + s x_2 + \frac{dx_2}{dz} + \alpha_4 x_2 = \alpha_3\tilde{\mathcal{R}}_1 u + \tilde{\mathcal{R}}_2^{-1}x_2 = 0$$

where, by using the RDE (24)

$$\begin{aligned} u = \tilde{\mathcal{R}}_1^{-1}(x_1 + \gamma x_2) &= \left(s x_1 + \frac{dx_1}{dz} + \alpha_1 x_1 + \alpha_2 x_2\right) \\ &+ \left(\frac{d\gamma}{dz} + \alpha_1\gamma - \alpha_4\gamma + \alpha_3\gamma^2 - \alpha_2\right)x_2 \\ &+ \gamma\left(\alpha_3 x_1 + s x_2 + \frac{dx_2}{dz} + \alpha_4 x_2\right) \\ &= s x_1 + \frac{dx_1}{dz} + \alpha_1 x_1 + \alpha_2 x_2. \end{aligned}$$

□

Proof of Theorem 5.1: First let us show that $\hat{R}(s)$, given by (61), satisfies the spectral factorization identity (43), or equivalently, for all $u, v \in L^2(0,\ 1)$

$$\langle \hat{G}(s)u,\ \hat{G}(-\overline{s})v\rangle + \langle u,\ v\rangle = \langle \hat{R}(s)u,\ \hat{R}(-\overline{s})v\rangle.$$

So let us consider arbitrary functions $u, v \in L^2(0,\ 1)$. By a straightforward computation, one gets the following identity: $\langle \hat{R}(s)u,\ \hat{R}(-\overline{s})v\rangle =$

$$\begin{aligned}\langle u,\ v\rangle &- \beta\langle(\psi_1 I + [\psi_1\gamma - \psi_2]\tilde{\mathcal{R}}_2(s)\alpha_3 I)\tilde{\mathcal{R}}_1(s)u, v\rangle\\ &- \beta\,\langle u,\ (\psi_1 I + [\psi_1\gamma - \psi_2]\tilde{\mathcal{R}}_2(-\overline{s})\alpha_3 I)\tilde{\mathcal{R}}_1(-\overline{s})v\rangle\\ &+ \beta^2\langle(\psi_1 I + [\psi_1\gamma - \psi_2]\tilde{\mathcal{R}}_2(s)\alpha_3 I)\tilde{\mathcal{R}}_1(s)u,\\ &\quad(\psi_1 I + [\psi_1\gamma - \psi_2]\tilde{\mathcal{R}}_2(-\overline{s})\alpha_3 I)\tilde{\mathcal{R}}_1(-\overline{s})v\rangle.\end{aligned}$$

Let x_1, x_2, y_1 and y_2 be the auxiliary functions defined in Lemma 5.1. Then it follows from identities (52)–(54) that $\langle \hat{R}(s)u,\ \hat{R}(-\overline{s})v\rangle =$

$$\begin{aligned}\langle u,\ v\rangle &- \beta\left\langle \psi_1 x_1 + \psi_2 x_2, -\overline{s}y_1 + \frac{dy_1}{dz} + \alpha_1 y_1 + \alpha_2 y_2\right\rangle\\ &- \beta\,\left\langle \psi_2 x_1 + \psi_3 x_2, \alpha_3 y_1 - \overline{s}y_2 + \frac{dy_2}{dz} + \alpha_4 y_2\right\rangle\\ &- \beta\left\langle s x_1 + \frac{dx_1}{dz} + \alpha_1 x_1 + \alpha_2 x_2,\ \psi_1 y_1 + \psi_2 y_2\right\rangle\\ &- \beta\left\langle \alpha_3 x_1 + s x_2 + \frac{dx_2}{dz} + \alpha_4 x_2,\ \psi_2 y_1 + \psi_3 y_2\right\rangle\\ &+ \beta^2\,\langle(\psi_1 x_1 + \psi_2 x_2),\ (\psi_1 y_1 + \psi_2 y_2)\rangle\,.\end{aligned}$$

Now let us consider three new functions $\phi_1 := -\beta\psi_1$, $\phi_2 := -\beta\psi_2$ and $\phi_3 := -\beta\psi_3$. By observing that each term that includes the complex variable s can be canceled, it follows that

$$\begin{aligned}\langle \hat{R}(s)u,\ \hat{R}(-\overline{s})v\rangle = \langle u,\ v\rangle &+ \left\langle \Phi x, \frac{dy}{dz}\right\rangle - \langle \Phi x, \mathcal{M}y\rangle\\ &+ \left\langle \frac{dx}{dz}, \Phi y\right\rangle - \langle \mathcal{M}x, \Phi y\rangle\langle S\Phi x, \Phi y\rangle.\end{aligned}$$

Now observe that $x_{1|_{z=0}} = x_{2|_{z=0}} = y_{1|_{z=0}} = y_{2|_{z=0}} = 0$ and recall that, since the matrix Φ is solution of the RDE (59), $\phi_1(1) = \phi_2(1) = \phi_3(1) = 0$. These observations lead to the following relations:

$$\begin{aligned}\langle \hat{R}(s)u,\ \hat{R}(-\overline{s})v\rangle = \langle u,\ v\rangle &- \left\langle \frac{d\Phi}{dz}x, y\right\rangle - \langle \mathcal{M}^*\Phi x, y\rangle\\ &-\langle \Phi\mathcal{M}x, y\rangle + \langle \Phi S\Phi x, y\rangle.\end{aligned}$$

It follows by the matrix RDE (59) that:

$$\begin{aligned}&\langle \hat{R}(s)u, \hat{R}(-\overline{s})v\rangle\\ &\quad= \langle u,\ v\rangle + \langle Qx, y\rangle\\ &\quad= \langle u,\ v\rangle + \langle \beta(w_1 x_1 + w_2 x_2), \beta(w_1 y_1 + w_2 y_2)\rangle\\ &\quad= \langle u,\ v\rangle + \langle \hat{G}(s)u,\ \hat{G}(-\overline{s})v\rangle.\end{aligned}$$

Hence, $\hat{R}(s)$ satisfies the spectral factorization identity. It remains to be shown that $\hat{R}(s)$ is in $H^\infty(\mathcal{L}(L^2(0,1)))$ together with its inverse and that $\hat{R}(\infty) = I$. First by construction of $\hat{R}(s)$, it is easy to see that $\hat{R} \in H^\infty(\mathcal{L}(L^2(0,1)))$ since A generates an exponentially stable C_0-semigroup : see Theorem 3.2. In addition $\hat{R}(\infty) = I$, since $(sI - A)^{-1}$ converges strongly towards 0 as $s \to \infty$ along the positive real axis. Now let us prove that $\hat{R}(s)^{-1} \in H^\infty(\mathcal{L}(L^2(0,1)))$. Observe that the inverse of $\hat{R}(s)$ can be expressed as follows:

$$\hat{R}^{-1}(s) = I + \mathcal{K}(sI - A - B\mathcal{K})^{-1}B. \tag{78}$$

By Lemma 5.3, the operator $A + B\mathcal{K}$ generates an exponentially stable C_0-semigroup. Thus, by [11, Theorem 5.1.5, p. 222], $(sI - A - B\mathcal{K})^{-1} \in H^\infty(\mathcal{L}(L^2(0,1)))$, hence, $\hat{R}^{-1} \in H^\infty(\mathcal{L}(L^2(0,1)))$. One can conclude that $\hat{R}$ is the standard spectral factor of $I + \hat{G}_*\hat{G}$ and $\mathcal{K}$ is an LQ-feedback of the linearized plug flow reactor. □

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