Proceedings of the 17th World Congress
The International Federation of Automatic Control
Seoul, Korea, July 6-11, 2008

Control of Time-Varying Distributed Parameter Plug Flow Reactor by LQR ⋆

Ilyasse Aksikas, **Adrian M. Fuxman**, **J. Fraser Forbes**

Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB, T6G 2G
e-mail: {aksikas; afuxman; fraser.forbes }@ualberta.ca

Abstract: The linear quadratic (LQ) optimal control problem is studied for a partial differential equation model of a time-varying plug flow tubular reactor. First some properties of the linearized model around a specific equilibrium profile are studied. Next, an LQ-control feedback is computed by using the corresponding operator Riccati differential equation, whose solution can be obtained via a related matrix Riccati partial differential equation. The controller is applied to the nonlinear reactor system and tested numerically.

Keywords: LQ-optimal control, plug flow reactor, time-varying infinite-dimensional systems, evolution systems.

1. INTRODUCTION

The dynamics of nonisothermal plug flow reactors are usually described by nonlinear partial differential equations derived from mass and energy balances (see. e.g., Aksikas et al., [2007], Laabissi et al., [2001], and references therein). The main source of nonlinearities in the dynamics of a (bio)-chemical reaction are often due to the kinetics terms of the model equations.

In Aksikas et al., [2007], the linear-quadratic control problem was studied for a plug flow reactor model with time-invariant rate of reaction by using the method of spectral factorization (Callier et al., [1992]). In this paper, we are interested in the time-varying case by using the well-known Riccati equation approach (Curtain et al., [1995], Bensoussan et al., [2007] and Pandolfi., [1992]). Time-varying rates of reaction arise from loss of catalyst activity which is an important issue in catalytic reactors. The literature provides several models for catalyst deactivation. For the purpose of this paper, we will adopt a simple exponential decay model form.

The contributions of this paper can be summarized as follows. In section 2, we recall some basic results on evolution systems and linear quadratic control problem for infinite dimensional time-varying systems. Section 3, describes both the dynamics of the time-varying plug flow reactor that we are interested in, its steady state profile and its linearized model around this profile. In designing an LQ-controller, some useful results on the dynamical properties of the linearized model are established in Section 4. The optimal control design problem is the subject of Section 5. An LQ-control feedback is computed by using the corresponding operator Riccati differential equation, whose solution can be obtained via a related matrix Riccati partial differential equation. Finally, the controller is applied to the nonlinear closed-loop system and tested numerically in Section 6.

2. BASIC RESULTS

2.1 Evolution Systems

Evolution systems theory generalizes the concept of one parameter semigroup $T_A(t)$ (generated by a given operator A) for the non-autonomous case, i.e. in the case where $A(t)$ depends on t: see e.g., Pazy. [1983], Acquistapace et al., [1984] and Tanabe., [1975].

Definition 1. Let H be a Hilbert space. A two parameter family of bounded linear operators $U(t,s),\ 0 \le s \le t \le T$, on H is called an evolution system if the following two conditions are satisfied:

(i) $U(s,s) = I,\ U(t,r)U(r,s) = U(t,s)$ for $0 \le s \le r \le t \le T$.
(ii) $(t,s) \to U(t,s)$ is strongly continuous for $0 \le s \le r \le t \le T$.

The following concept is needed for the existence and uniqueness of an evolution system for a time-varying initial value problem:

Definition 2. Let H be a Hilbert space. A family $A(t),\ t \in [0,T]$ of infinitesimal generators of C_0-semigroup on H is called stable if there are constants $M \ge 1$ and ω such that

$$\rho(A(t)) \supset]\omega, \infty[\text{ for } t \in [0,T]$$

and

$$\|\Pi_{j=1}^{k} R(\lambda : A(t_j))\| \le M(\lambda - \omega)^{-k} \text{ for} \lambda > \omega$$

and every finite sequence $0 \le t_1 \le t_2 \le \ldots, \le t_k \le T, k = 1, 2, \ldots$.

The following perturbation theorem is a useful criterion to prove that a given family of infinitesimal generators is stable ([Pazy. , 1983, Theorem 2.3. p. 132]).

⋆ Paper accepted for presentation as a regular paper at IFAC World Congress 2008.

978-1-1234-7890-2/08/$20.00 © 2008 IFAC 10.3182/20080706-5-KR-1001.3532

Theorem 3. Let $\{A(t)\}_{t\in[0,T}$ be a stable family of infinitesimal generators. Let $D(t), 0 \le t \le T$ be bounded linear operators on H. If $\|D(t)\| \le K$ for all $0 \le t \le T$ then $\{A(t)+D(t)\}_{t\in[0,T]}$ is a stable family of infinitesimal generators.

[Pazy. , 1983, Theorem 4.6, p.143] shows that if $\{A(t)\}_{t\in[0,T]}$ satisfies some conditions then one can associate a unique evolution system to $\{A(t)\}_{t\in[0,T]}$. One special case in which the conditions of [Pazy. , 1983, Theorem 4.6, p.143] can be easily verified is the case where $D(A(t)) = D_0$ is independent of t.

Theorem 4. Let $\{A(t)\}_{t\in[0,T]}$ be a stable family of infinitesimal generators of C_0-semigroup on H. If $D(A(t)) = D_0$ is independent of t and for every $v \in D_0, A(t)v$ is continuously differentiable in H then there exists a unique evolution system $U_A(t,s), 0 \le s \le t \le T$, satisfying

(i) $\|U_A(t,s)\| \le Me^{\omega(t-s)}$, for $0 \le s \le t \le T$.
(ii) $\dfrac{\partial}{\partial t}U_A(t,s)x = A(t)U_A(t,s)x$, for $x \in D_0, 0 \le s \le t \le T$.
(iii) $U_A(t,s)D_0 \subset D_0$ for $0 \le s \le t \le T$.

2.2 LQ-Optimal Control: Finite Time Horizon

Consider the system

$$\begin{cases} \dot{x}(t) \;=\; A(t)x(t) + B(t)u(t), \\ x(0) \;=\; x_0, \end{cases} \tag{1}$$

where $A(t) : D(A(t)) \subset H \to H$ and $B(t) \in \mathcal{L}(U;H)$ are linear operators. We make the following assumptions on the families $\{A(t)\}_{t\in[0,T]}$ and $\{B(t)\}_{t\in[0,T]}$:

i) $A(t)$ generates a C_0-semigroup in H for all $t \in [0,T]$,
ii) there exists a strongly continuous mapping $U_A(\cdot,\cdot)$: $\{(t,s) \in \mathbb{R}^2 : t \ge s\} \longrightarrow \mathcal{L}(H)$ such that $U_A^*(\cdot,\cdot)$ is also strongly continuous and

$$\frac{\partial}{\partial t}U_A(t,s)x = A(t)U_A(t,s)x, \quad U_A(s,s)x = x$$
$$\forall x \in D(A(t)), \quad 0 \le s \le t \le T, \tag{2}$$

iii) we have $\lim_{n\to\infty} U_{A_n}(t,s)x = U_A(t,s)x, \forall x \in H$ uniformly on the bounded sets of $\{(t,s) \in \mathbb{R}^2 : t \ge s\}$, where $U_{A_n}(t,s)$ is the evolution operator generated by the Yosida approximations of $A(t)$,
iv) $B(\cdot)u$ is continuous for all $u \in U$.

Under these assumptions problem (1) has a unique mild solution given by

$$x(t) = U(t,0)x_0 + \int_0^t U(t,s)Bu(s)ds.$$

Assumptions (2) are verified in many problems both parabolic and hyperbolic (see Acquistapace et al., [1984], Pazy. [1983] and Tanabe., [1975]).

We want to minimize the cost function

$$J(u) = \int_0^T \left\{|Cx(s)|^2 + |u(s)|^2\right\} ds + \langle P_0x(T), x(T)\rangle \tag{3}$$

over all controls $u \in L^2(0,\infty; L^2(0,1)$ subject to the differential equation constraint (1), where the operators B, C, and P_0 satisfy the following assumptions

$$P_0 \ge 0,\ C \in C_s([0,T]; \mathcal{L}(H;Y)),$$
$$B \in C_s([0,T]; \mathcal{L}(U;H)) \tag{4}$$

Let us consider the operator Riccati differential equation

$$\begin{cases} \dot{Q} + A^*Q + QA - QBB^*Q + C^*C = 0 \\ Q(T) = P_0 \quad \text{and} \quad Q(D(A)) \subset D(A^*). \end{cases} \tag{5}$$

Existence and uniqueness criteria for the solution of the operator Riccati differential equation are given by the following theorem, which is an immediate consequence of [Bensoussan et al., , 2007, Theorem 7.2 and Proposition 7.1, p. 416].

Theorem 5. Assume (2) and (4). Then the Riccati equation (5) has a unique nonnegative mild solution Q.

The solution of the linear-quadratic optimal control problem is given by the following well-known result.

Theorem 6. [Bensoussan et al., , 2007, Theorem 7.3, p.416] Assume (2) and (4), and let $x_0 \in H$. Then there exists a unique optimal pair (u^*, x^*) and $u^* \in C([0,T]; U)$ is related to x^* by the feedback formula

$$u^*(t) = -B^*(t)Q(t)x^*(t), \quad t \in [0,T].$$

Finally, the optimal cost $J(u^*)$ is given by

$$J(u^*) = \langle Q(0)x_0, x_0\rangle.$$

2.3 LQ-Optimal Control: Infinite Time Horizon

Let us consider the system (1). Here we want to minimize the cost function

$$J_\infty(u) = \int_0^\infty \left\{|Cx(s)|^2 + |u(s)|^2\right\} ds \tag{6}$$

over all controls $u \in L^2(0,\infty; U)$ subject to the differential equation constraint (1). First the following concept is needed.

Definition 7. $(A(t), B(t))$ is said to be $C(t)$-stabilizable if there exists $K \in \mathcal{L}(H;U)$, $M > 0$ and $\omega > 0$ such that

$$\|C(t)T_K(t,s)\| \le Me^{-\omega(t-s)},\ 0 \le s \le t,$$

where $T_K(\cdot,\cdot)$ is the evolution system generated by $A(t) + B(t)K(t)$.

Remark 8. Note that if $A(t)$ generates an exponentially stable evolution system then $(A(t), B(t))$ is $C(t)$-stabilizable for any bounded operator $C(t)$.

Theorem 9. [Bensoussan et al., , 2007, Theorem 5.2, p.507] Assume that conditions (2) and (4) are verified, and that (A,B) is C-stabilizable. Then the Riccati equation

$$\dot{Q} + A^*Q + QA - QBB^*Q + C^*C = 0, \text{ in } [0,\infty) \tag{7}$$

has a nonnegative bounded solution Q . This solution is minimal among all nonnegative bounded solutions of (7).

3. PLUG FLOW REACTOR MODEL

3.1 Nonlinear Model

Let us consider a nonisothermal plug flow tubular 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 PDE's derived from mass and energy balance principles. Here if the kinetics of the above reaction are characterized by first order time-varying kinetics with respect to the reactant concentration C (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 PDE's:

$$\frac{\partial T}{\partial \tau} = -v\frac{\partial T}{\partial \zeta} - \frac{\Delta H}{\rho C_p} k(\tau) C e^{-\frac{E}{RT}} - \beta_0 (T - T_c) \tag{8}$$

$$\frac{\partial C}{\partial \tau} = -v\frac{\partial C}{\partial \zeta} - k(\tau) C e^{-\frac{E}{RT}} \tag{9}$$

where $\beta_0 := \frac{4h}{\rho C_p d}$. In this paper, we adopt the simple deactivation model given by $k(\tau) = k_0 + k_1 e^{-\alpha\tau}$. The boundary conditions are given, for $\tau \geq 0$, by :

$$\begin{array}{rcl} T(0,\tau) & = & T_{in} \\ C(0,\tau) & = & C_{in}. \end{array} \tag{10}$$

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

$$\begin{array}{rcl} T(\zeta,0) & = & T_0(\zeta) \\ C(\zeta,0) & = & C_0(\zeta). \end{array} \tag{11}$$

In the equations above, v, ΔH, ρ, C_p, k, E, R, h, d, T_{in} and $C_{A,in}$ hold for the superficial fluid velocity, the heat of reaction, the density, the specific heat, the kinetic function, 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_0 denote the initial temperature and reactant concentration profiles respectively, such that $T_0(0) = T_{in}$ and $C_0(0) = C_{in}$.

Let us denote by T_{ss}, C_{ss} and $T_{c,ss}$ the temperature equilibrium, the reactant concentration equilibrium and the corresponding coolant temperature equilibrium, respectively. Then the corresponding steady-state equations of the PDEs model (8)-(11) are given by the following ordinary differential equations:

$$\begin{cases} v\dfrac{\partial T_{ss}}{\partial \zeta} & = -\dfrac{\Delta H}{\rho C_p} k_0 C_{ss} e^{-\frac{E}{RT_{ss}}} + \beta_0 (T_{c,ss} - T_{ss}), \\ v\dfrac{\partial C_{ss}}{\partial \zeta} & = -k_0 C_{ss} e^{-\frac{E}{RT_{ss}}}, \\ T_{ss}(0) & = T_{in},\ C_{ss}(0) = C_{in}. \end{cases} \tag{12}$$

3.2 Dimensionless Model

Let us consider the following dimensionless state variables $\theta_1(t)$ and $\theta_2(t)$, and dimensionless coolant temperature $\theta_c(t)$, $t \geq 0$ defined as follows:

$$\theta_1 = \frac{T - T_{in}}{T_{in}}, \quad \theta_2 = \frac{C_{in} - C}{C_{in}}, \text{ and } \theta_c = \frac{T_c - T_{in}}{T_{in}} \tag{13}$$

Let us consider also dimensionless time t and space z variables:

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

Then we obtain the following equivalent representation of the model (8)-(11):

$$\frac{\partial \theta_1}{\partial t} = -\frac{\partial \theta_1}{\partial z} + (h_0 + h_1 e^{\overline{\alpha} t})(1 - \theta_2) e^{\frac{\mu\theta_1}{1+\theta_1}} - \beta(\theta_1 - \theta_c) \tag{14}$$

$$\frac{\partial \theta_2}{\partial t} = -\frac{\partial \theta_2}{\partial z} + (l_0 + l_1 e^{\overline{\alpha} t})(1 - \theta_2) e^{\frac{\mu\theta_1}{1+\theta_1}} \tag{15}$$

where the parameters $\beta, \mu, \overline{\alpha}, l_0, l_1, h_0$ and h_1 are related to the original parameters as follows:

$$\beta = \frac{\beta_0 L}{v} \quad \mu = \frac{E}{RT_{in}}, \quad \overline{\alpha} = -\frac{\alpha L}{v} \tag{16}$$

$$l_{0,1} = \frac{k_{0,1} L}{v} \exp(-\mu), \text{ and } h_{0,1} = -\frac{\Delta H}{\rho C_p} \frac{C_{in}}{T_{in}} l_{0,1}. \tag{17}$$

The equivalent state-space description of the model (14)-(15) is given by the following time-varying semilinear infinite-dimensional system on the Hilbert space $H := L^2(0,1) \times L^2(0,1)$:

$$\begin{cases} \dot{\theta}(t) & = A_0 \theta(t) + N_0(t, \theta(t)) + B\theta_c(t) \\ \theta(0) & = \theta_0 \in D(A_0) \cap F_0 \end{cases} \tag{18}$$

where A_0 is the linear (unbounded) operator defined on its domain

$$D(A_0) := \{\theta \in H : \theta \text{ is a.c. }, \frac{d\theta}{dz} \in H \text{ and } \theta(0) = 0\} \tag{19}$$

(where a.c. means that θ is absolutely continuous) by

$$A_0\, \theta := \begin{bmatrix} -\dfrac{d.}{dz} - \beta I & 0 \\ 0 & -\dfrac{d.}{dz} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \tag{20}$$

and the nonlinear operator N_0 is defined on $[0, \infty) \times F_0$, where F_0 is the closed convex subset given by

$$F_0 := \{\theta \in H : \theta_1 \geq -1 \text{ and } 0 \leq \theta_2 \leq 1\}$$

(where the inequalities hold almost everywhere on $[0,1]$) by

$$N_0(t, \theta) := \begin{bmatrix} (h_0 + h_1 e^{-\overline{\alpha} t})(1 - \theta_2) e^{\frac{\mu\theta_1}{1+\theta_1}} \\ (l_0 + l_1 e^{-\overline{\alpha} t})(1 - \theta_2) e^{\frac{\mu\theta_1}{1+\theta_1}} \end{bmatrix}. \tag{21}$$

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

$$B_0 = \beta \begin{bmatrix} I \\ 0 \end{bmatrix}. \tag{22}$$

In terms of dimensionless variables, let us denote by $\theta_{ss} := (\theta_{1,ss}, \theta_{2,ss})^T \in H$ and $\theta_{c,ss} \in L^2[0,1]$ the equilibrium profile of the system (14)-(15).

Now we are in a position to establish a result for the existence and uniqueness of the solution of the nonautonomous equation (18).

Theorem 10. For any $\theta_0 \in D(A_0) \cap F_0$, the initial value problem (18) has a unique mild solution on $[0, \infty)$.

Proof: To prove this result it suffices to prove that the nonlinear operator N_0 is uniformly Lipshitz, whence we can apply [Pazy. , 1983, Theorem 1.2, p. 184].

3.3 Linearized Model

Now we are interested in the linearization of the nonlinear model (14)-(15) around the equilibrium profile θ_{ss}. Let us consider the state transformation

$$x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} \theta_1(t) - \theta_{1,ss} \\ \theta_2(t) - \theta_{2,ss} \end{bmatrix} \tag{23}$$

The linearization of the system (14)-(15) around the equilibrium θ_{ss} leads to the following linear time-varying infinite-dimensional system on the Hilbert space H:

$$\begin{cases} \dot{x}(t) \ = \ A(t)x(t) + Bu(t) \\ x(0) \ = \ x_0 \in H \ . \end{cases} \tag{24}$$

Here $\{A(t)\}_{t\geq 0}$ is the family of linear operators defined on their domains:

$$D(A(t)) = \{x \in H : x \text{ is a.c. }, \ \frac{dx}{dz} \in H \text{ and } x(0) = 0\} \tag{25}$$

by

$$A(t) = \begin{bmatrix} -\frac{d.}{dz} + \alpha_1(t,z)I & \alpha_2(t,z)I \\ \alpha_3(t,z)I & -\frac{d.}{dz} + \alpha_4(t,z)I \end{bmatrix}, \tag{26}$$

where the functions α_i are given by

$$\alpha_1(t,z) = -\beta + (h_0 + h_1 e^{-\overline{\alpha}t}) \frac{\mu(1-\theta_{2,ss})}{(1+\theta_{1,ss})^2} \exp\left(\frac{\mu\theta_{1,ss}}{1+\theta_{1,ss}}\right),$$

$$\alpha_2(t,z) = -(h_0 + h_1 e^{-\overline{\alpha}t}) \exp\left(\frac{\mu\theta_{1,ss}}{1+\theta_{1,ss}}\right),$$

$$\alpha_3(t,z) = (l_0 + l_1 e^{-\overline{\alpha}t}) \frac{\mu(1-\theta_{2,ss})}{(1+\theta_{1,ss})^2} \exp\left(\frac{\mu\theta_{1,ss}}{1+\theta_{1,ss}}\right)$$

and

$$\alpha_4(z) = -(l_0 + l_1 e^{-\overline{\alpha}t}) \exp\left(\frac{\mu\theta_{1,ss}}{1+\theta_{1,ss}}\right).$$

The operator B is given by (22).

Remark 11. Note that the domain of the operator $A(t)$ is independent of time.

4. TRAJECTORY AND STABILITY ANALYSIS

In this section, we are interested in the trajectory and the exponential stability of the linearized model described in the previous section. The following lemma is useful in order to prove the existence and uniqueness of the trajectory of the linearized model (24).

Lemma 12. The family of operators $\{A(t)\}_{t\geq 0}$ is a stable family of infinitesimal geneartors.

Proof: Note that the operator $A(t)$ can be written as

$$A(t) = A_0 + D(t) = \begin{bmatrix} -\frac{d.}{dz} & 0 \\ 0 & -\frac{d.}{dz} \end{bmatrix} + \begin{bmatrix} \alpha_1(t,z)I & \alpha_2(t,z)I \\ \alpha_3(t,z)I & \alpha_4(t,z)I \end{bmatrix}.$$

The operator A_0 is a stable family of infinitesimal generators and $D(t), t \geq 0$ is bounded linear operators, then, by using the perturbation theorem (Theorem 3), the operator $A(t)$ is a stable family of infinitesimal geneartors.

Theorem 13. There exists a unique evolution system $U_A(\cdot,\cdot) : \{(t,s) \in I\!R^2 : t \geq s\} \longrightarrow \mathcal{L}(H)$ such that

$$\frac{\partial}{\partial t} U_A(t,s)x = A(t)U_A(t,s)x, \ \forall x \in D(A(t)), \ 0 \leq s \leq t.$$

Moreover, there are constants $M \geq 1$ and w such that

$$\|U_A(t,s)\| \leq M e^{w(t-s)}, \ 0 \leq s \leq t.$$

Proof: By Lemma 12 $A(t)$ is a stable family of infinitesimal generators of C_0-semigroup on H. On the other hand, note that $D(A(t)$ is independent of t (Remark 11), then the rest of the proof is a consequence of Theorem 4.

Theorem 14. The family of operators $\{A(t)\}_{t\geq 0}$ generates an exponentially stable evolution system.

Proof: This result can be proved by two ways. The first one is based on the corresponding Lyapunov equation and it suffices to prove that the latter has a nonnegative solution. The second one is based on [Pazy. , 1983, Theorem 8.1, p.173].

5. OPTIMAL CONTROL DESIGN

This section deals with the computation of an LQ-optimal feedback operator for the linearized plug flow reactor model (24)-(26), (22) by using the corresponding operator Riccati equation. First let us define an output function $y(.)$ by

$$y(t) = Cx(t) := [\, w_1 I \ \ w_2 I \,]\, x(t), \quad t \geq 0, \tag{27}$$

where $w_1, w_2 : [0, \ 1] \to I\!R$ are continuous functions. In view of the definition (3) of the corresponding quadratic cost and the linearized model state definition (23), these functions can be interpreted as weighting factors for estimates of the distance between the initial model state and the chosen equilibrium profile.

It turns out that the solution of corresponding operator Riccati differential equation is based on the solution of a matrix Riccati partial differential equation.

Lemma 15. Let us consider the follwing matrix functions on $[0, \infty) \times [0, 1]$

$$M(t,z) = -\begin{bmatrix} \alpha_1(t,z) & \alpha_2(t,z) \\ \alpha_3(t,z) & \alpha_4(t,z) \end{bmatrix}, Q = \begin{bmatrix} w_1^2 & w_1 w_2 \\ w_1 w_2 & w_2^2 \end{bmatrix},$$

and $S := diag(\beta^2, 0)$ and let us consider the matrix Riccati partial differential equation:

$$\begin{aligned} \frac{\partial \Psi}{\partial t} \ &= -\frac{\partial \Psi}{\partial z} + M^*\Psi + \Psi M - Q + \Psi S \Psi, \\ \Psi(t,1) \ &= \ 0, \ t \in [0, \infty). \end{aligned} \tag{28}$$

Then the latter has a nonnegative solution on $[0,\infty)\times[0,1]$.

Proof: By using the method of characteristics, the matrix Riccati partial differential equation becomes the following matrix Riccati differential equation along the characteristics

$$\begin{aligned} \frac{d\Psi}{dr} &= M^*\Psi + \Psi M + Q - \Psi S \Psi, \\ \Psi(1) &= 0. \end{aligned} \tag{29}$$

Then by using [Aboukandil et al., , 2003, Corollary 6.7.36], it can be shown that equation (29) has a nonnegative solution.

Now we are in a position to state the following theorem.

Theorem 16. Let us consider the linearized plug flow reactor model, with control operator B given by (22) and observation operator C given by (27). Let

$$\Psi(t,z) = \begin{bmatrix} \psi_1(t,z) & \psi_2(t,z) \\ \psi_2(t,z) & \psi_3(t,z) \end{bmatrix} = \Psi^*(t,z) \geq 0 \tag{30}$$

be the nonnegative solution of the matrix partial differential equation (28). Then $Q(t) := \Psi(t,z)I$ is a nonnegative solution of the operator Riccati differential equation (7). Moreover, the optimal control is given by

$$u_{opt}(t,z) = -\beta\psi_1(t,z)x_1(t,z) - \beta\psi_2(t,z)x_2(t,z).$$

Proof: By assuming that the solution of the operator Riccati equation (7) has the form $Q(t) = \Psi(t,z)I$, it can be shown by straightforward calculation that if Ψ is a nonnegative solution of the matrix Riccati partial differential equation (28) then Q is a nonnegative solution of equation(7).

6. NUMERICAL SIMULATIONS

This section provides with numerical simulations of the nonlinear closed-loop reactor model in (8) and (9). The model parameter values used for numerical simulations are given in Table 1. The operating conditions chosen are:

$$T_{in} = 340K,\ C_{in} = 0.02mol\cdot l^{-1},\ T_c(z,t) = 400K \tag{31}$$

Table 1. Model Parameters.

Parameter	Value
v	$0.025\ m\cdot s^{-1}$
L	$1\ m$
E	$11250\ cal\cdot mol^{-1}$
k_0	$10^5\ s^{-1}$
k_1	$10^5\ s^{-1}$
R	$1.986\ cal\cdot mol^{-1}\cdot K^{-1}$
$\frac{4h}{\rho C_p d}$	$0.2\ s^{-1}$
$\frac{\Delta H}{\rho C_p}$	$-4250\ K\cdot l\cdot mol^{-1}$
α	0.1

Using the operating conditions in (31), the steady state distribution is computed (see Figure 1) to formulate the LQ-feedback controller. With the choice of weighting functions $w_1(z) = 1$ and $w_2(z) = 1$, the LQ-state feedback function in Figure 2 and Figure 3 is obtained. To implement the LQ-controller, we use 100 equally distributed points along the reactor at which the temperature is observed and the jacket temperature is adjusted.

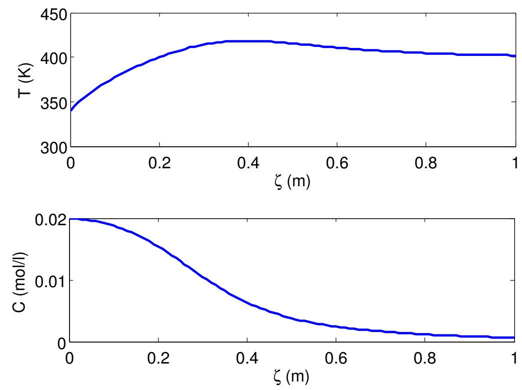

Fig. 1. Steady state profile.

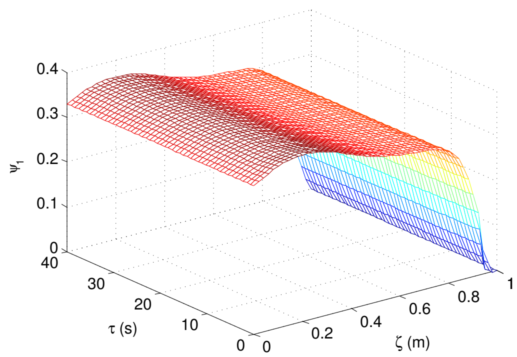

Fig. 2. LQ-feedback function Ψ_1 for $w_1(z) = 1$ and $w_2(z) = 1$.

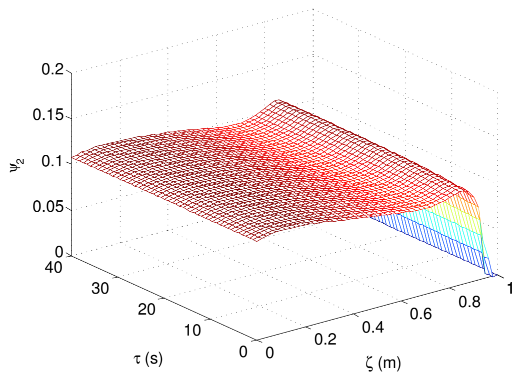

Fig. 3. LQ-feedback function Ψ_2 for $w_1(z) = 1$ and $w_2(z) = 1$.

To illustrate the control performance of the LQ controller, we set both the initial temperature and concentration profiles to the inlet temperature and concentration, respectively and we simulate the closed-loop response. The resulting fluid temperature, reactant concentration and jacket temperature along the reactor are shown in Figures 4, 5 and 6, respectively. It can be observed that the state converges numerically to the chosen equilibrium profile.

7. CONCLUDING REMARKS

In this paper, the linear quadratic optimal control problem has been studied for a plug flow tubular reactor with time-varying rate of reaction. To design the LQ-controller, some useful results on evolution systems and linear quadratic control problem for time-varying infinite dimensional sys-

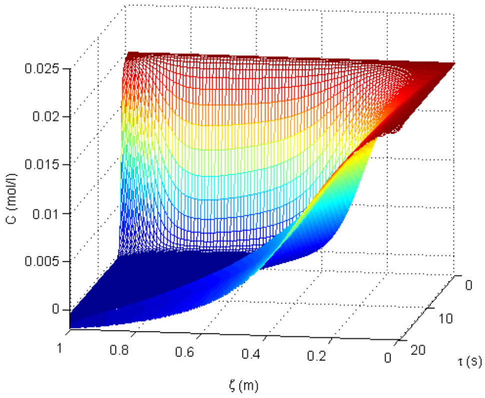

Fig. 4. Closed-loop concentration distribution.

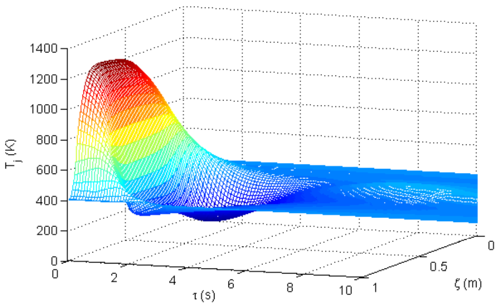

Fig. 5. Closed-loop jacket temperature distribution.

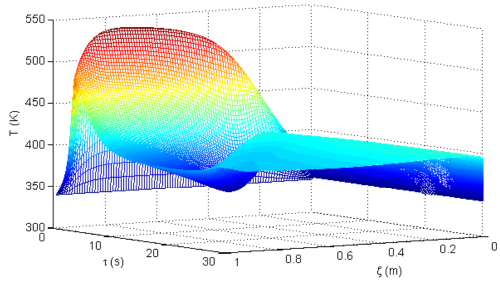

Fig. 6. Closed-loop temperature distribution.

tems have been reviewed. An LQ-control feedback has been computed by using an operator Riccati differential equation, whose solution can be obtained via a related matrix Riccati partial differential equation. The controller has been tested numerically on a nonlinear model for a plug flow reactor.

Work is continuing on stability and other controller design issues for plug flow reactor models with deactivity catalysts.

REFERENCES

H. Aboukandil, G. Freiling, V. Ionescu and G. Jank Matrix Riccati Equations in Control and Systems Theory. *Birkhauser Verlag*, Basel, 2003.

P. Acquistapace and B. Terreni Some existence and regularity results for abstract non-autonomous parabolic equations. *J. Math. Anal. Appl.*, 99, pp. 9–64, 1984.

I. Aksikas Analysis and LQ-Optimal Control of Infinite-Dimensional Semilinear Systems: Application to a Plug Flow Reactor PhD., Université Catholique de Louvain, Belgium, 2005.

I. Aksikas, J.J Winkin, and D. Dochain Optimal LQ-Feedback regulation of a nonisothermal plug flow reactor model by spectral factorization. *IEEE Transactions on Automatic Control*, Vol. 52, NO. 7, pp. 1179-1193, 2007.

A. Bensoussan, G. Da Prato, M.C. Delfour, and S.K. Mitter Representation and Control of Infinite Dimensional Systems. *Birkhauser*, Boston, 2nd edition, 2007.

F.M. Callier and J.J. Winkin LQ-Optimal control of infinite-dimensional systems by spectral factorization. *Automatica*, Vol. 28, No. 4, pp.757-770, 1992.

P.D. Christofides Nonlinear and Robust Control of Partial Differential Equation Systems: Methods and Application to Transport-Reaction Processes. *Birkhauser*, Boston, 2001.

R.F. Curtain, and H.J. Zwart An Introduction to Infinite-Dimensional Linear Systems Theory. *Springer-Verlag*, New York, 1995.

G. Da Prato, and A. Ichikawa Quadratic control for linear time-varying systems. *SIAM J. Control and Optimization*, Vol. 28, 2, pp. 359-381, 1990.

M. Laabissi, M.E. Achhab, J. Winkin and D. Dochain Trajectory analysis of nonisothermal tubular reactor nonlinear models. *System & Control Letters*, Vol. 42, pp. 169-184, 2001.

Z. Luo, B. Guo, and O. Morgul Stability and Stabilization of Infinite-Dimensional Systems with Applications. *Springer*, London, 1999.

L. Pandolfi Existence of solutions to the Riccati equation for time-varying distributed systems. *IMA Journal of Mathematical Control & Information*, Vol. 9, pp. 265-273, 1992.

A. Pazy Semigroup of Linear Operators and Application to Partial Diferential Equations. *Springer-Verlag*, New York, 1983.

V. Ngoc Phat Stabilization of linear continuous time-varying systems with state delays in Hilbert spaces. *Electronic Journal of Differential Equations*, Vol. 2001, No. 67, pp.1-13, 2001.

H. Tanabe Equations of Evolution. *Pitman*, London, 1979; English Transl., Iwanami, Tokyo, 1975.

J. Winkin, D. Dochain, and P. Ligarius Dynamical analysis of distributed parameter tubular reactors. *Automatica*, Vol. 36, pp. 349–361, 1998.