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Optimal boundary control of coupled parabolic PDE–ODE systems using infinite-dimensional representation

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ABSTRACT

The optimal boundary control problem is studied for coupled parabolic PDE–ODE systems. The linear quadratic method is used and exploits an infinite-dimensional state-space representation of the coupled PDE–ODE system. Linearization of the nonlinear system is established around a steady-state profile. Using appropriate state transformations, the linearized system has been 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 linear quadratic control problem has been solved using the corresponding Riccati equation and the solution of the corresponding eigenvalue problem. The results were applied to the case study of a catalytic cracking reactor with catalyst deactivation. Numerical simulations are performed to illustrate the performance of the proposed controller.

1. Introduction

Many chemical and biochemical processes are modelled by coupled PDEs and ODEs. An example of such processes is the hybrid bioreactor that is used for the treatment of volatile organic compounds such as benzene. This process consists of the bubble column bioreactor, which may be best described by a set of ODEs, interconnected with the biofilter, which is described by a set of PDEs. More examples for processes modelled by coupled PDEs–ODEs can be found in [1–4]. Composite PDE–ODE models can also be used to describe the transportation delay accompanied by other chemical processes such as chemical reactions or mixing, where differential-difference equations fail to model the system [5]. In such systems, the transportation delay can be modelled by a set of PDEs and the other portion of the system can be described by a set of 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, since 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 of this coupling. These systems are called cascaded PDE–ODE systems and their control has been the subject of a few recent studies (e.g. [6,7]). The second type of coupling takes place in the domain of the PDE, which means the parameters of the distributed dynamics (e.g., the coefficients) are functions of the states of the lumped parameter system. Examples of this kind of coupling include a catalytic reactor with catalyst deactivation, where the deactivation kinetics are described by a set of ODEs, or a heat exchanger with a time varying heat transfer coefficient, where the fouling dynamics are described by a set of ODEs. Most biochemical processes are also modelled by a set of coupled PDE–ODE with in-domain coupling (e.g., in situ bioremediation).

A common approach for controlling distributed parameter systems is to convert the set of PDEs to a set of ODEs using discretization techniques (e.g. finite difference or finite element methods). These discretization methods may result in models that do not accurately capture all of the dynamic properties of the original system. In order to ensure accurate finite-dimensional models, a very fine discretization is needed and can result in high-order state-space systems, which in turn can lead to computationally demanding controllers.

In recent years, research on control of DPS has focused on methods that deal with infinite-dimensional nature of these systems [8,9]. In the aforementioned work, distributed parameter systems are formulated in a state-space form, similar to lumped parameter systems, by introducing a suitable infinite-dimensional space setting and associated operators. This approach allows infinite-dimensional controllers to be synthesized directly from the infinite-dimensional realization of the system [8,10,11].

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For parabolic PDEs, Christofides [12] studied nonlinear order reduction and control of nonlinear systems. For diffusion–convection–reaction systems, which are described by parabolic PDEs, Dubljevic et al. [13] used modal decomposition to derive finite-dimensional systems that capture the dominant dynamics of the original PDE which are subsequently used for low dimensional controller design. Also, boundary control of systems described by single invariant parabolic PDEs has been studied by Dubljevic and Christofides [14], and in [15,16], the boundary 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.

Control problems of coupled hyperbolic PDE–ODE have been studied in some recent works [17–19]. In [19], the problem of optimal regulation of large space structures governed by coupled system of hyperbolic PDEs and ODEs has been studied. The problem is solved by developing some optimality conditions that are based on the Gâteau differential of the performance index with respect to the control. In [18], a new optimal control approach for a distributed system governed by first-order hyperbolic partial differential equations coupled with a lumped parameter system that accurately models a closed-circuit wind tunnel. A general theory has been developed to analyse an optimal control problem of this class of system. The theory is applied to a predictive optimal control design to regulate the test section Mach number during a continuous pitch motion of a test model. The predictive optimal control is found to have a modified Riccati solution. In [17], the LQ control problem for a class of composite hyperbolic PDEs and ODEs is formulated and solved by using the state-space approach. The solution of the LQ control problem is achieved by solving the matrix Riccati equations that result from the operator Riccati equation of the infinite-dimensional state-space representation. The designed optimal control policy is implemented on an interacting CSTR–PFR system through a numerical study.

In this work, we are interested in the boundary (LQ) control of a system described by a set of nonlinear parabolic PDEs and ODEs, using the infinite-dimensional state-space description. An important advantage of LQ control is that it uses a state feedback law, in which the state feedback gain is calculated off-line by using LTI system's dynamics and thereby the amount of on-line calculations is reduced, significantly. 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 in the study of infinite-dimensional optimal controller for such systems. The approach developed in [17] cannot be implemented in the case of parabolic PDEs due to the nature of the corresponding operator Riccati equation. The latter cannot be transformed into a matrix Riccati equation as in the hyperbolic PDEs case. Here, the operator Riccati equation will be solved by using the eigenvalues and eigenvectors of the system generator.

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. Appropriate state transformations are used to write the linearized system as a well posed infinite-dimensional system. In Section 3, the eigenvalue problem is solved by adopting the method used for the heat equation of composite media [20]. Section 4 deals with the optimal control problem, which is solved using the corresponding Riccati equation. In Section 5, we consider the case study of a tubular reactor wherein the Van de Vusse reaction takes place. This reaction 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. The triangular structure simplifies the computation of the spectrum of the system. 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

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

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

Comment 1The approach developed here can be extended to the case where the matrices $\mathbf{D}_0$ and $\mathbf{V}$ are diagonalizable. Indeed, state transformation can be used to return to the case where the matrices are diagonal. Moreover, in most chemical engineering processes, $\mathbf{D}_0$ and $\mathbf{V}$ are symmetric and then diagonalizable.

The nonlinear system (1)–(2) can be linearized around the steady state profile (z_{ss}, k_{ss}) and the resulting linear system is given by:

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

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

Here, the boundary and initial conditions can be written as follows:

$$\begin{aligned} &\mathbf{D}_0 \frac{\partial \tilde{z}}{\partial \xi}|_{\xi=0} = \mathbf{V}\left(\tilde{z}_{|_{\xi=0}} - \tilde{z}_{in}\right) \quad \text{and} \quad \frac{\partial \tilde{z}}{\partial \xi}|_{\xi=l} = 0 \\ &\tilde{z}(\xi, 0) = \tilde{z}_0 \qquad\qquad\qquad\qquad \text{and} \quad \tilde{k}(0) = \tilde{k}_0, \end{aligned} \tag{4}$$

where $\tilde{z} = z - z_{ss}$ and $\tilde{k} = k - k_{ss}$ 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.

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

Comment 2At this stage, one can remark that Eq. (3b) can be solved and injected in Eq. (3a), however, this will convert Eq. (3a) into a state-space equation with an independent term represented by $\mathbf{N}_2(\xi)\tilde{k}$ and can be considered as external disturbance. In this case, we will need to develop an optimal controller that takes into consideration disturbance part. To avoid this issue, we prefer to keep the system in its standard state-space equation.

Eq. (3a) is of type diffusion–convection–reaction PDE. In view of solving the eigenvalue 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:

$$\theta = \mathbf{T}\tilde{z} = \exp\left(-\frac{\mathbf{D}_0^{-1}\mathbf{V}}{2}\xi\right)\tilde{z} \tag{5}$$

By using this transformation, the PDE system (3a)–(3b) can be described in terms of the new state θ by the following linear diffusion–reaction parabolic PDE coupled with a linear ODE (more details about this conversion can be found in Appendix A):

$$\frac{\partial\theta}{\partial t} = \mathbf{D}\frac{\partial^2\theta}{\partial\xi^2} + \mathbf{M}_1(\xi)\theta + \mathbf{M}_2(\xi)\tilde{k} \tag{6a}$$

$$\frac{d\tilde{k}}{dt} = \mathbf{M}_0\tilde{k} \tag{6b}$$

where the matrices $\mathbf{M}_1$, $\mathbf{M}_2$ and $\mathbf{D}$ are given by

$$\mathbf{M}_1(\xi) = \mathbf{T}\left[\mathbf{N}_1(\xi) - \frac{1}{4}\mathbf{V}\mathbf{D}_0^{-1}\mathbf{V}\right]\mathbf{T}^{-1}, \quad \mathbf{M}_2(\xi) = \mathbf{T}\mathbf{N}_2(\xi) \quad \text{and}$$
$$\mathbf{D} = \mathbf{T}\mathbf{D}_0\mathbf{T}^{-1}.$$

The boundary and initial conditions are:

$$\begin{aligned} &\mathbf{D}\frac{\partial\theta}{\partial\xi}|_{\xi=0} = \frac{\mathbf{V}}{2}\theta_{|_{\xi=0}} - \mathbf{T}\mathbf{V}\tilde{z}_{in}, \quad \mathbf{D}\frac{\partial\theta}{\partial\xi}|_{\xi=l} = -\frac{\mathbf{V}}{2}\theta_{|_{\xi=l}} \\ &\theta(\xi,0) = \mathbf{T}^{-1}\tilde{z}_0 := \theta_0 \qquad \tilde{k}(0) = \tilde{k}_0 \end{aligned} \tag{7}$$

Now, we are in a position to formulate the system (6)–(7) as an abstract boundary control problem on the infinite-dimensional space $H = \mathcal{H} \oplus \mathcal{K}$. First, let us put $u = \mathbf{V}\tilde{x}_{in}$ and define a new state vector

$$x = \begin{bmatrix} x_d \\ x_l \end{bmatrix} := \begin{bmatrix} \theta \\ \tilde{k} \end{bmatrix} \tag{8}$$

The abstract equation is given by the following boundary control system

$$\begin{cases} \dot{x}(t) &= \mathfrak{A}x(t), \quad x(0) = x_0 \\ \mathfrak{B}x(t) &= u(t) \\ y(t) &= \mathfrak{C}x(t) \end{cases} \tag{9}$$

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

$$\mathcal{D}(\mathfrak{A}) = \left\{x \in H : x_d \text{ and } \frac{dx_d}{d\xi} \text{ are absolutely continuous, } \frac{d^2x_d}{d\xi^2} \in \mathcal{H}, \ \mathbf{D}\frac{dx_d}{d\xi}_{|_{\xi=l}} = -\frac{\mathbf{V}}{2}x_{d_{|_{\xi=l}}}\right\} \tag{10}$$

and is given by

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

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

$$\mathfrak{B}x(\cdot) = \left[-\mathbf{D}\frac{\partial\cdot}{\partial\xi} + \frac{\mathbf{V}}{2}\cdot|0\right]\begin{bmatrix} x_d \\ x_l \end{bmatrix}_{\xi=0} \tag{12}$$

Since $\mathbf{M}_2$ in Eq. (11) is generally non-zero, x_d and x_l are coupled. By introducing the following transformation, the system can be transformed into decoupled subsystems:

$$\Lambda = \left[\begin{array}{c|c} I & J \\ \hline 0 & I \end{array}\right] \in \mathcal{L}(H) \quad \& \quad \hat{x} = \Lambda x \tag{13}$$

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

$$\hat{\mathfrak{A}} = \Lambda\mathfrak{A}\Lambda^{-1} = \left[\begin{array}{c|c} \mathfrak{A}_{11} & -\mathfrak{A}_{11}J + \mathfrak{A}_{12} + J\mathfrak{A}_{22} \\ \hline 0 & \mathfrak{A}_{22} \end{array}\right] \tag{14}$$

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.

$$-\mathfrak{A}_{11}J + \mathfrak{A}_{12} + J\mathfrak{A}_{22} = 0 \tag{15}$$

Comment 3Eq. (15) is a Sylvester equation and admits a unique solution if and only if $\sigma(-\mathfrak{A}_{11}) \cap \sigma(\mathfrak{A}_{22}) = \emptyset$ [21]. The solution is given by

$$J = \int_0^\infty T_{11}(t)\mathfrak{A}_{12}T_{22}(t)dt, \tag{16}$$

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

Thanks to Sylvester equation (15) and its solution (16), the resulting decoupled system is given by the following infinite-dimensional boundary system:

$$\begin{cases} \dot{\hat{x}}(t) = \hat{\mathfrak{A}}\hat{x}(t), \quad \hat{x}(0) = \hat{x}_0 \\ \hat{\mathfrak{B}}\hat{x}(t) = u(t) \\ y(t) = \hat{\mathfrak{C}}\hat{x}(t), \end{cases} \tag{17}$$

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

System (17) is in the form of a standard abstract boundary control problem. Then by following a similar approach to [16,15], it can be converted to a well-posed infinite-dimensional system with bounded input and output operators. Here is the procedure (see [8, p. 122]). Define a new operator $\mathcal{A}$ as

$$\begin{aligned} \mathcal{A}\hat{x} &= \hat{\mathfrak{A}}\hat{x} \\ \mathcal{D}(\mathcal{A}) &= \mathcal{D}(\hat{\mathfrak{A}}) \cap ker(\hat{\mathfrak{B}}) = \left\{\hat{x} \in H : \hat{x} \text{ and } \frac{d\hat{x}}{d\xi} \text{ are a.c., } \frac{d^2\hat{x}}{d\xi^2} \in H \text{ and } \mathbf{D}\frac{d\hat{x}_d}{d\xi}|_{\xi=0} = \frac{\mathbf{V}}{2}\hat{x}_d|_{\xi=0}, \mathbf{D}\frac{d\hat{x}_d}{d\xi}|_{\xi=l} = -\frac{\mathbf{V}}{2}x_d|_{\xi=l}\right\} \end{aligned} \tag{18}$$

where a.c. means absolutely continuous. If $\mathcal{A}$ generates a C_0-semigroup on H and there exists a $B \in \mathcal{L}(U, H)$ such that the following condition holds:

$$Bu \in \mathcal{D}(\hat{\mathfrak{A}}) \quad \text{and} \quad \forall u \in U, \hat{\mathfrak{B}}Bu = u, \tag{19}$$

then system (17) can be transformed into the following infinite-dimensional system with bounded input operator on the state space $\mathbf{H} = U \oplus H$

$$\begin{cases} \dot{\mathbf{x}}(t) = \mathrm{A}\mathrm{x}(t) + \mathrm{B}\mathrm{u}(t) \\ \mathbf{y}(t) = \mathrm{C}\mathrm{x}(t) \end{cases} \tag{20}$$

where the operators $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are given as follows:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 \\ \hat{\mathfrak{A}}B & \mathcal{A} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} I \\ -B \end{bmatrix}, \quad \mathbf{C} = \mathfrak{C}\begin{bmatrix} B & I \end{bmatrix} \tag{21}$$

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

Comment 4Consider $\tilde{B} = \Lambda^{-1}B$, then Condition (19) becomes

$$\tilde{B}u \in \mathcal{D}(\hat{\mathfrak{A}}) \quad \text{and} \quad \mathfrak{B}\tilde{B}u = u.$$

One can assume that $\tilde{B} = [B_d \mid B_l]^T$. Then the following conditions are equivalent to (19)

$$\mathbf{D}\frac{dB_d(0)}{d\xi} - \frac{\mathbf{V}}{2}B_d(0) = I, \quad \mathbf{D}\frac{dB_d(l)}{d\xi} + \frac{\mathbf{V}}{2}B_d(l) = 0, \quad B_l \in \mathcal{K} \tag{22}$$

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

$$B = \Lambda\tilde{B} = \begin{bmatrix} B_d + JB_l \\ B_l \end{bmatrix}. \tag{23}$$

Comment 5The infinite-dimensional system (20) is in the form of a standard infinite-dimensional system and 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 (20) and 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 eigenvalue problem for the system (20).

3. Eigenvalue problem

In the analysis developed in this paper, we will use the concepts of (1) Riesz basis, which is a sequence of vectors in a Hilbert space **H** such that there exists an equivalent inner product on **H** with respect to which this sequence is an orthonormal basis of **H** and (2) Riesz spectral operator, which is a closed linear operator with simple eigenvalues such that the sequence of eigenvectors is a Riesz basis and the closure of the set of its eigenvalues is totally disconnected. The use of these concepts is motivated by the fact that many dynamical PDE systems are generated by non-self-adjoint operators whose eigenvectors may not be orthogonal, but that do form a Riesz basis. Moreover, elements of the state space **H** can be uniquely represented as a linear combination of the Riesz basis (even if the basis is not orthogonal) by using the corresponding bi-orthogonal sequence (i.e. the eigenvectors of the adjoint operator).

In this section, the solution of the eigenvalue problem that was introduced in [15,16] is extended to the case of coupled PDE–ODE systems. There is no general algorithm for analytical solution of an eigenvalue 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 many 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 diagonal, which is extensible to diagonalizable case.

In this work, we are interested in the analytical solution of the eigenvalue problem, therefore the simplifying assumptions were necessary. One can use the results developed here with eigenvalues calculated by numerical methods which can be used for more generic form of the operator $\mathfrak{A}_{11}$. Here, the eigenvalue problem of interest is given by the following equation:

$$\mathbf{A}\phi = \lambda\phi \tag{24}$$

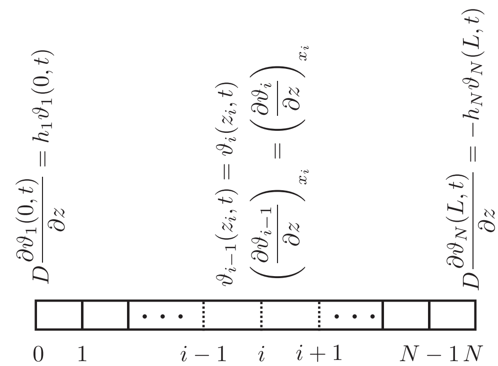

Fig. 1. Approximation of the reactor as a composite media.

where the operator **A** is given by (21) and

$$\mathcal{A} = \begin{bmatrix} \mathcal{A}_{11} & 0 \\ 0 & \mathcal{A}_{22} \end{bmatrix}$$

$$\mathcal{A}_{11} := \begin{bmatrix} F_{11} & 0 \\ F_{21} & F_{22} \end{bmatrix} = \begin{bmatrix} \mathbf{d}_1 \dfrac{d^2}{d\xi^2} + \mathbf{h}_{11} & 0 \\ \mathbf{h}_{21} & \mathbf{d}_2 \dfrac{d^2}{d\xi^2} + \mathbf{h}_{22} \end{bmatrix} \tag{25}$$

$$\mathcal{A}_{22} = \begin{bmatrix} \alpha_{11} & 0 \\ 0 & \alpha_{22} \end{bmatrix}$$

Observe that the operator $\mathcal{A}$ is a block diagonal operator, therefore the set of eigenvalues consists of the eigenvalues of the two operators on its diagonal, i.e.

$$\sigma(\mathcal{A}) = \sigma(\mathcal{A}_{11}) \cup \sigma(\mathcal{A}_{22}).$$

Since $\mathcal{A}_{11}$ is a lower triangular operator according to assumption 2, $\sigma(\mathcal{A}_{11}) = \sigma(F_{11}) \cup \sigma(F_{22})$, then $\sigma(\mathcal{A}) = \sigma(F_{11}) \cup \sigma(F_{22}) \cup \sigma(\mathcal{A}_{22})$. Note that F_{11} and F_{22} have the following form:

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

where I is the identity operator. It can be shown that the resolvent operator of F is compact, then, the spectrum of the operator F consists only of isolated eigenvalues with finite multiplicities [8, Lemma A.4.19]. However, the calculation of this spectrum is a challenging issue due to the fact that **h** depends on the space variable ξ. In [16], the spectrum is calculated by dividing the space interval into a finite number N of subintervals $[\xi_{i-1}, \xi_i]$, in which it is assumed that the values of **h** are constant and are denoted by $\mathbf{h}_i$ (see Fig. 1).

The procedure of [16] will be adopted here. The explicit expressions of the eigenvalues and eigenfunctions of the operator F are given in Appendix B. Let λ_n and ϕ_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} (see Appendix B). Then the eigenvalues of the operator $\mathcal{A}_{11}$ consists of eigenvalues of F_{11} and F_{22}, i.e.

$$\sigma(\mathcal{A}_{11}) = \sigma(F_{11}) \cup \sigma(F_{22}) = \{\lambda_n, \mu_n, n = 1, \ldots, \infty\}. \tag{26}$$

Thanks to the triangular form of the operator $\mathcal{A}_{11}$, we can easily find the associated eigenfunctions, which are given by

$$\left\{ \begin{bmatrix} \phi_n \\ (\lambda_n I - F_{22})^{-1} F_{21}\phi_n \end{bmatrix}, \begin{bmatrix} 0 \\ \psi_n \end{bmatrix} \right\}, \quad n = 1, \ldots, \infty \tag{27}$$

Similar procedure can be used to compute the corresponding bi-orthonormal eigenfunctions. Indeed, we can solve the eigenvalue problem for the adjoint operator $\mathcal{A}_{11}^*$, which leads to:

$$\left\{ \begin{bmatrix} \phi_n \\ 0 \end{bmatrix}, \begin{bmatrix} (\mu_n I - F_{11})^{-1} F_{21} \psi_n \\ \psi_n \end{bmatrix} \right\}, \quad n = 1, \ldots, \infty \tag{28}$$

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

$$\sigma(\mathcal{A}) = \{\lambda_n, \mu_n, \alpha_{11}, \alpha_{22}\}, \quad n = 1, \ldots, \infty \tag{29}$$

and the associated eigenfunctions are

$$\tilde{\Phi}_n = \left\{ \begin{bmatrix} \phi_n \\ (\lambda_n I - F_{22})^{-1} F_{21} \phi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \psi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\} \tag{30}$$

The corresponding bi-orthonormal eigenfunctions are

$$\tilde{\Psi}_n = \left\{ \begin{bmatrix} \phi_n \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} (\mu_n I - F_{11})^{-1} F_{21} \psi_n \\ \psi_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\} \tag{31}$$

Assume that the operator $\mathcal{A}$ has eigenvalues $\{\sigma_k, k \geq 1\}$ and biorthonormal pair $\{(\tilde{\Phi}_k, \tilde{\Psi}_k), k \geq 1\}$. The spectrum of the operator $\mathbf{A}$ is given by $\sigma(\mathbf{A}) = \sigma(\mathcal{A}) \cup \{0\}$ and the eigenvalue $\sigma_0 = 0$ has a multiplicity m, where m is the number of manipulated variables. The corresponding eigenfunction for σ_0 can be computed by solving the equation $\mathbf{A}\Phi_0 = 0$. Due to the special form of the operator $\mathbf{A}$, the expression of the eigenfunction Φ_0 is given as follows

$$\Phi_0 = \begin{bmatrix} 1 \\ -\mathcal{A}^{-1}(\hat{\mathfrak{A}}B) \end{bmatrix} = \begin{bmatrix} 1 \\ \sum_{k=0}^{\infty} -\dfrac{1}{\sigma_k} \langle \hat{\mathfrak{A}}B, \tilde{\Psi}_k \rangle \tilde{\Phi}_k \end{bmatrix}, \tag{32}$$

The right hand side of the previous equation is an immediate consequence of the expression of the resolvent operator of $\mathcal{A}$ in terms of its eigenvalues and eigenfunctions (see [8, Eq 2.35, p. 41]). On the other hand, the corresponding eigenfunctions for σ_n, $n \geq 1$ are given by

$$\Phi_n = \begin{bmatrix} 0 \\ \tilde{\Phi}_n \end{bmatrix} \tag{33}$$

Finally, the corresponding bi-orthonormal eigenfunctions of $\mathbf{A}$ are

$$\Psi_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \Psi_n = \begin{bmatrix} \dfrac{1}{\sigma_n} (\hat{\mathfrak{A}}B)^* \tilde{\Psi}_n \\ \tilde{\Psi}_n \end{bmatrix}. \tag{34}$$

4. Infinite-horizon optimal control

In this section, we are interested in solving the optimal control problem. In order to do so, we need to investigate the dynamical properties of the system. The following theorem states a result about the generation property of the extended system. This is a consequence of the fact that a Riesz spectral operator generates a C_0-semigroup if and only if $\sup_{n \geq 1} Re(\lambda_n) < \infty$.

Theorem 1. *Consider the operator* $\mathbf{A}$ *given by Eq. (20). Then* $\mathbf{A}$ *is the infinitesimal generator of a* C_0*-semigroup on* $\mathbf{H}$.

Proof. Here, we will prove that the operator $\mathcal{A}_{11}$ is a Riesz spectral operator (see [23]). In Section 3, it has been shown that F_{11} and F_{22} are Riesz spectral operators and they both have real countable and distinct eigenvalues. Therefore, they generate C_0-semigroups T_{11} and T_{22}, respectively.

According to [8, Lemma 3.2.2, p. 114], the operator $\mathcal{A}_{11}$ is the generator of a C_0-semigroup on $\mathcal{H}$ denoted $\mathcal{T}_{11}(t)$ and is given by

$$\mathcal{T}_{11}(t) = \begin{bmatrix} T_{11}(t) & 0 \\ T_{21}(t) & T_{22}(t) \end{bmatrix} \tag{35}$$

where the operator T_{21} is given by

$$T_{21}(t)x_1 = \int_0^t T_{22}(t-s) F_{21} T_{11}(s) x_1 ds \tag{36}$$

On the other hand, the operator $\mathcal{A}_{22}$ is a diagonal finite-dimensional operator and therefore it is the generator of a C_0-semigroup on $\mathcal{K}$ given by $\mathcal{T}_{22} = \exp(-\mathcal{A}_{22} t)$. As a consequence, the (diagonal) operator $\mathcal{A}$ is the infinitesimal generator of the following C_0-semigroup:

$$\mathcal{T}(t) = \begin{bmatrix} \mathcal{T}_{11}(t) & 0 \\ 0 & \mathcal{T}_{22}(t) \end{bmatrix} \tag{37}$$

According to Section 3, it has been shown that the eigenvalues of the operator $\mathbf{A}$ consist of eigenvalues of $\mathcal{A}$ and 0 with finite multiplicity m. Moreover, the eigenfunctions of $\mathbf{A}$ and its adjoint are bi-orthonormal. Therefore, they form a Riesz basis for $\mathbf{H}$. Furthermore, $\mathbf{A}$ is a Riesz spectral operator and then it is the generator of a C_0-semigroup given by

$$\mathbf{T}(t) = \begin{bmatrix} I & 0 \\ \mathcal{S}(t) & \mathcal{T}(t) \end{bmatrix} \tag{38}$$

where $\mathcal{S}(t)x = \int_0^t \mathcal{T}(s) \tilde{\mathfrak{A}} B x ds$. □

The next corollary is immediate consequence of [8, Theorem 5.2.10]. It gives a necessary and sufficient conditions for the extended system $\sum(\mathbf{A}, \mathbf{B}, \mathbf{C})$ to be β-exponentially stabilizable and β-exponentially detectable..

Corollary 1. *Consider the linear system* $\sum(\mathbf{A}, \mathbf{B}, \mathbf{C})$ *given by Eq. (20). Assume that* $\mathbf{B}$ *and* $\mathbf{C}$ *are finite rank operators defined by*

$$\mathbf{B}u = \sum_{i=1}^{m} b_i u_i \quad \text{and} \quad \mathbf{C}x = (\langle x, c_1 \rangle \quad \cdots \quad \langle x, c_k \rangle)$$

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

$$\text{rank}(\langle b_1, \Psi_n \rangle \quad \cdots \quad \langle b_m, \Psi_n \rangle) = 1. \tag{39}$$

A necessary and sufficient condition for $\sum(\mathbf{A}, -, \mathbf{C})$ *to be* β*-exponentially detectable is that for all n such that* $\lambda_n \in \sigma_\beta^+(A)$

$$\text{rank}(\langle c_1, \Phi_n \rangle \quad \cdots \quad \langle c_k, \Phi_n \rangle) = 1. \tag{40}$$

Proof. $\mathbf{A}$ is a Riesz spectral operator and its eigenvalues consist of eigenvalues of $\mathcal{A}$ and 0 with finite multiplicity m. Diagonal entries of $\mathcal{A}$ are Sturm–Liouville operators and the spectrum of $\mathcal{A}$ is finitely bounded (i.e., there exists a ω such that all $\lambda \in \sigma(\mathcal{A}) < \omega$). Therefore, for any arbitrary β and ϵ, $\sigma_{\beta-\epsilon}^+(A^e)$ comprises finitely many eigenvalues and the first condition of Theorem 5.2.10 in [8] holds. Then, the necessary and sufficient condition for β-exponential stabilizability of $\sigma(\mathbf{A}, \mathbf{B}, -)$ reduces to (39). The β-exponential detectability can be proved in a similar way. □

Now, we are interested in the design of linear quadratic (LQ) state feedback optimal controller for the infinite-dimensional system (20)–(21). The aim is to minimize the quadratic cost function:

$$\mathbf{J}(\mathbf{u}) = \int_0^\infty \langle \mathbf{y}(s), \mathbf{y}(s)\rangle + \langle \mathbf{u}(s), \mathbf{u}(s)\rangle ds \tag{41}$$

It is known that the solution of this optimal control problem can be obtained by solving the following algebraic Riccati equation (ARE) [8]:

$$\langle \mathrm{A}\mathbf{x}_1, \Pi\mathbf{x}_2\rangle + \langle \Pi\mathbf{x}_1, \mathrm{A}\mathbf{x}_2\rangle + \langle \mathbf{x}_1, \mathbf{C}^*\mathrm{C}\mathbf{x}_2\rangle - \langle \Pi\mathbf{x}_1, \mathrm{BB}^*\Pi\mathbf{x}_2\rangle = 0 \tag{42}$$

When ($\mathbf{A}$, $\mathbf{B}$) is exponentially stabilizable and ($\mathbf{C}$, $\mathbf{A}$) is exponentially detectable, the algebraic Riccati equation (42) has an unique non-negative self-adjoint solution $\Pi \in \mathcal{L}(\mathbf{H})$ and for any initial state $\mathbf{x}_0 \in \mathbf{H}$ the quadratic cost is minimized by the optimal control $\mathbf{u}_o$ given by

$$\mathbf{u}_o(s) = -\mathbf{B}^*\Pi\mathbf{x}(s). \tag{43}$$

Let us set $\mathbf{x}_1 = \Phi_m$ and $\mathbf{x}_2 = \Phi_n$ 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:

$$(\sigma_m + \sigma_n)\Pi_{nm} + \mathbf{C}_{nm} - \sum_{k,l=0}^{\infty} \mathbf{B}_{kl}\Pi_{nl}\Pi_{km} = 0 \tag{44}$$

where $\mathbf{C}_{nm} = \langle \mathbf{C}\Phi_n, \mathbf{C}\Phi_m\rangle$, and $\mathbf{B}_{nm} = \langle \mathbf{B}^*\Phi_n, \mathbf{B}^*\Phi_m\rangle$. For more mathematical details of how to convert the Riccati equation (42) into (44), please see Appendix C.

5. 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 [24]. The reaction scheme is given by equations

$$A \overset{k_1}{\to} B \overset{k_2}{\to} C \qquad A \overset{k_3}{\to} C \tag{45}$$

with the kinetic equations given by

$$\begin{aligned} r_A &= -(k_1 + k_3)y_A^2 = -k_0 y_A^2 \\ r_B &= k_1 y_A^2 - k_2 y_B \end{aligned} \tag{46}$$

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

$$\frac{dk_1}{dt} = \alpha k_1 + \beta, \qquad k_1(0) = k_{1_0} \tag{47}$$

The above equation for the rate of deactivation of the catalyst is equivalent to the common exponential decay assumption that is used 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 [25]. The model of the reactor will be:

$$\begin{aligned} \frac{\partial y_A}{\partial t} &= D_a \frac{\partial^2 y_A}{\partial \xi^2} - v\frac{\partial y_A}{\partial \xi} + r_A, \\ \frac{\partial y_B}{\partial t} &= D_a \frac{\partial^2 y_B}{\partial \xi^2} - v\frac{\partial y_B}{\partial \xi} + r_B, \\ \frac{dk_1}{dt} &= \alpha k_1 + \beta \end{aligned} \tag{48}$$

Initial and boundary conditions are:

$$\begin{aligned} D_a \frac{\partial y_A}{\partial \xi}|_{\xi=0} &= v\left(y_A|_{\xi=0} - y_{A_{in}}\right), \\ D_a \frac{\partial y_B}{\partial \xi}|_{\xi=0} &= v\left(y_B|_{\xi=0} - y_{B_{in}}\right), \\ \frac{\partial y_A}{\partial \xi}|_{\xi=l} &= 0, \\ \frac{\partial y_B}{\partial \xi}|_{\xi=l} &= 0, \\ y_A(\xi, 0) &= y_{A_0}(\xi), \\ y_B(\xi, 0) &= y_{B_0}(\xi), \\ k_1(0) &= k_{1_0} \end{aligned} \tag{49}$$

By defining the new state and input variables

$$x(t) = \begin{bmatrix} x_1 \\ x_2 \\ \hline x_3 \end{bmatrix} = \begin{bmatrix} e^{-\frac{v\xi}{2D_a}}(y_A - y_{A_{ss}}) \\ e^{-\frac{v\xi}{2D_a}}(y_B - y_{B_{ss}}) \\ \hline k_1 - k_{1_{ss}} \end{bmatrix} \in \mathbf{H} := L^2(0,l)^2 \oplus R, \tag{50}$$

$$u(t) = v\left(y_{A_{in}} - y_{A_{in,ss}}\right) \tag{51}$$

the set of equations (48) can be linearized and then converted to a diffusion–reaction system by using the transformation given in Eq. (5). The resulting system is

$$\frac{\partial}{\partial t}\begin{bmatrix} x_1 \\ x_2 \\ \hline x_3 \end{bmatrix} = \left[\begin{array}{cc|c} D_a\frac{\partial^2}{\partial \xi^2} - \hat{k}_1(\xi) & 0 & -y_{A_{ss}}^2 \\ 2k_{1_{ss}}y_{A_{ss}}(\xi) & D_a\frac{\partial^2}{\partial \xi^2} - \hat{k}_2 & y_{A_{ss}}^2 \\ \hline 0 & 0 & \alpha \end{array}\right]\begin{bmatrix} x_1 \\ x_2 \\ \hline x_3 \end{bmatrix} \tag{52}$$

with the following initial and boundary conditions

$$\begin{aligned} D_a \frac{\partial}{\partial \xi}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{\xi=0} &= \frac{v}{2}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{\xi=0} - \begin{bmatrix} u \\ 0 \end{bmatrix} \\ D_a \frac{\partial}{\partial \xi}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{\xi=l} &= -\frac{v}{2}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{\xi=l} \\ x(\xi, 0) &= x_0 \end{aligned} \tag{53}$$

where

$\hat{k}_1(\xi) = -\frac{v^2}{4D_a} - 2\left(k_{1_{ss}} + k_3\right) y_{A_{ss}}$ and $\hat{k}_2 = -\frac{v^2}{4D_a} - k_2$

The infinite-dimensional representation of the system (52)–(53) on the Hilbert space **H** has the form (9), where the operator $\mathfrak{A}$ is given by:

$$\mathfrak{A} = \left[\begin{array}{cc|c} D_a\frac{\partial^2}{\partial\xi^2} - \hat{k}_1(\xi) & 0 & -y_{A_{ss}}^2 \\ 2k_{1_{ss}} y_{A_{ss}}(\xi) & D_a\frac{\partial^2}{\partial\xi^2} - \hat{k}_2 & y_{A_{ss}}^2 \\ \hline 0 & 0 & \alpha \end{array}\right] \quad (54)$$

$$\mathcal{D}(\mathfrak{A}) = \left\{ x \in \mathbf{H} : x \text{ and } \frac{dx}{d\xi} \text{ are a.c.}, \frac{dx^2}{d\xi^2} \in \mathbf{H}, D_a\frac{dx_1}{d\xi}|_{\xi=l} = -\frac{v}{2}x_1|_{\xi=l}, D_a\frac{dx_2}{d\xi}|_{\xi=l} = -\frac{v}{2}x_2|_{\xi=l}, D_a\frac{dx_1}{d\xi}|_{\xi=0} = \frac{v}{2}x_1|_{\xi=0} \right\} \quad (55)$$

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

$$\mathfrak{B}x(\cdot) = \left[\begin{array}{cc|c} -D_a\frac{\partial}{\partial\xi} + \frac{v}{2} & 0 & 0 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \\ \hline x_3 \end{array}\right]_{\xi=0} \quad (56)$$

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

$$\mathfrak{C} = \mathfrak{C}_0 I = [0 \quad 1 \mid 0] \quad (57)$$

By performing the transformation (13), the operator $\mathfrak{A}$ can be converted to a block diagonal form and the decoupled infinite-dimensional system (17) will be computed. Using Eq. (16), the operator J in Eq. (13) is

$$J = \int_0^{\infty} \mathfrak{T}_{11}(t)\mathfrak{A}_{12}\mathfrak{T}_{22}(t)dt \quad (58)$$

$\mathfrak{T}_{11}$ 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

$$\mathfrak{A}_{11} = \begin{bmatrix} D_a\frac{\partial^2}{\partial\xi^2} - \hat{k}_1(\xi) & 0 \\ 2k_{1_{ss}} y_{A_{ss}}(z) & D_a\frac{\partial^2}{\partial\xi^2} - \hat{k}_2 \end{bmatrix}, \quad \mathfrak{A}_{12} = \begin{bmatrix} -y_{A_{ss}}^2 \\ y_{A_{ss}}^2 \end{bmatrix}, \quad \mathfrak{A}_{22} = [\alpha] \quad (59)$$

- **Computation of** $\mathfrak{T}_{11}$: The operator $\mathfrak{A}_{11}$ is a lower triangular operator and as discussed in Section 4 generates the C_0-semigroup $\mathfrak{T}_{11}$ given by

$$\mathfrak{T}_{11}(t) = \begin{bmatrix} T_{11}(t) & 0 \\ T_{21}(t) & T_{22}(t) \end{bmatrix} \quad (60)$$

where T_{11} and T_{22} are the semigroups generated by the diagonal elements of $-\mathfrak{A}_{11}$ and are given by

$$T_{11}(t)x = \sum_{n=1}^{\infty} e^{-\lambda_n t}\langle x, \phi_n\rangle\phi_n \quad (61)$$

$$T_{22}(t)x = \sum_{n=1}^{\infty} e^{-\mu_n t}\langle x, \psi_n\rangle\psi_n \quad (62)$$

λ_n, μ_n, ϕ_n and ψ_n can be calculated using the approach discussed in Section 3. $T_{21}(t)$ can be calculated using $T_{11}(t)$ and $T_{22}(t)$ by

$$T_{21}(t)x = \int_0^t T_{22}(t-s)FT_{11}(s)xds \quad (63)$$

where F is the off-diagonal element of $\mathfrak{A}_{11}$ and is equal to $2k_{1_{ss}} y_{A_{ss}}(\xi)$. By performing simple calculations, $T_{21}(t)$ becomes

$$T_{21}(t)x = \sum_{n,m=1}^{\infty} -\frac{e^{-\lambda_m t} - e^{-\mu_n t}}{\lambda_m - \mu_m}\langle x, \phi_m\rangle\langle F\phi_m, \psi_n\rangle\psi_n \quad (64)$$

- **Computation of** $\mathfrak{T}_{22}$: $\mathfrak{A}_{22}$ is a scalar and the semigroup generated by it is

$$\mathfrak{T}_{22} = e^{\alpha t} \quad (65)$$

- **Computation of** J: Using Eqs. (58) and (60)–(65), and assuming that $\mathfrak{A}_{12} = \begin{bmatrix} N_1 \\ N_2 \end{bmatrix}$, the operator J can be computed as:

$$J = \begin{bmatrix} J_1 \\ J_2 \end{bmatrix} \quad (66)$$

$$J_1 x = \sum_{n=1}^{\infty} \frac{\langle N_1 x, \phi_n\rangle\phi_n}{\lambda_n + \alpha} \quad (67)$$

$$J_2 x = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{\langle N_1 x, \phi_n\rangle\langle F\phi_n, \psi_m\rangle\psi_m}{(\lambda_n + \alpha)(\mu_m + \alpha)} + \sum_{m=1}^{\infty} \frac{\langle N_2 x, \psi_m\rangle\psi_m}{\mu_m + \alpha} \quad (68)$$

Finally, 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:

$$\begin{cases} \frac{d\hat{x}(t)}{dt} = \hat{\mathfrak{A}}\hat{x}(t) \\ \hat{x}(0) = \hat{x}_0 \\ \hat{\mathfrak{B}}\hat{x}(t) = u(t) \\ y(t) = \hat{\mathfrak{C}}\hat{x}(t) \end{cases} \quad (69)$$

The abstract boundary control problem (69), can be converted to a well-posed infinite-dimensional system with bounded input and output operators using Eqs. (18)–(21). In Eq. (21), B can be calculated using the discussion in Comment 4. Since $\tilde{B}$ is any arbitrary function that satisfies conditions (22), 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 (22), B_1 and B_2 are:

$$B_1 = \frac{-2}{4D_a l + vl^2}\xi^2 + \frac{2}{v} \quad (70)$$

$$B_2 = -\frac{1}{4D_a l + vl^2}\xi^2 + \frac{1}{4D_a + vl}\xi + \frac{2D_a}{4D_a v + v^2 l} \quad (71)$$

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

$$B = \begin{bmatrix} B_1 + J_1 B_l \\ B_2 + J_2 B_l \\ B_l \end{bmatrix} \quad (72)$$

6. 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

Table 1
Model parameters.

Parameter	Value	Unit
k_{1_0}	18.1	(h weight fraction)$^{-1}$
k_2	1.7	h^{-1}
k_3	4.8	(h weight fraction)$^{-1}$
D_a	0.5	m^2 h^{-1}
v	2	m hr^{-1}
$y_{A_{in}}$	0.7	weight fraction
$y_{B_{in}}$	0	weight fraction
α	−0.001	h^{-1}
β	9.05×10^{-3}	

reactor given in Eqs. (46)–(49). Values of the model parameters are given in Table 1 [24].

The control objective is regulation of 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 Eqs. (46)–(49), 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 non-self-adjoint form of Eqs. (52)–(53). As it has been shown in Section 3, the operator **A** is a Riesz spectral operator and its eigenfunctions constitute a Riesz basis. The advantage here is that the Riccati equation (42) can be solved without having the normal orthogonal basis. Indeed, thanks to the eigenvalues and eigenfunctions of the operator **A**, the Riccati equation has been converted into the set of algebraic equation (44). Spectra of operators A_{11} and A_{22} were calculated using the algorithm discussed in Section 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. The first five eigenvalues of the operator A_{11} are:

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

and the first five eigenvalues of A_{22} are:

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

Finally, the spectrum of **A** was computed using Eqs. (32) and (33). The first six eigenvalues of **A** are:

$$\sigma(\mathbf{A}) = \{0, -0.001, -2.39 \times 10^{-5}, -2.04 \times 10^{-6}, -1.34 \times 10^{-4}, -1.096 \times 10^{-5}\} \quad (73)$$

and the associated eigenfunctions are shown in Figs. 2 and 3. Once the eigenvalues and eigenfunctions of the operator **A** are calculated, the LQ-feedback controller can be computed using Eq. (44). 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, Eq. (44) 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**, the effect of higher order eigenvalues on the system dynamic 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

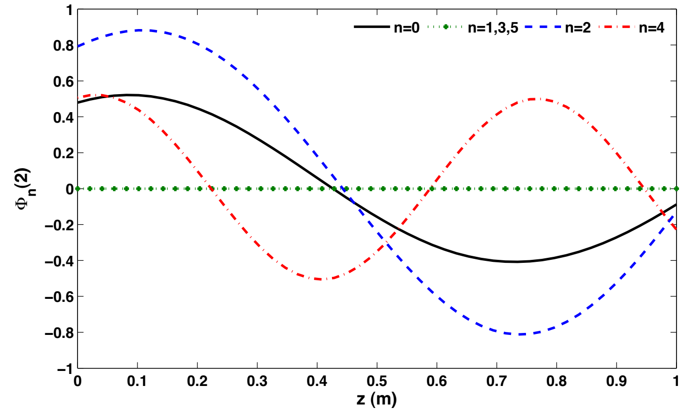

Fig. 2. Second element of $\hat{\phi}_n$.

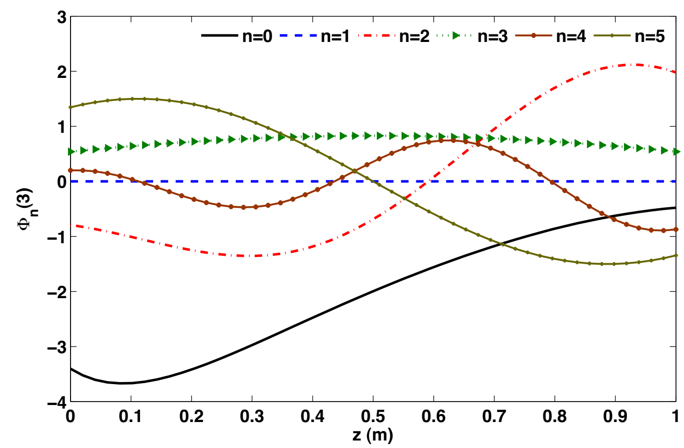

Fig. 3. Third element of $\hat{\phi}_n$.

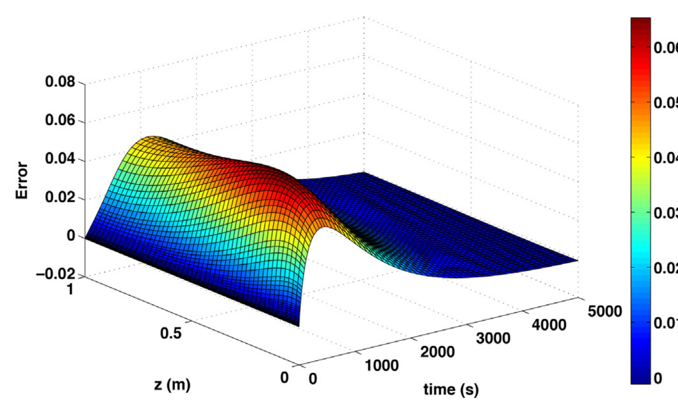

Fig. 4. Closed loop trajectory of error $y_B - y_{B_{ss}}$.

system was performed using COMSOL®. The closed loop trajectory of error is shown in Fig. 4 and the optimal input trajectory is shown in Fig. 5. Fig. 4 illustrates that, as catalyst deactivates, the controller is able to regulate the trajectory of y_B at the desired steady state trajectory.

7. Summary

The 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

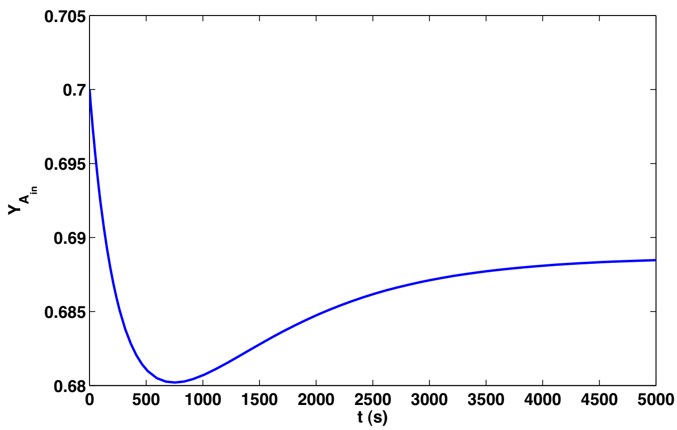

Fig. 5. Optimal input trajectory.

distributed parameter systems consisting of coupled parabolic and hyperbolic PDEs, as well as ODEs. The coupled PDE–ODEs were converted to a decoupled form using an exact transformation. Conditions on existence of this transformation were studied. The decoupled system was then formulated as a well-posed infinite-dimensional system by extension of the approach introduced in [16,15]. It was shown that the resulting system is a Riesz spectral system and by using this fact the stabilizability of the system was shown under some conditions. 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.

Appendix A. Convection term elimination

In this appendix, we will give more details about how to convert Eq. (3a) into Eq. (6a) by using the state transformation (5). Using Eq. (3a), the derivative of the function θ with respect to time can be written as follows:

$$\frac{\partial\theta}{\partial t}=\mathbf{T}\frac{\partial\tilde{z}}{\partial t}=\mathbf{T}\left(\mathbf{D}_0\frac{\partial^2\tilde{z}}{\partial\xi^2}-\mathbf{V}\frac{\partial\tilde{z}}{\partial\xi}+\mathbf{N}_1(\xi)\tilde{z}+\mathbf{N}_2(\xi)\tilde{k}\right) \quad (A.1)$$

Note that $\tilde{z}$ can be written as a function of θ by using the inverse transformation of $\mathbf{T}$, which is given by

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

By injecting Eq. (A.2) in Eq. (A.1), one gets the following

$$\begin{aligned}\frac{\partial\theta}{\partial t} &= \mathbf{T}\mathbf{D}_0\frac{\partial^2(\mathbf{T}^{-1}\theta)}{\partial\xi^2}-\mathbf{T}\mathbf{V}\frac{\partial(\mathbf{T}^{-1}\theta)}{\partial\xi}+\mathbf{T}\mathbf{N}_1(\xi)\mathbf{T}^{-1}\theta+\mathbf{T}\mathbf{N}_2(\xi)\tilde{k}\\ &= \mathbf{T}\mathbf{D}_0\frac{d^2\mathbf{T}^{-1}}{d\xi^2}\theta+2\mathbf{T}\mathbf{D}_0\frac{d\mathbf{T}^{-1}}{d\xi}\frac{\partial\boldsymbol{\theta}}{\partial\xi}+\mathbf{T}\mathbf{D}_0\mathbf{T}^{-1}\frac{\partial^2\theta}{\partial\xi^2}-\mathbf{T}\mathbf{V}\frac{d\mathbf{T}^{-1}}{d\xi}\theta\\ &\quad -\mathbf{T}\mathbf{V}\mathbf{T}^{-1}\frac{\partial\theta}{\partial\xi}+\mathbf{T}\mathbf{N}_1(\xi)\mathbf{T}^{-1}\theta+\mathbf{T}\mathbf{N}_2(\xi)\tilde{k}\end{aligned}$$

It can be easily observed from the expression of $\mathbf{T}^{-1}$ that

$$\frac{d\mathbf{T}^{-1}}{d\xi}=\frac{\mathbf{D}_0^{-1}\mathbf{V}}{2}\exp\left(\frac{\mathbf{D}_0^{-1}\mathbf{V}}{2}\xi\right)=\frac{\mathbf{D}_0^{-1}\mathbf{V}}{2}\mathbf{T}^{-1}$$

$$\frac{d^2\mathbf{T}^{-1}}{d\xi^2}=\frac{\mathrm{D}_0^{-1}\mathrm{V}\mathrm{D}_0^{-1}\mathrm{V}}{4}=\frac{\mathrm{D}_0^{-1}\mathrm{V}\mathrm{D}_0^{-1}\mathrm{V}}{4}\mathbf{T}^{-1}$$

Plugging these expressions into the previous equation, one has

$$\begin{aligned}\frac{\partial\theta}{\partial t} &=\mathbf{T}\frac{\mathbf{V}\mathbf{D}_0^{-1}\mathbf{V}}{4}\mathbf{T}^{-1}\theta+\mathbf{T}\mathbf{V}\mathbf{T}^{-1}\frac{\partial\boldsymbol{\theta}}{\partial\xi}+\mathbf{T}\mathbf{D}_0\mathbf{T}^{-1}\frac{\partial^2\theta}{\partial\xi^2}\\ &\quad-\mathbf{T}\mathbf{V}\frac{\mathbf{D}_0^{-1}\mathbf{V}}{2}\mathbf{T}^{-1}\theta-\mathbf{T}\mathbf{V}\mathbf{T}^{-1}\frac{\partial\theta}{\partial\xi}+\mathbf{T}\mathbf{N}_1(\xi)\mathbf{T}^{-1}\theta+\mathbf{T}\mathbf{N}_2(\xi)\tilde{k}\\ &=\mathbf{T}\mathbf{D}_0\mathbf{T}^{-1}\frac{\partial^2\theta}{\partial\xi^2}+\left(\mathbf{T}\mathbf{N}_1(\xi)\mathbf{T}^{-1}-\mathbf{T}\frac{\mathbf{V}\mathbf{D}_0^{-1}\mathbf{V}}{4}\mathbf{T}^{-1}\right)\theta+\mathbf{T}\mathbf{N}_2(\xi)\tilde{k}\end{aligned}$$

which leads to Eq. (6a).

Appendix B. Eigenvalues and eigenfunctions of F_{11} and F_{22}

In this appendix, we are interested in giving the expression of the eigenvalues and eigenfunctions of the operators F_{11} and F_{22}. Note that they both have the following form

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

The fact that **h** is a function of space makes the eigenvalue problem challenging. Here, the length of the reactor is divided to a finite number of segments. It is assumed that at each segment the value of **h** is constant. Full description of this approach and more details can be found in [16, Section 3]. The eigenvalues λ_i are given by

$$\lambda_i^2=\mathbf{d}\omega_i^2+\mathbf{h}_i$$

where $\{\omega_i\}_{i\geq1}$ is the set of solutions of the following resolvent equation:

$$\tan(\omega_i l)=\frac{4\mathbf{d}\omega_i v}{4\mathbf{d}^2\omega_i^2-v^2}$$

and the corresponding eigenfunctions are given by

$$\phi_i(\xi)=a_1\rho_i\sin(\omega_i\xi)+\eta_i\cos(\omega_i\xi)$$

where $\rho_1=1$; $\rho_i=s_{i,i-1}s_{i-1,i-2}\ldots s_{2,1}$ and

$$\begin{aligned}s_{i,i-1} &= \frac{\sin(\omega_{i-1}\xi_i)+\eta_{i-1}\cos(\omega_{i-1}\xi_i)}{\sin(\omega_i\xi_i)+\eta_i\cos(\omega_i\xi_i)}\\ s_{N,N-1} &= \frac{1}{h_N}\frac{\sin(\omega_{N-1}\xi_N)+\eta_{N-1}\cos(\omega_{N-1}\xi_N)}{\sin(\omega_N\xi_N)+\eta_N\cos(\omega_N\xi_N)}\\ \eta_1 &= -\frac{v\sin(\omega_1\xi_1)-2\mathbf{h}_1\omega_1\cos(\omega_1\xi_1)}{v\cos(\omega_1\xi_1)+2\mathbf{h}_1\omega_1\sin(\omega_1\xi_1)}\\ \eta_i &= \frac{\cos(\omega_i\xi_i)(\sin(\omega_{i-1}\xi_i)+\eta_{i-1}\cos(\omega_{i-1}\xi_i))-\sin(\omega_i\xi_i)(\cos(\omega_{i-1}\xi_i)-\eta_i\sin(\omega_{i-1}\xi_i))}{\sin(\omega_i\xi_i)(\sin(\omega_{i-1}\xi_i)+\eta_{i-1}\cos(\omega_{i-1}\xi_i))+\cos(\omega_i\xi_i)(\cos(\omega_{i-1}\xi_i)-\eta_i\sin(\omega_{i-1}\xi_i))}.\end{aligned}$$

Appendix C. Conversion of Riccati equation (42) into (44)

In this appendix, we are interested in converting the operator Riccati equation (42) into the set of algebraic equations (44).

Let us set $\mathbf{x}_1 = \Phi_m$ and $\mathbf{x}_2 = \Phi_n$ and assume that $\Pi_{nm} = \langle \Phi_n, \Pi\Phi_m \rangle$. The Riccati equation (42) can be written as

$$\langle \mathrm{A}\Phi_m, \Pi\mathbf{\Phi}_n \rangle + \langle \Pi\mathbf{\Phi}_m, \mathrm{A}\Phi_n \rangle + \langle \mathbf{\Phi}_m, \mathbf{C}^*\mathrm{C}\Phi_n \rangle - \langle \Pi\mathbf{\Phi}_m, \mathrm{BB}^*\Pi\mathbf{\Phi}_n \rangle = 0 \quad \text{(C.1)}$$

Using the fact that σ_n is an eigenvalue of the operator $\mathbf{A}$ and Φ_n is the corresponding eigenvector, one has

$$\begin{aligned}\langle \mathrm{A}\Phi_m, \Pi\mathbf{\Phi}_n \rangle + \langle \Pi\mathbf{\Phi}_m, \mathrm{A}\Phi_n \rangle &= \langle \sigma_m\mathbf{\Phi}_m, \Pi\mathbf{\Phi}_n \rangle + \langle \Pi\mathbf{\Phi}_m, \sigma_n\mathbf{\Phi}_n \rangle \\ &= \sigma_m\langle \mathbf{\Phi}_m, \Pi\mathbf{\Phi}_n \rangle + \sigma_n\langle \Pi\mathbf{\Phi}_m, \mathbf{\Phi}_n \rangle \\ &= \sigma_m\Pi_{nm} + \sigma_n\Pi_{nm} = (\sigma_m + \sigma_n)\Pi_{nm}.\end{aligned}$$

Now let us calculate the last term of the Riccati equation (C.1). In order to do so, we will use the fact that any element in the space can be written uniquely in the Riesz basis, particularly, we will use

$$\mathrm{BB}^*x = \sum_{k=0}^{\infty} \langle \mathrm{BB}^*x, \Phi_k \rangle \Phi_k$$

Therefore, one has

$$\begin{aligned}\langle \Pi\mathbf{\Phi}_m, \mathrm{BB}^*\Pi\mathbf{\Phi}_n \rangle &= \left\langle \Pi\mathbf{\Phi}_m, \sum_{k=0}^{\infty} \langle \mathrm{BB}^*\Pi\mathbf{\Phi}_n, \Phi_k \rangle \Phi_k \right\rangle \\ &= \sum_{k=0}^{\infty} \langle \mathrm{BB}^*\Pi\mathbf{\Phi}_n, \Phi_k \rangle \langle \Pi\mathbf{\Phi}_m, \Phi_k \rangle \\ &= \sum_{k=0}^{\infty} \langle \Pi\mathbf{\Phi}_n, \mathrm{BB}^*\Phi_k \rangle \Pi_{km} \\ &= \sum_{k=0}^{\infty} \left\langle \Pi\mathbf{\Phi}_n, \sum_{l=0}^{\infty} \langle \mathrm{BB}^*\Phi_k, \Phi_l \rangle \Phi_l \right\rangle \Pi_{km} \\ &= \sum_{k,l=0}^{\infty} \langle \mathrm{BB}^*\Phi_k, \Phi_l \rangle \langle \Pi\mathbf{\Phi}_n, \Phi_l \rangle \Pi_{km} \\ &= \sum_{k,l=0}^{\infty} \mathbf{B}_{kl}\Pi_{nl}\Pi_{km}\end{aligned}$$

where $\mathbf{B}_{kl} = \langle \mathbf{BB}^*\Phi_k, \Phi_l \rangle = \langle \mathbf{B}^*\Phi_k, \mathbf{B}^*\Phi_l \rangle$. Moreover, if we put $\mathbf{C}_{nm} = \langle \Phi_n, \mathbf{C}^*\mathbf{C}\Phi_m \rangle$, then the Riccati equation (C.1) can be written as a set of the following algebraic equations:

$$(\sigma_m + \sigma_n)\Pi_{nm} + \mathbf{C}_{nm} - \sum_{k,l=0}^{\infty} \mathbf{B}_{kl}\Pi_{nl}\Pi_{km} = 0 \quad \text{(C.2)}$$

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