Preprints of the 19th World Congress
The International Federation of Automatic Control
Cape Town, South Africa. August 24-29, 2014

Boundary optimal control of coupled parabolic PDE-ODE systems

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Abstract: This paper deals with boundary optimal control problem for coupled parabolic PDE-ODE systems. The problem is studied using infinite-dimensional state space representation of the coupled PDE-ODE system. Linearization of the non-linear system is established around a steady state profile. Using some state transformations, the linearized system is formulated as a well-posed infinite-dimensional system with bounded input and output operators. It has been shown that the resulting system is a Riesz Spectral system. The LQ-control problem is studied on the basis of the solution of the corresponding eigenvalues problem. The results have been applied to the case study of catalytic cracking reactor with catalyst deactivation. Numerical simulations are performed to illustrate the performances of the developed controller.

1. INTRODUCTION

Many chemical and biochemical processes are modelled by coupled parabolic PDEs and ODEs. Two types of coupling can exist between PDEs and ODEs. The first one arises through the boundary conditions of the distributed portion of the process. Indeed, the boundary conditions are functions of the state variables of the lumped parameter system. A tubular reactor and a well mixed reactor in series is a simple example for this coupling. These kind of systems are called cascaded PDE-ODE systems and their control was the subject of few recent studies (Krstic [2009], Susto and Krstic [2010]). The second type of coupling takes place in the domain of the PDE, which means the parameters of the distributed part (e.g., the coefficients) are functions of the states of the lumped parameter system. Examples of this kind of coupling include catalytic reactor with catalyst deactivation, where the deactivation kinetics is described by a set of ODEs, or a heat exchanger with a time varying heat transfer coefficient. Most biochemical processes are also modelled by a set of coupled PDE-ODE with in-domain coupling (e.g., in-situ bioremediation).

In this work, we are interested in the boundary control of a system described by a set of nonlinear parabolic PDEs and ODEs using the infinite dimensional state space description. To the best of authors knowledge, there is no published work on the infinite dimensional optimal control of coupled parabolic PDEs-ODEs with in-domain coupling and this work is the first step on the study of infinite dimensional optimal controller for these systems. In Mohammadi et al. [2011, 2012], the control problem for parabolic PDEs with spatially varying coefficients has been studied and the corresponding Riccati equation has been solved by using the eigenvalues and eigenfunctions of the system generator. Here, the previous work is extended to the case of coupled parabolic PDEs and ODEs. Note that control problem of hyperbolic PDEs has been treated in Aksikas et al. [2008] for time-invariant case and in Aksikas et al. [2009] for time-varying case.

The paper is organized as follows. Section 2 focuses on the mathematical description of the system of interest. The nonlinear system is to be linearized around a steady state profile. Some state transformations are used to write the linearized system as a well posed infinite-dimensional system. In section 3, the eigenvalues problem is solved by adopting the method used for the heat equation of composite media (de. Monte [2002]). The generation and stabilizability properties are the focus of Section 4. Some necessary and sufficient conditions are given to guarantee the β-stabilizability of the system. Section 5 deals with the linear quadratic problem. By using the system spectral properties, the operator Riccati equation is converted to a set of coupled algebraic equations which can be solved numerically. In Section 6, we consider the case study of a tubular reactor wherein the Van de Vusse reaction takes place. This reaction scheme consists of two series parallel reactions. The mass balance for the reactor results in a set of coupled nonlinear parabolic PDEs, in particular a triangular operator. It is also assumed that the parameters of the reactive term are modelled by a set of ODEs which represent the deactivation kinetics.

2. MATHEMATICAL MODEL DESCRIPTION

Let us consider the following set of quasi-linear parabolic PDEs coupled (in-domain) with a set of nonlinear ODEs:

$$\begin{cases} \dfrac{\partial z}{\partial t} = \mathbf{D}_0 \dfrac{\partial^2 z}{\partial \xi^2} - \mathbf{V}\dfrac{\partial z}{\partial \xi} + \mathbf{F}(k, z) \\ \dfrac{dk}{dt} = g(k) \end{cases} \tag{1}$$

with the following initial and boundary conditions

$$\mathbf{D}_0 \frac{\partial z}{\partial \xi}|_{\xi=0} = \mathbf{V}(z_{|_{\xi=0}} - z_{in}) \qquad \text{and} \qquad \frac{\partial z}{\partial \xi}|_{\xi=l} = 0$$
$$z(\xi, 0) = z_0 \qquad \text{and} \qquad k(0) = k_0 \tag{2}$$

where $z(.,t) = \left[z_1(.,t) \cdots z_n(.,t) \right]^T \in \mathcal{H} := L^2(0,l)^n$ denotes the vector of state variables of the distributed parameter portion, $k = \left[k_1(t) \cdots k_m(t) \right]^T \in \mathcal{K} := \mathbb{R}^m$ denotes the vector of state variables for the lumped parameter portion of the model. $\xi \in [0,l] \in \mathbb{R}$ and $t \in [0,\infty)$ denote position and time, respectively. $\mathbf{D}_0$ and $\mathbf{V}$ are matrices of appropriate sizes. $\mathbf{F}$ is a Lipschitz continuous nonlinear operator from $\mathcal{H} \oplus \mathcal{K}$ into $\mathcal{H}$. g is a vector of appropriate size whose entries are functions defined in $\mathbb{R}$.

In a catalytic reactor, $\mathbf{F}$ represents the reaction terms and g represents the deactivation kinetics.

The nonlinear system (1)-(2) can be linearized around the steady state profile and the resulting linear system is:

$$\frac{\partial \tilde{z}}{\partial t} = \mathbf{D}_0 \frac{\partial^2 \tilde{z}}{\partial \xi^2} - \mathbf{V}\frac{\partial \tilde{z}}{\partial \xi} + \mathbf{N}_1(\xi)\tilde{z} + \mathbf{N}_2(\xi)\tilde{k} \tag{3a}$$

$$\frac{d\tilde{k}}{dt} = \mathbf{M}_0 \tilde{k} \tag{3b}$$

where $\tilde{z}$ and $\tilde{k}$ are the state variables in deviation form and $\mathbf{N}_1, \mathbf{N}_2$ and $\mathbf{M}_0$ are the Jacobians of the nonlinear terms evaluated at the steady state.

$$\mathbf{N}_1(\xi) = \frac{\partial \mathbf{F}(k,z)}{\partial z}|_{ss}, \mathbf{N}_2(\xi) = \frac{\partial \mathbf{F}(k,z)}{\partial k}|_{ss} \text{ and } \mathbf{M}_0 = \frac{dg}{dk}|_{ss}.$$

The equation (3a) is of type diffusion-convection-reaction PDE. In view of solving the eigenvalues problem, it is much easier to convert the equation to a diffusion-reaction type. In order to do so, let us consider the following transformation

$$\theta = \mathbf{T}\tilde{z} = \exp\left(-\frac{\mathbf{D}_0^{-1}\mathbf{V}}{2}\xi \right)\tilde{z} \tag{4}$$

The resulting system is:

$$\frac{\partial \theta}{\partial t} = \mathbf{D}\frac{\partial^2 \theta}{\partial \xi^2} + \mathbf{M}_1(\xi)\theta + \mathbf{M}_2(\xi)\tilde{k} \tag{5a}$$

$$\frac{d\tilde{k}}{dt} = \mathbf{M}_0 \tilde{k} \tag{5b}$$

where

$$\mathbf{M}_1(\xi) = \mathbf{T}\left[\mathbf{N}_1(\xi) - \frac{1}{4}\mathbf{V}\mathbf{D}_0^{-1}\mathbf{V} \right]\mathbf{T}^{-1}$$

and

$$\mathbf{M}_2(\xi) = \mathbf{T}\mathbf{N}_2(\xi), \quad \mathbf{D} = \mathbf{T}\mathbf{D}_0\mathbf{T}^{-1}$$

Let us put $u = \mathbf{V}\tilde{x}_{in}$ and define a new state vector

$$x = \begin{bmatrix} x_d \\ x_l \end{bmatrix} := \begin{bmatrix} \theta \\ \tilde{k} \end{bmatrix} \tag{6}$$

Now, we are in a position to formulate the system (5) as an abstract boundary control problem on the infinite-dimensional space $H = \mathcal{H} \oplus \mathcal{K}$ given by

$$\begin{cases} \dot{x}(t) = \mathfrak{A}x(t), x(0) = x_0 \\ \mathfrak{B}x(t) = u(t) \\ y(t) = \mathfrak{C}x(t) \end{cases} \tag{7}$$

where $\mathfrak{A}$ is a linear operator defined on the domain

$$\mathcal{D}(\mathfrak{A}) = \{x \in H : x_d \text{ and } \frac{dx_d}{d\xi} \text{ are absolutely continuous,}$$

$$\frac{d^2x_d}{d\xi^2} \in \mathcal{H}, \quad \mathbf{D}\frac{dx_d}{d\xi}_{|\xi=l} = -\frac{\mathbf{V}}{2}x_{d|\xi=l}\} \tag{8}$$

and is given by

$$\mathfrak{A} = \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\frac{d^2 .}{d\xi^2} + \begin{bmatrix} \mathbf{M}_1 & \mathbf{M}_2 \\ \mathbf{0} & \mathbf{M}_0 \end{bmatrix} \cdot I := \begin{bmatrix} \mathfrak{A}_{11} & \mathfrak{A}_{12} \\ 0 & \mathfrak{A}_{22} \end{bmatrix} \tag{9}$$

The boundary operator $\mathfrak{B} : H \to U := \mathbb{R}^n$ is given by

$$\mathfrak{B}x(.) = \left[-\mathbf{D}\frac{\partial \cdot}{\partial \xi} + \frac{\mathbf{V}}{2}\cdot \middle| 0 \right]\left[\frac{x_d}{x_l} \right]_{\xi=0} \tag{10}$$

Since $\mathbf{M}_2$ in Equation (9) is generally non-zero, x_d and x_l are coupled. By introducing the following transformation, the system can be transformed to decoupled subsystems:

$$\Lambda = \left[\begin{array}{c|c} I & J \\ \hline 0 & I \end{array} \right] \in \mathcal{L}(H) \quad \& \quad \hat{x} = \Lambda x \tag{11}$$

The operator $\mathfrak{A}$ will be transformed to

$$\hat{\mathfrak{A}} = \Lambda\mathfrak{A}\Lambda^{-1} = \left[\begin{array}{c|c} \mathfrak{A}_{11} & -\mathfrak{A}_{11}J + \mathfrak{A}_{12} + J\mathfrak{A}_{22} \\ 0 & \mathfrak{A}_{22} \end{array} \right] \tag{12}$$

with $\mathcal{D}(\hat{\mathfrak{A}}) = \mathcal{D}(\mathfrak{A})$. Therefore, if there exists a J that satisfies the following equation, operator $\hat{\mathfrak{A}}$ will be decoupled.

$$-\mathfrak{A}_{11}J + \mathfrak{A}_{12} + J\mathfrak{A}_{22} = 0 \tag{13}$$

Remark: The Equation (13) is a Sylvester equation and admits a unique solution if and only if $\sigma(-\mathfrak{A}_{11}) \cap \sigma(\mathfrak{A}_{22}) = \emptyset$. Laub [2005] . The solution is given by

$$J = \int_0^\infty T_{11}(t)\mathfrak{A}_{12}T_{12}(t)dt \tag{14}$$

where T_{11} and T_{22} are C_0-semigroups generated by $-\mathfrak{A}_{11}$ and $\mathfrak{A}_{22}$, respectively (see Emirsajlow [1999]).

The resulting decoupled system is given by

$$\begin{cases} \dot{\hat{x}}(t) = \hat{\mathfrak{A}}\hat{x}(t), \quad \hat{x}(0) = \hat{x}_0 \\ \hat{\mathfrak{B}}\hat{x}(t) = u(t) \\ y(t) = \hat{\mathfrak{C}}\hat{x}(t) \end{cases} \tag{15}$$

where $\hat{\mathfrak{B}} = \mathfrak{B}\Lambda^{-1}$ and $\hat{\mathfrak{C}} = \mathfrak{C}\Lambda^{-1}$.

System (15) is in the form of a standard abstract boundary control problem, then by following a similar approach to Mohammadi et al. [2011, 2012] it can be converted to a well-posed infinite dimensional system with bounded input and output operators. The procedure is given below.
Define a new operator $\mathcal{A}$ by

$$\mathcal{A}\hat{x} = \hat{\mathfrak{A}}\hat{x}$$

$$\mathcal{D}(\mathcal{A}) = \mathcal{D}(\hat{\mathfrak{A}}) \cap \ker(\hat{\mathfrak{B}})$$

$$= \{\hat{x} \in H : \hat{x} \text{ and } \frac{d\hat{x}}{d\xi} \text{ are a.c.}, \frac{d^2\hat{x}}{d\xi^2} \in H$$

$$\text{and } \mathbf{D}\frac{d\hat{x}_d}{d\xi}|_{\xi=0} = \frac{\mathbf{V}}{2}\hat{x}_d|_{\xi=0}, \mathbf{D}\frac{d\hat{x}_d}{d\xi}|_{\xi=l} = -\frac{\mathbf{V}}{2}x_d|_{\xi=l}\} \tag{16}$$

If $\mathcal{A}$ generates a C_0-semigroup on H and there exists a B such that the following condition holds:

$$Bu \in \mathcal{D}(\hat{\mathfrak{A}}) \quad \text{and} \quad \forall u \in U, \, \hat{\mathfrak{B}}Bu = u, \tag{17}$$

then system (15) can be transformed into the following infinite dimensional system with bounded input operator on the state space $H^e = H \oplus U$

$$\begin{cases} \dot{x}^e(t) = A^e x^e(t) + B^e \tilde{u}(t) \\ y^e(t) = C^e x^e(t) \end{cases} \tag{18}$$

where

$$A^e = \begin{bmatrix} 0 & 0 \\ \hat{\mathfrak{A}}B & \mathcal{A} \end{bmatrix}, \quad B^e = \begin{bmatrix} I \\ -B \end{bmatrix}, \quad C^e = \mathfrak{C}\left[B \;\; I \right] \tag{19}$$

and $\tilde{u}(t) = \dot{u}(t)$ and $x^e(t) = \left[\, u(t) \quad \hat{x}(t) - Bu(t) \,\right]^T$ are the new input and state variables.

Remark: Consider $\tilde{B} = \Lambda^{-1}B$, then the condition (17) becomes $\tilde{B}u \in \mathcal{D}(\hat{\mathfrak{A}})$ and $\mathfrak{B}\tilde{B}u = u$.

One can assume that $\tilde{B} = \left[\, B_d | B_l \,\right]^T$, then the following conditions are equivalent to (17)

$$\begin{aligned} &\mathbf{D}\frac{dB_d(0)}{d\xi} - \frac{\mathbf{V}}{2}B_d(0) = I \\ &\mathbf{D}\frac{dB_d(l)}{d\xi} + \frac{\mathbf{V}}{2}B_d(l) = 0 \\ &B_l \in \mathcal{K} \end{aligned} \tag{20}$$

B_d can be any function that satisfies the above conditions. For simplicity one can assume that B_d is a matrix of polynomials. B_l is any arbitrary matrix in $\mathcal{K}$. Finally B can be calculated by

$$B = \Lambda\tilde{B} = \begin{bmatrix} B_d + JB_l \\ B_l \end{bmatrix} \tag{21}$$

The infinite dimensional system (18) is in the form of a standard infinite dimensional system and now we are in the position to proceed with dynamical properties and optimal control design for this system. It should be mentioned that, since all of the transformations introduced in this section are exact and there was no approximation involved, all of the dynamical properties of the original linearized system are preserved. Hence, we can perform analysis and controller formulation on the transformed system (18), and then apply the designed controller to the original system. In order to study the dynamical properties and solve the control problem, we need to solve the eigenvalues problem for the system (18).

3. EIGENVALUES PROBLEM

In this section, the solution of the eigenvalues problem that was introduced in Mohammadi et al. [2011, 2012] is extended to the case of coupled PDE-ODE systems. There is no general algorithm for analytical solution of eigenvalues problem for a general form of parabolic operator. Therefore, in this section we will consider the following assumptions:

(1) $\mathbf{N}_1$ in (3a) is lower triangular, which leads to lower triangular form of $\mathfrak{A}_{11}$. In most chemical engineering processes, one can use a transformation to triangularize the system.
(2) The number of state variables in (3a) is two. Extension to more than two variables is straightforward.
(3) Assume that $\mathbf{M}_0$ is diagonalizable. Then without loss of generality, we can assume that $\mathbf{M}_0$ is diagonal.

Then the eigenvalue problem of interest will be:

$$A^e\phi = \lambda\phi \tag{22}$$

where A^e is given by (19) and

$$\begin{aligned} &\mathcal{A} = diag(\mathcal{A}_{11}, \mathcal{A}_{22}) \\ &\mathcal{A}_{11} := \begin{bmatrix} F_{11} & 0 \\ F_{21} & F_{22} \end{bmatrix} = \begin{bmatrix} d_{11}\dfrac{d^2}{d\xi^2} + h_{11} & 0 \\ h_{21} & d_{22}\dfrac{d^2}{d\xi^2} + h_{22} \end{bmatrix} \\ &\mathcal{A}_{22} = diag(\alpha_{11}, \alpha_{22}) \end{aligned} \tag{23}$$

3.1 Eigenvalues and Eigenfunctions of $\mathcal{A}$

The operator $\mathcal{A}$ is a block diagonal operator, therefore $\sigma(\mathcal{A}) = \sigma(\mathcal{A}_{11}) \cup \sigma(\mathcal{A}_{22})$. Since $\mathcal{A}_{11}$ is a lower triangular operator $\sigma(\mathcal{A}_{11}) = \sigma(F_{11}) \cup \sigma(F_{22})$. Then, $\sigma(\mathcal{A}) = \sigma(F_{11}) \cup \sigma(F_{22}) \cup \sigma(\mathcal{A}_{22})$. Observe that F_{11} and F_{22} have the same following form:

$$d\frac{d^2}{d\xi^2} + h(\xi) \cdot I$$

Since h depend on the space variable ξ, then calculation of the spectrum is a challenging issue. In Mohammadi et al. [2012], the spectrum is calculated by dividing the space interval into finite number N of subintervals $[\xi_{i-1}, \xi_i]$, in which it is assumed that the values of h are constant, denoted by h_i. Let λ_n and χ_n be eigenvalues and eigenfunctions of the operator F_{11} and μ_n and ψ_n be eigenvalues and eigenfunctions of the operator F_{22}. Then according to Mohammadi et al. [2012], the eigenvalues of the operator $\mathcal{A}_{11}$ are

$$\sigma(\mathcal{A}_{11}) = \sigma(F_{11}) \cup \sigma(F_{22}) = \{\lambda_n, \mu_n,\ n = 1, \cdots, \infty\} \tag{24}$$

and the associated eigenfunctions are:

$$\left\{ \begin{bmatrix} \chi_n \\ (\lambda_n I - \mathcal{A}_{22})^{-1}\mathcal{A}_{21}\chi_n \end{bmatrix}, \begin{bmatrix} 0 \\ \psi_n \end{bmatrix} \right\} \quad n = 1, \cdots, \infty \tag{25}$$

The corresponding bi-orthonormal eigenfunctions can be computed by solving the eigenvalue problem for $\mathcal{A}_{11}^*$ and are given by:

$$\left\{ \begin{bmatrix} \chi_n \\ 0 \end{bmatrix}, \begin{bmatrix} (\mu_n I - \mathcal{A}_{11})^{-1}\mathcal{A}_{21}\psi_n \\ \psi_n \end{bmatrix} \right\} \quad n = 1, \cdots, \infty \tag{26}$$

$\mathcal{A}_{22}$ is a diagonal matrix and its eigenvalues are $\{\alpha_{11}, \alpha_{22}\}$ with the associated eigenvectors $\{[1,0]^T, [0,1]^T\}$. Finally:

$$\sigma(\mathcal{A}) = \{\lambda_n, \mu_n, \alpha_{11}, \alpha_{22}\} \quad n = 1, \cdots, \infty \tag{27}$$

and the associated eigenfunctions are

$$\left\{ \begin{bmatrix} \chi_n \\ (\lambda_n I - \mathcal{A}_{22})^{-1}\mathcal{A}_{21}\chi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \psi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\} \tag{28}$$

The corresponding bi-orthonormal eigenfunctions are

$$\left\{ \begin{bmatrix} \chi_n \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} (\mu_n I - \mathcal{A}_{11})^{-1}\mathcal{A}_{21}\psi_n \\ \psi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\} \tag{29}$$

3.2 Eigenvalues and Eigenfunctions of A^e

Assume that the operator $\mathcal{A}$ has eigenvalues $\{\sigma_k, k \geq 1\}$ and biorthonormal pair $\{(\phi_k, \psi_k), k \geq 1\}$. The spectrum of the operator A^e is given by $\sigma(A^e) = \sigma(\mathcal{A}) \cup \{0\}$ and $\lambda_0 = 0$ has a multiplicity of m, where m is the number of manipulated variables. The corresponding eigenfunctions for λ_0 are given for $i = 1, \cdots, m$ by

$$\Phi_0^i = \begin{bmatrix} e_i \\ -\mathcal{A}^{-1}(\hat{\mathfrak{A}}B) \end{bmatrix} = \begin{bmatrix} e_i \\ \sum_{k=0}^{\infty} \frac{1}{\sigma_k} \langle \hat{\mathfrak{A}}B, \psi_k \rangle \phi_k \end{bmatrix}, \quad (30)$$

where $e_i, i = 1, \cdots, m$ is the orthonormal basis for $U = \mathbb{R}^n$. The corresponding bi-orthonormal eigenfunctions of A^e are

$$\Psi_0^i = \begin{bmatrix} e_i \\ 0 \end{bmatrix}, \quad i = 1, \cdots, m \quad (31)$$

For $\lambda \in \sigma(\mathcal{A})$, the associated bi-orthonormal pair are

$$\Phi_n = \begin{bmatrix} 0 \\ \phi_n \end{bmatrix} \quad \& \quad \Psi_n = \begin{bmatrix} \frac{1}{\sigma_n} (\hat{\mathfrak{A}}B)^* \psi_n \\ \psi_n \end{bmatrix} \quad (32)$$

4. SYSTEM PROPERTIES

In this section, we will investigate the generation and stabilizability properties of the extended system. Let us start by the generation property.

Theorem 1. Consider the operator $\mathcal{A}$ given by Equation (23). Then $\mathcal{A}$ is the infinitesimal generator of a C_0-semigroup on H. Consequently, the operator A^e given by Equation (18) is an infinitesimal generator of C_0-semigroup on H^e.

The next theorem gives a necessary and sufficient condition for the extended system to be β-exponentially stablizable.

Theorem 2. Consider the linear system $\sum(A^e, B^e, C^e)$ given by Equation (18). Assume that B is a finite rank operator defined by

$$Bu = \sum_{i=1}^{m} b_i u_i$$

A necessary and sufficient condition for $\sum(A^e, B^e, -)$ to be β-exponentially stabilizable is that for all n such that $\lambda_n \in \sigma_\beta^+(A)$

$$\operatorname{rank} \begin{pmatrix} \langle b_1, \psi_{n_1} \rangle & \cdots & \langle b_m, \psi_{n_1} \rangle \\ \vdots & & \vdots \\ \langle b_1, \psi_{n_{rn}} \rangle & \cdots & \langle b_m, \psi_{n_{rn}} \rangle \end{pmatrix} = r_n \quad (33)$$

where r_n is the multiplicity of the eigenvalue λ_n.

5. LQ CONTROL OF PDE-ODE SYSTEMS

This section deals with the design of linear quadratic (LQ) state feedback optimal controller for the infinite dimensional system (18)-(19). The aim is to minimize the quadratic cost function:

$$\mathbf{J}(\tilde{u}) = \int_0^\infty \langle y^e(s), y^e(s) \rangle + \langle \tilde{u}(s), R\tilde{u}(s) \rangle ds \quad (34)$$

where $R = R_0 \cdot I$ and R_0 is a self-adjoint positive matrix. It is known that the solution of this optimal control problem can be obtained by solving the following algebraic Riccati equation (ARE) (Curtain and Zwart [1995]):

$$\begin{aligned} \langle A^e x_1, \Pi x_2 \rangle + \langle \Pi x_1, A^e x_2 \rangle + \langle C^e x_1, C^e x_2 \rangle \\ - \langle B^{e^*} \Pi x_1, R^{-1} B^{e^*} \Pi x_2 \rangle = 0 \end{aligned} \quad (35)$$

When (A^e, B^e) is exponentially stabilizable and (C^e, A^e) is exponentially detectable, the algebraic Riccati Equation (35) has a unique non-negative self-adjoint solution $\Pi \in \mathcal{L}(H^e)$ and for any initial state $x_0 \in H^e$ the quadratic cost is minimized by the optimal control u_o given by

$$u_o(s) = -R^{-1} B^{e^*} \Pi x(s). \quad (36)$$

Let us set $x_1 = \Phi_m$ and $x_2 = \Phi_n$ and assume that $\Pi_{nm} = \langle \Phi_n, \Pi \Phi_m \rangle$. Therefore the solution of the optimal control problem for this system can also be found by solving the set of algebraic equations given by:

$$(\sigma_n + \sigma_m)\Pi_{nm} + C_{nm} - \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \Pi_{nk} \Pi_{lm} B_{nm} = 0 \quad (37)$$

where

$C_{nm} = \langle C^e \Phi_n, C^e \Phi_m \rangle$, and $B_{nm} = \langle R^{-1} B^e \Psi_n, B^e \Psi_m \rangle$.

6. CASE STUDY: CRACKING REACTOR

In this section, the proposed approach is applied to a catalytic cracking reactor with the assumption that the catalyst deactivates with time.

6.1 Model description

The reaction scheme is given by Equations

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \quad \text{and} \quad A \xrightarrow{k_3} C \quad (38)$$

with the kinetic equations given by

$$r_A = -(k_1 + k_3) y_A^2 = -k_0 y_A^2 \quad \text{and} \quad r_B = k_1 y_A^2 - k_2 y_B$$

It is assumed that the catalyst deactivation will only affect the pre-exponential factor of the main reaction, and k_1 will be modelled by

$$\frac{dk_1}{dt} = \alpha k_1 + \beta, \qquad k_1(0) = k_{1_0} \quad (39)$$

The above equation for the rate of deactivation of the catalyst, is equivalent to the exponential decay assumption, which is a common assumption for modelling catalyst deactivation. It is in agreement with the observation that the catalyst deactivation consists of three phases: rapid initial deactivation, slow deactivation and stabilization (Kallinikos et al. [2008]). The model of the reactor will be:

$$\begin{aligned} \frac{\partial y_A}{\partial t} &= D_a \frac{\partial^2 y_A}{\partial \xi^2} - v \frac{\partial y_A}{\partial \xi} + r_A, \\ \frac{\partial y_B}{\partial t} &= D_a \frac{\partial^2 y_B}{\partial \xi^2} - v \frac{\partial y_B}{\partial \xi} + r_B, \\ \frac{dk_1}{dt} &= \alpha k_1 + \beta \end{aligned} \quad (40)$$

Initial and boundary conditions are:

$$\begin{aligned} & D_a \frac{\partial y_A}{\partial \xi}|_{\xi=0} = v(y_A|_{\xi=0} - y_{A_{in}}), \\ & D_a \frac{\partial y_B}{\partial \xi}|_{\xi=0} = v(y_B|_{\xi=0} - y_{B_{in}}), \\ & \frac{\partial y_A}{\partial \xi}|_{\xi=l} = 0, \frac{\partial y_B}{\partial \xi}|_{\xi=l} = 0, \\ & y_A(\xi, 0) = y_{A_0}(\xi), y_B(\xi, 0) = y_{B_0}(\xi), \text{ and } k_1(0) = k_{1_0} \end{aligned} \quad (41)$$

By defining the new state and input variables

$$\theta(t) = \begin{bmatrix} y_A - y_{A_{ss}} \\ y_B - y_{B_{ss}} \\ k_1 - k_{1_{ss}} \end{bmatrix}, \quad u(t) = v(y_{A_{in}} - y_{A_{in,ss}}) \quad (42)$$

the set of equations (40) can be linearized and then converted to a diffusion-reaction system by using the transformation given in Equation (4).

The infinite dimensional representation of the linearized system on the Hilbert space H has the form (7), where the operator $\mathfrak{A}$ is given by:

$$\mathfrak{A} = \left[\begin{array}{cc|c} D_a \dfrac{\partial^2}{\partial \xi^2} - \hat{k}_1(\xi) & 0 & -y^2_{A_{ss}} \\ 2k_{1_{ss}} y_{A_{ss}}(\xi) & D_a \dfrac{\partial^2}{\partial \xi^2} - \hat{k}_2 & y^2_{A_{ss}} \\ \hline 0 & 0 & \alpha \end{array}\right] \tag{43}$$

$$\begin{aligned} \mathcal{D}(\mathfrak{A}) = \{ x \in H : x \text{ and } \frac{dx}{d\xi} \text{ are a.c.}, \frac{dx^2}{d\xi^2} \in H, \\ D_a \frac{dx_1}{d\xi}|_{\xi=l} = -\frac{v}{2} x_1|_{x=l}, \\ D_a \frac{dx_2}{d\xi}|_{\xi=l} = -\frac{v}{2} x_2|_{x=l}, D_a \frac{dx_1}{d\xi}|_{\xi=0} = \frac{v}{2} x_1|_{x=0} \} \end{aligned} \tag{44}$$

and the boundary operator $\mathfrak{B}$ by

$$\mathfrak{B}x(.) = \left[-D_a \frac{\partial}{\partial \xi} + \frac{v}{2} \;\; 0 \middle| 0 \right] \left[\begin{array}{c} x_1 \\ x_2 \\ \hline x_3 \end{array}\right]_{\xi=0} \tag{45}$$

Assuming that, the control variable is x_2, the output operator $\mathfrak{C}$ is:

$$\mathfrak{C} = \mathfrak{C}_0 I = [\, 0 \;\; 1 | 0 \,] \tag{46}$$

By performing the transformation (11), the operator $\mathfrak{A}$ can be converted to a block diagonal form and the decoupled infinite dimensional system (15) will be computed. Using Equation (14), the operator J in Equation (11) is

$$J = \int_0^\infty \mathfrak{T}_{11}(t) \mathfrak{A}_{12} \mathfrak{T}_{22} \tag{47}$$

$\mathfrak{T}_{11}$ and $\mathfrak{T}_{22}$ are the C_0-semigroups generated by $-\mathfrak{A}_{11}$ and $\mathfrak{A}_{22}$. The operators $\mathfrak{A}_{11}, \mathfrak{A}_{22}$ and $\mathfrak{A}_{12}$ are given by

$$\begin{aligned} \mathfrak{A}_{11} &= \begin{bmatrix} D_a \dfrac{\partial^2}{\partial \xi^2} - \hat{k}_1(\xi) & 0 \\ 2k_{1_{ss}} y_{A_{ss}}(z) & D_a \dfrac{\partial^2}{\partial \xi^2} - \hat{k}_2 \end{bmatrix}, \\ \mathfrak{A}_{12} &= \begin{bmatrix} -y^2_{A_{ss}} \\ y^2_{A_{ss}} \end{bmatrix}, \quad \mathfrak{A}_{22} = [\, \alpha \,] \end{aligned} \tag{48}$$

By defining $\hat{\mathfrak{A}} = \Lambda \mathfrak{A} \Lambda^{-1}, \hat{\mathfrak{B}} = \mathfrak{B} \Lambda^{-1}$ and $\hat{\mathfrak{C}} = \mathfrak{C} \Lambda^{-1}$, the decoupled abstract boundary control problem becomes:

$$\begin{cases} \dfrac{d\hat{x}(t)}{dt} = \hat{\mathfrak{A}} \hat{x}(t), \; \hat{x}(0) = \hat{x}_0 \\ \hat{\mathfrak{B}} \hat{x}(t) = u(t) \\ y(t) = \hat{\mathfrak{C}} \hat{x}(t) \end{cases} \tag{49}$$

The abstract boundary control problem (49), can be converted to a well-posed infinite dimensional system with bounded input and output operators using Equations (16)-(19). In the Equation (19), B can be calculated using the discussion in Remark 2. Since $\tilde{B}$ is any arbitrary function that satisfies conditions (20), we assume that $B_d = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}$ and B_1 and B_2 are both second order polynomials. Using the conditions (20), B_1 and B_2 are:

$$B_1 = \frac{-2}{4D_a l + vl^2} \xi^2 + \frac{2}{v} \tag{50}$$

$$B_2 = -\frac{1}{4D_a l + vl^2} \xi^2 + \frac{1}{4D_a + vl} \xi + \frac{2D_a}{4D_a v + v^2 l} \tag{51}$$

B_l is any arbitrary number in $\mathbb{R}$ and we assume that $B_l = 1$. Finally B becomes:

$$B = \begin{bmatrix} B_1 + J_1 B_l \\ B_2 + J_2 B_l \\ B_l \end{bmatrix} \tag{52}$$

7. NUMERICAL SIMULATIONS

In this section the performance of the proposed approach is demonstrated. The LQ controller discussed in the previous section was studied via a simulation that used a nonlinear model of the reactor given in Equations (40)-(41). Values of the model parameters can be found in Weekman [1969].

The control objective is to regulate the trajectory of y_B at the desired steady state profile. Deactivation of catalyst has a negative impact on y_B and our objective is to calculate the optimal values of inlet y_A to keep trajectory of y_B at the desired profile and eliminate the effect of deactivation. Using the nominal operating conditions, and the model given in Equations (40)-(41), the steady-state profiles of y_A and y_B were computed. Then, the nonlinear model was linearized around the stationary states and transformed to the self-adjoint form of Equations (39)-(41). Spectra of operators A_{11} and A_{22} were calculated using the algorithm discussed in §3. In order to compute the spectrum of A_{11}, it was assumed that the length of the reactor is divided into 50 equally-spaced sections and the coefficient of the reaction term is constant in each section. First five eigenvalues of the operator A_{11} are:

$$\begin{aligned} \lambda = \{ &-2.39 \times 10^{-5}, -1.34 \times 10^{-4}, -4.46 \times 10^{-4}, \\ &-1.12 \times 10^{-3}, -2.35 \times 10^{-3} \} \end{aligned}$$

First five eigenvalues of A_{22} are:

$$\begin{aligned} \lambda = \{ &-2.04 \times 10^{-6}, -1.096 \times 10^{-5}, -5.68 \times 10^{-5}, \\ &-2.08 \times 10^{-4}, -5.78 \times 10^{-4} \} \end{aligned}$$

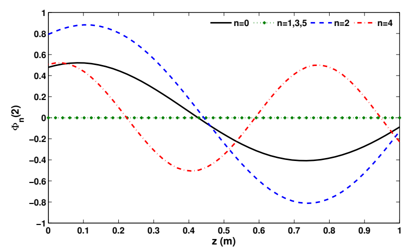

Fig. 1. Second element of $\hat{\phi}_n$

Finally, the spectrum of A^e was computed using Equations (30)-(32). The first six eigenvalues of A^e is:

$$\begin{aligned} \sigma(A^e) = \{ &0, -0.001, -2.39 \times 10^{-5}, -2.04 \times 10^{-6}, \\ &-1.34 \times 10^{-4}, -1.096 \times 10^{-5} \} \end{aligned} \tag{53}$$

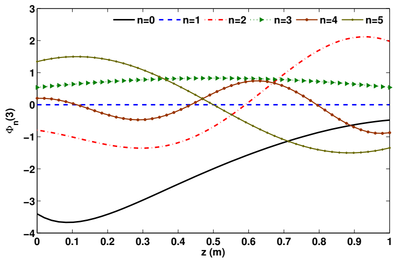

Fig. 2. Third element of $\hat{\phi}_n$

and the associated eigenfunctions are shown in Figures 1-2. Once the eigenvalues and eigenfunctions of the operator A^e are calculated, the LQ-feedback controller can be computed using Equation (37). Note that since Π is a self-adjoint operator, $\langle \phi_n, \Pi\phi_m\rangle = \langle \phi_m, \Pi\phi_n\rangle$, therefore $\Pi_{nm} = \Pi_{mn}$. As a result, Equation (37) gives $\frac{n(n+1)}{2}$ coupled algebraic equations that should be solved simultaneously where n is the number of modes that are used to formulate the controller. Since there are two orders of magnitude difference between the first and sixth eigenvalues of the operator A^e, the effect of higher order eigenvalues on the dynamic of the system is considered to be negligible; therefore, in this work the first five modes were used for numerical simulation. The computed LQ controller was applied to the nonlinear model of the reactor. Simulation of the nonlinear system was performed using COMSOL®. The closed loop trajectory of error is shown in Figure 3 and the optimal input trajectory is shown in Figure 4. Figure 3 illustrates that, as catalyst deactivates, the controller is able to regulate the trajectory of y_B at the desired steady state trajectory.

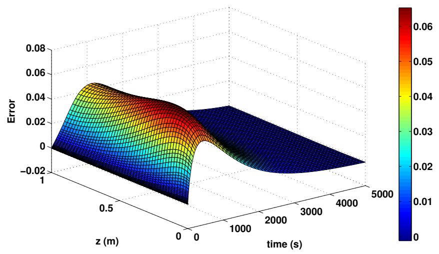

Fig. 3. Closed loop trajectory of error $y_B - y_{B_{ss}}$

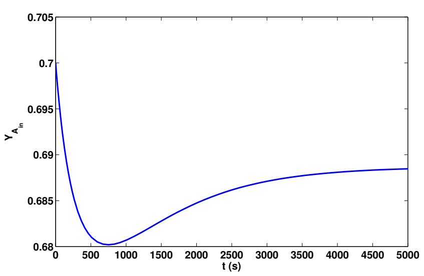

Fig. 4. Optimal input trajectory

8. SUMMARY

The infinite dimensional LQ controller for boundary control of an infinite dimensional system modelled by coupled Parabolic PDE-ODE equations was studied. This work is an important step in formulation of an optimal controller for the most general form of distributed parameter systems consisting of coupled parabolic and hyperbolic PDEs, as well as ODEs. The LQ controller was applied to a catalytic fixed bed reactor, where the rate of catalyst deactivation was modelled by an ODE. The closed loop performance of the controller was studied via numerical simulations. It was illustrated that the formulated controller is able to eliminate the effect of the catalyst deactivation.

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