Extension of Kalman Filtering to Semilinear PDE Systems-Application to Pulp and Paper

Ivan Francisco Yupanqui Tello * † Alain Vande Wouver * Daniel Coutinho †

* *Systems, Estimation, Control, and Optimization (SECO), University of Mons, Belgium.*

† *Postgraduate Program in Engineering of Automation and Systems, Federal University of Santa Catarina, Brazil.*

E-mails: *ivanfrancisco.yupanquitello@umons.ac.be*, *alain.vandewouwer@umons.ac.be*, *daniel.coutinho@ufsc.br*

***Abstract*—This paper deals with the observer design of nonlinear tubular chemical reactor models. The analysis is performed on a linearized version of the model around a steady-state profile, in which some coefficients are a function of the spatial variable. The study starts from a general model of chemical tubular reactors that will serve as a benchmark model for the formulation in the infinite dimensional Hilbert state space. The optimal output injection operator associated to the proposed observer is computed via the solution of the infinite-dimensional Riccati equation in the space variable. The performance of the observer is illustrated through numerical experiments of an industrial pulp bleaching tubular reactor model.**

***Index Terms*—distributed parameter systems, boundary observation, optimal observer, pulp bleaching tubular reactor**

I. Introduction

Distributed chemical reaction systems correspond to processes involving reactions with phases that are not well mixed, thus resulting in spatial dependencies. Chemical tubular reactors (CTR) are a prime example of such systems, see e.g. [10]. The dependent variables of this model are typically concentrations and temperatures. These variables, which depend on time and spatial coordinates, are described by partial differential equations (PDEs) consisting of material and heat balances that couple the effects of advection, reaction, diffusion along with initial and boundary conditions. The time and space dependence makes the analysis of distributed reaction systems more complex. In addition, depending on the type of boundary conditions, these systems can be more or less difficult to analyze.

On-line state observation is particularly critical in spatially distributed reactors due to the high dimensionality associated with the dynamic representation. In this class of systems, the mass and energy balances result into a nonlinear set of partial differential equations [1]. In addition the observer must be supplied with several (online) state measurements along the spatial domain which is normally not feasible due to the limited number of sensors [11]. In this work, we are interested in boundary observation of a distributed chemical tubular reactor system described by a set of nonlinear parabolic PDEs. By linearizing the nonlinear equations in the vicinity of the system steady state profile, a set of linear parabolic PDEs with spatially varying coefficients is derived. Then, the state estimation problem can be transformed into a well-posed abstract boundary problem. The spectrum of the resulting linear operator is computed by solving an eigenvalue problem using the differential transformation technique. Finally, by using the spectral properties of the system, the infinite-dimensional Riccati equation is converted into a set of coupled algebraic equations, which can be solved numerically.

The majority of the previous work on boundary problems of infinite-dimensional systems concentrated on cases that are described by a single spatially invariant parabolic PDE [2], [8]. This work investigates an approach for systems that are described by a set of PDEs with spatially varying coefficients which can model the linear approximation of several chemical engineering processes. A case study involving the industrial pulp bleaching tubular reactor model is used to illustrate the proposed method. The reaction scheme facilitates the triangularization of the state operator, which simplifies the computation of the spectrum of the system.

The paper is organized as follows. Section II focuses on the mathematical description of the system of interest. In Section III, the general formulation of the optimal state observation problem for infinite dimensional systems is presented. The solution of the infinite-dimensional Riccati equation provides the optimal output injection operator. In Section IV, the industrial pulp bleaching tubular reactor model is presented. In Section V, the eigenvalue problem of the state operator of the linearized system is addressed. Section VI deals with the solution of the infinite-dimensional Riccati equation associated with the system in question. Throughout this work, the mathematical notation is standard for infinite dimensional systems; see, for instance, [4].

II. Mathematical Model Description and Formulation

In particular, the dynamics of an axial dispersion tubular reactor for one isothermal reaction is given by the following general dynamical model:

$$\theta_t(z,t) = \Gamma\theta_{zz}(z,t) - \Upsilon\theta_z(z,t) + F(\theta(z,t)) \tag{1}$$

subject to the following boundary and initial conditions

$$\begin{array}{lcl} \Gamma\theta_z(0,t) &=& \Upsilon(\theta(0,t)-u_{in}(t)) \\ \theta_z(l,t) &=& 0 \\ \theta(z,0) &=& \theta_0(z) \end{array} \tag{2}$$

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where $\theta(\cdot,t)=[\theta_1(\cdot,t),...,\ \theta_n(\cdot,t)]^T\in H=L_2^n(0,l)$ denotes the vector of state variables that represents the components concentration of the process, $z\in[0,l]$ (where l is the reactor length) and $t\in[0,\infty)$ denote the spatial and time variables, respectively. Γ and Υ are n-dimensional diagonal matrices of nonzero constant entries that represent the diffusion coefficients and the constant advective velocity respectively. F is assumed to be a locally Lipschitz continuous function from a specific subset of H into H. The associated state estimation problem for system (1)-(2) consists in designing a dynamical observer on the basis of its mathematical model, the measurement $\theta(0,t)$, and the input signal $u_{in}(t)\in\mathbb{R}^n$ which produces a convergent state estimate $\hat{\theta}(z,t)$ such that $\lim_{t\to\infty}\theta(z,t)-\hat{\theta}(z,t)\ =\ 0$. In order to design a linear observer having local convergence properties, the nonlinear system (1)-(2) is linearized around the steady state profile $(\theta_{ss}(z),u_{ss})$ and the resulting linear system is given by:

$$\tilde{\theta}_t(z,t)=\Gamma\tilde{\theta}_{zz}(z,t)-\Upsilon\tilde{\theta}_z(z,t)+K_0(z)\tilde{\theta}(z,t) \tag{3}$$

subject to the following boundary and initial conditions

$$\begin{array}{rcl}\Gamma\tilde{\theta}_z(0,t) & = & \Upsilon(\tilde{\theta}(0,t)-\tilde{u}_{in}(t))\\ \tilde{\theta}_z(l,t) & = & 0\\ \tilde{\theta}(z,0) & = & \tilde{\theta}_0(z)\end{array} \tag{4}$$

where $K_0(z)=\frac{\partial F}{\partial\theta}(\theta_{ss}(z))$, and $\tilde{\theta}(z,t)=\theta(z,t)-\theta_{ss}(z)$ and $\tilde{u}_{in}(t)=u_{in}(t)-u_{ss}$ are the state vector and control input deviations with respect to their steady state profiles, respectively. The equation in (3) 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. To this end, consider the following transformation:

$$x(z,t)=T\tilde{\theta}(z,t)=\exp\left(-\frac{1}{2}\Gamma^{-1}\Upsilon z\right)\tilde{\theta}(z,t). \tag{5}$$

By using the above transformation, the PDE system (3)-(4) can be described in terms of a new state vector $x(z,t)$ leading to the following linear diffusion-reaction coupled parabolic PDE:

$$x_t(z,t)=\Gamma x_{zz}(z,t)+K(z)x(z,t) \tag{6}$$

subject to the boundary and initial conditions given by

$$\begin{array}{rcl}\Gamma x_z(0,t) & = & \frac{1}{2}\Upsilon x(0,t)-\Upsilon\tilde{u}_{in}(t)\\ \Gamma x_z(l,t) & = & -\frac{1}{2}\Upsilon x(l,t)\\ x(z,0) & = & T^{-1}\tilde{\theta}_0(z),\end{array} \tag{7}$$

where the matrix $K(z)$ is given by

$$K(z)=K_0(z)-\tfrac{1}{4}\Upsilon\Gamma_0^{-1}\Upsilon \tag{8}$$

A. Infinite-dimensional formulation

We can formulate the system as an abstract boundary system on the infinite-dimensional space H [4] by considering that $u(t)=\Upsilon\tilde{u}_{in}(t)$ yielding the following state space representation:

$$\begin{array}{rcl}\dot{x}(t) & = & \mathfrak{U}x(t)\quad x(0)=x_0\\ \mathfrak{B}x(t) & = & u(t)\\ y(t) & = & \mathfrak{C}x(t)\end{array} \tag{9}$$

where $x(\cdot,t)\in H$ and the operators $\mathfrak{U}:D(\mathfrak{U})\to H$, $\mathfrak{B}:D(\mathfrak{B})\to\mathbb{R}^n$, $\mathfrak{C}:D(\mathfrak{C})\to\mathbb{R}^n$ are defined as

$$\begin{aligned}&\mathfrak{U}=\Gamma\frac{d^2}{dz^2}+K(z)\cdot I\\ &D(\mathfrak{U})=\Big\{x\in H: x,\ \frac{dx}{dz}\text{ are a.c. },\frac{d^2x}{dz^2}\in H\\ &\qquad\qquad\text{and }\ \Gamma\frac{dx}{dz}(l)+\frac{1}{2}\Upsilon x(l)=0\Big\}\\ &\mathfrak{B}x=\left[-\Gamma\tfrac{dx}{dz}(0)+\tfrac{1}{2}\Upsilon x(0)\right]\\ &\mathfrak{C}x=\left[x(0)\right].\end{aligned} \tag{10}$$

Problems with boundary control inputs occur frequently in applications, but unfortunately they do not fit into the standard formulation with bounded control operators. However, for sufficiently smooth control inputs $u(t)$ it is possible to reformulate such problem on an equivalent form with a new bounded control operator as described in [4]. Firstly, a new operator $\mathcal{A}$ is defined by

$$\mathcal{A}x=\mathfrak{U}x, \tag{11}$$

$$\begin{aligned}D(\mathcal{A})&=D(\mathfrak{U})\cap\ \ker\mathfrak{B}\\ &=\Big\{x\in H: x,\ \frac{dx}{dz}\ \text{ are a.c.},\ \frac{d^2x}{dz^2}\in H\quad\text{and}\\ &\qquad\Gamma\frac{dx}{dz}(0)-\frac{\Upsilon}{2}x(0)=0,\ \Gamma\frac{dx}{dz}(l)+\frac{\Upsilon}{2}x(l)=0\Big\}.\end{aligned}$$

By using standard results of C_0-semigroup theory (see, e.g., [4] and [5]), it can be shown that, if the entries of $K(z)$ are bounded, then $\mathcal{A}$ is the infinitesimal generator of a C_0-semigroup on H. Assume that there exists an operator $B\in\mathscr{L}(\mathbb{R}^n,H)$ such that for all $u\in\mathbb{R}^n$, $Bu\in D(\mathfrak{U})$ and $\mathfrak{B}Bu=u$.

By introducing the new state $\xi(t)=x(t)-Bu(t)$, the following resulting system with distributed bounded control operator is equivalent to system (9) in the sense of [4].

$$\begin{aligned}&\dot{\xi}(t)=\mathcal{A}\xi(t)+\mathfrak{U}Bu(t)-B\dot{u}(t)\quad\xi(0)=\xi_0\\ &y(t)=\mathfrak{C}\xi(t)+\mathfrak{C}Bu(t).\end{aligned} \tag{12}$$

Therefore, the proposed Luenberger-type observer is formally given by

$$\dot{\hat{\xi}}(t)=\mathcal{A}\hat{\xi}(t)+\mathfrak{U}Bu(t)-B\dot{u}(t)+\mathcal{L}(\hat{y}(t)-y(t))\quad\hat{\xi}(0)=\hat{\xi}_0$$

$$\hat{y}(t)=\mathfrak{C}\hat{\xi}(t)+\mathfrak{C}Bu(t) \tag{13}$$

in such a way that the dynamics of the observer error $e(t)=\hat{\xi}(t)-\xi(t)=\hat{x}(t)-x(t)$ satisfies

$$e(t)=(\mathcal{A}+\mathcal{L}\mathfrak{C})e(t)\quad e(0)=e_0. \tag{14}$$

The convergence of the observer (13) is achieved by finding an bounded operator $\mathcal{L}\in\mathscr{L}(\mathbb{R}^n,H)$ which ensures the exponential stability of the corresponding error dynamics (14). Finally, we can recover the estimation of the original state by using $\hat{x}(t) = \hat{\xi}(t) + Bu(t)$.

III. Optimal state observation

This section is devoted to present the optimal state observation approach for system (12) considering noisy measurements. The fundamental result for infinite-dimensional linear systems is the well-known Kalman filter [4]. Considering system (12) with noisy measured output and $\mathfrak{C} \in \mathscr{L}(H, \mathbb{R}^n)$ described by

$$\begin{aligned} \dot{\xi}(t) &= \mathcal{A}\xi(t) + \mathfrak{U}Bu(t) - B\dot{u}(t) \\ y(t) &= \mathfrak{C}\xi(t) + \mathfrak{C}Bu(t) + v(t) \end{aligned} \tag{15}$$

where it is assumed that $v(t) \in L_2([0,\infty], \mathbb{R}^n)$ is uncorrelated white Gaussian noise with mean zero and covariance $V = V^* > 0$. The goal is to estimate the states of system (15) in an optimal sense. Thus, the observer system (13) with $\mathcal{L} \in \mathscr{L}(\mathbb{R}^n, H)$ that minimizes the estimation cost

$$J_e = \lim_{t\to\infty} \mathbb{E}[\|e(t)\|^2]$$

is called Kalman filter, where $\mathbb{E}[X]$ is the expectation of X.

Theorem 3.1: ([4]) $\mathcal{L} = -\hat{\Pi}\mathfrak{C}^* V^{-1}$ is the unique output injection operator of the Kalman filter (13), where $\hat{\Pi}$ is a self adjoint non-negative operator $\hat{\Pi} \in \mathscr{L}(H)$ and the unique solution of the infinite-dimensional Ricatti equation

$$\langle \hat{\Pi}\xi_1, \mathcal{A}^*\xi_2\rangle + \langle \mathcal{A}^*\xi_1, \hat{\Pi}\xi_2\rangle - \langle \mathfrak{C}\hat{\Pi}\xi_1, V^{-1}\mathfrak{C}\hat{\Pi}\xi_2\rangle = 0 \tag{16}$$

for all $\xi_1,\ \xi_2 \in D(\mathcal{A}^*)$.

IV. The pulp bleaching tubular reactor

The bleaching reactor model consists of a set of nonlinear coupled PDEs. The two reactants in the model are chlorine dioxide (C) and lignin (L). The reaction term is a bilinear term. The PDEs describing the reactor dynamics are [6]:

$$\begin{aligned} L_t(z,t) &= \gamma L_{zz}(z,t) - vL_z(z,t) - k_L L(z,t)C(z,t) \\ C_t(z,t) &= \gamma C_{zz}(z,t) - vC_z(z,t) - k_c L(z,t)C(z,t) \end{aligned} \tag{17}$$

and the boundary conditions are:

$$\begin{aligned} \gamma L_z(0,t) &= v(L(0,t) - L_{in}(t) - L_0) \\ \gamma C_z(0,t) &= v(C(0,t) - C_{in}(t) - C_0) \\ L_z(h,t) &= 0 \\ C_z(h,t) &= 0 \end{aligned} \tag{18}$$

where C_{in}, L_{in}, h, C_0 and L_0 are the inlet chlorine and lignin concentrations, the bleaching tower height, and constant adjustment parameters determined from the kinetic studies carried out by [9]. The model described by (17)-(18) takes the form of (1) by considering

$$\theta(z,t) = \begin{bmatrix} L(z,t) \\ C(z,t) \end{bmatrix},\ u_{in}(t) = \begin{bmatrix} L_{in}(t) + L_0 \\ C_{in}(t) + C_0 \end{bmatrix},\ \Gamma = \begin{bmatrix} \gamma & 0 \\ 0 & \gamma \end{bmatrix},$$
$$\Upsilon = \begin{bmatrix} v & 0 \\ 0 & v \end{bmatrix},\ F(\theta) = \begin{bmatrix} k_L L(z,t)C(z,t) \\ k_c L(z,t)C(z,t) \end{bmatrix}.$$

The adopted numerical values for the process parameters are taken from Table I (see [6]).

TABLE I
NUMERICAL VALUES OF THE PROCESS PARAMETERS

Parameter	Value
h	1 m
k_C	0.006
k_L	0.0035
L_{inss}	31 Kappa
L_0	9 Kappa
C_{inss}	2.5 g/l
v	1/30 m/min
γ	0.5/30 m^2/min

The steady state profiles of $L(z,t)$ and $C(z,t)$ are shown in Figure 1. They were obtained by solving numerically the steady equation related to (17)-(18) and considering the parameters given in Table I.

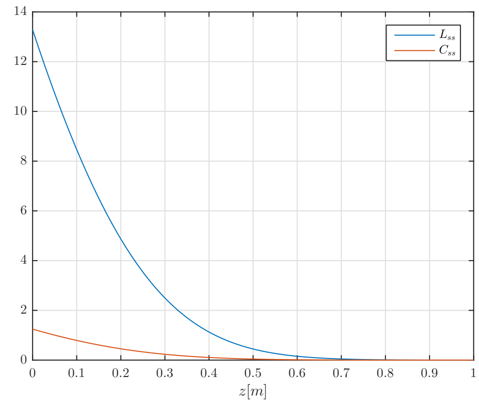

Fig. 1. Steady state profiles.

The linearized model, according to (3)-(4), can be written as follows:

$$\begin{aligned} \begin{bmatrix} \tilde{L}_t(z,t) \\ \tilde{C}_t(z,t) \end{bmatrix} &= \begin{bmatrix} \gamma & 0 \\ 0 & \gamma \end{bmatrix} \begin{bmatrix} \tilde{L}_{zz}(z,t) \\ \tilde{C}_{zz}(z,t) \end{bmatrix} - \begin{bmatrix} v & 0 \\ 0 & v \end{bmatrix} \begin{bmatrix} \tilde{L}_z(z,t) \\ \tilde{C}_z(z,t) \end{bmatrix} \\ &\quad + \begin{bmatrix} -k_L C_{ss}(z) & -k_L L_{ss}(z) \\ -k_C C_{ss}(z) & -k_C L_{ss}(z) \end{bmatrix} \begin{bmatrix} \tilde{L}(z,t) \\ \tilde{C}(z,t) \end{bmatrix} \end{aligned} \tag{19}$$

subject to the following boundary conditions

$$\begin{aligned} \begin{bmatrix} \gamma & 0 \\ 0 & \gamma \end{bmatrix} \begin{bmatrix} \tilde{L}_z(0,t) \\ \tilde{C}_z(0,t) \end{bmatrix} &= \begin{bmatrix} v & 0 \\ 0 & v \end{bmatrix} \left(\begin{bmatrix} \tilde{L}(z,t) \\ \tilde{C}(z,t) \end{bmatrix} - \begin{bmatrix} \tilde{L}_{in}(t) \\ \tilde{C}_{in}(t) \end{bmatrix} \right) \\ \begin{bmatrix} \tilde{L}_z(h,t) \\ \tilde{C}_z(h,t) \end{bmatrix} &= 0. \end{aligned} \tag{20}$$

A. System triangularization

Due to the coupling of the state variables in both equations, a first step then consists in introducing a state transformation (which corresponds to a system triangularization) so that the first PDE becomes independent of the second one in order to facilitate the computation of the eigenvalues and eigenvectors of the state operator. Hence, let us consider the following state transformation:

$$\eta_1(z,t) = k_C\tilde{L}(z,t) - k_L\tilde{C}(z,t), \quad \eta_2(z,t) = \tilde{C}(z,t) \quad (21)$$

This change of variable yields the following set of PDEs:

$$\begin{aligned}\begin{bmatrix}\eta_{1t}(z,t)\\ \eta_{2t}(z,t)\end{bmatrix} &= \begin{bmatrix}\gamma & 0\\ 0 & \gamma\end{bmatrix}\begin{bmatrix}\eta_{1zz}(z,t)\\ \eta_{2zz}(z,t)\end{bmatrix} - \begin{bmatrix}\upsilon & 0\\ 0 & \upsilon\end{bmatrix}\begin{bmatrix}\eta_{1z}(z,t)\\ \eta_{2z}(z,t)\end{bmatrix}\\ &+ \begin{bmatrix}0 & 0\\ -C_{ss}(z) & -k_CL_{ss}(z) - k_LC_{ss}(z)\end{bmatrix}\begin{bmatrix}\eta_1(z,t)\\ \eta_2(z,t)\end{bmatrix} \quad (22)\end{aligned}$$

subject to the following boundary conditions

$$\begin{aligned}\begin{bmatrix}\gamma & 0\\ 0 & \gamma\end{bmatrix}\begin{bmatrix}\eta_{1z}(0,t)\\ \eta_{2z}(0,t)\end{bmatrix} &= \begin{bmatrix}\upsilon & 0\\ 0 & \upsilon\end{bmatrix}\left(\begin{bmatrix}\eta_1(0,t)\\ \eta_2(0,t)\end{bmatrix} - \begin{bmatrix}\eta_{1in}(t)\\ \eta_{2in}(t)\end{bmatrix}\right)\\ \begin{bmatrix}\eta_{1z}(h,t)\\ \eta_{2z}(h,t)\end{bmatrix} &= 0 \quad (23)\end{aligned}$$

This transformation has eliminated the reaction term from the first PDE and is related to the notion of reaction invariants. We also can convert (22)-(23) into a reaction-diffusion type set of PDEs if we define the vector variable $x(z,t)$ according to the transformation proposed in (5) leading to

$$\begin{bmatrix}x_1(z,t)\\ x_2(z,t)\end{bmatrix} = \mathrm{e}^{-\frac{\upsilon}{2\gamma}z}\begin{bmatrix}\eta_1(z,t)\\ \eta_2(z,t)\end{bmatrix}. \quad (24)$$

B. Infinite-dimensional formulation

By using the formulation described in Section II-A, we can initially represent the system, in the new state variables defined in (24), as an abstract boundary system on the Hilbert space $H = L^2(0,1) \oplus L^2(0,1)$ according to

$$\begin{aligned}\dot{x}(t) &= \mathfrak{A}x(t) \quad x(0) = x_0\\ \mathfrak{B}x(t) &= u(t)\\ y(t) &= \mathfrak{C}x(t)\end{aligned} \quad (25)$$

where $x(t) = \left\{\begin{bmatrix}x_1(\cdot,t)\\ x_2(\cdot,t)\end{bmatrix},\ 0 \le z \le l\right\} \in H$ and the operators $\mathfrak{A} : D(\mathfrak{A}) \to H$, $\mathfrak{B} : D(\mathfrak{B}) \to \mathbb{R}^2$, $\mathfrak{C} : D(\mathfrak{C}) \to \mathbb{R}^2$ are defined as

$$\mathfrak{A} = \begin{bmatrix}\gamma\frac{d^2}{dz^2} - \hat{k}_1 & 0\\ -C_{ss}(z) & \gamma\frac{d^2}{dz^2} - \hat{k}_2(z)\end{bmatrix} = \begin{bmatrix}\mathfrak{A}_{11} & 0\\ \mathfrak{A}_{21} & \mathfrak{A}_{22}\end{bmatrix}$$

$$\begin{aligned}D(\mathfrak{A}) = \Big\{x \in H : x,\ \frac{dx}{dz} \text{ are a.c. },\ \frac{d^2x}{dz^2} \in H \text{ and}\\ \gamma\frac{dx_1}{dz}(h) + \frac{\upsilon}{2}x_1(h) = 0,\\ \gamma\frac{dx_2}{dz}(h) + \frac{\upsilon}{2}x_2(h) = 0\Big\}\end{aligned}$$

$$\mathfrak{B}x = \begin{bmatrix}-\gamma\frac{dx_1}{dz}(0) + \frac{\upsilon}{2}x_1(0)\\ -\gamma\frac{dx_2}{dz}(0) + \frac{\upsilon}{2}x_2(0)\end{bmatrix}$$

$$\mathfrak{C}x = \begin{bmatrix}x_1(0)\\ x_2(0)\end{bmatrix} \quad (26)$$

with $\hat{k}_1 = \frac{\upsilon^2}{4\gamma}$ and $\hat{k}_2(z) = k_CL_{ss}(z) + k_LC_{ss}(z) + \frac{\upsilon^2}{4\gamma}$. Then, the equivalent system with bounded control operators is defined according to (12) by considering

$$\mathcal{A} = \begin{bmatrix}\gamma\frac{d^2}{dz^2} - \hat{k}_1 & 0\\ -C_{ss}(z) & \gamma\frac{d^2}{dz^2} - \hat{k}_2(z)\end{bmatrix} = \begin{bmatrix}\mathcal{A}_{11} & 0\\ \mathcal{A}_{21} & \mathcal{A}_{22}\end{bmatrix}$$

$$\begin{aligned}D(\mathcal{A}) = \Big\{x \in H : x,\ \frac{dx}{dz} \text{ are a.c. },\ \frac{d^2x}{dz^2} \in H \text{ and}\\ -\gamma\frac{dx_1}{dz}(0) + \frac{\upsilon}{2}x_1(0) = -\gamma\frac{dx_2}{dz}(0) + \frac{\upsilon}{2}x_2(0) = 0,\\ \gamma\frac{dx_1}{dz}(h) + \frac{\upsilon}{2}x_1(h) = \gamma\frac{dx_2}{dz}(h) + \frac{\upsilon}{2}x_2(h) = 0\Big\}\end{aligned}$$

and selecting

$$B = \begin{bmatrix}\frac{-2}{4\gamma+\upsilon h}z + \frac{4\gamma+2\upsilon h}{4\gamma\upsilon+\upsilon^2 h} & 0\\ 0 & \frac{-2}{4\gamma+\upsilon h}z + \frac{4\gamma+2\upsilon h}{4\gamma\upsilon+\upsilon^2 H}\end{bmatrix}. \quad (27)$$

Notice that B is such that $Bu \in \mathfrak{A}$ and $\mathfrak{B}Bu = u$.

V. Eigenvalues and eigenfunctions computation

The study of the spectrum of $\mathcal{A}$ allows the design of an observer with a certain decay rate of convergence as well as one in optimal sense. This section summarizes the computation of the eigenvalues and eigenvectors of operator $\mathcal{A}$.

Notice that $-\mathcal{A}_{11}$ and $-\mathcal{A}_{22}$ are both Sturm-Liouville operators, which are self-adjoint with respect to an appropriate inner product. It also implies that A_{11} and A_{22} are both Riesz-spectral operators [5].

A. Eigenvalues and eigenfunctions of $\mathcal{A}_{11}$ and $\mathcal{A}_{22}$

Now, let λ_n and χ_n be the eigenvalues and eigenfunctions of the operator $\mathcal{A}_{11}$, and μ_n and ψ_n be the eigenvalues and eigenfunctions of the operator $\mathcal{A}_{22}$. Then, it follows that:

- $\mathcal{A}_{11}$ is a linear operator with constant coefficients and its eigenvalues are given by

$$\lambda_n = -\gamma w_n^2 - \hat{k}_1, \text{ with } \tan(w_nh) = \frac{4\gamma w_n\upsilon}{4\gamma^2w_n^2 - \upsilon^2}$$

and the corresponding eigenfunctions are given by

$$\chi_n = \cos(w_n z) + \frac{\upsilon}{2\gamma w_n}\sin(w_n z).$$

- $\mathcal{A}_{22}$ is a linear operator with reaction coefficient depending on z, consequently the calculation of its spectrum is a challenging issue. This problem can be carried out by using the differential transformation [3]. The main stages can be summarized as follows:

Firstly, the eigenvalue μ and its corresponding eigenvectors ψ satisfy

$$\begin{aligned} \gamma \tfrac{d^2\psi}{dz^2}(z) - \hat{k}_2(z)\psi(z) &= \mu\psi(z) \\ -\gamma\psi_z(0) + \tfrac{\upsilon}{2}\psi(0) &= 0 \\ \gamma\psi_z(h) + \tfrac{\upsilon}{2}\psi(h) &= 0. \end{aligned} \tag{28}$$

The differential transformation $\overline{\psi}(k)$ and its inverse $\psi(z)$ are defined as

$$\overline{\psi}(k) = \tfrac{1}{k!}\tfrac{d^k\psi}{dz}(0), \quad \psi(z) = \textstyle\sum_{k=0}^{\infty} z^k\overline{\psi}(k). \tag{29}$$

Taking the differential transformation to (28), we obtain

$$\begin{aligned} \overline{\psi}(k+2) &= \frac{1}{\gamma(k+1)(k+2)}(\mu\overline{\psi}(k) \\ &\quad + \sum_{l=0}^{k}\hat{k}_2(z)\overline{\psi}(k-l)) \end{aligned} \tag{30}$$

$$\gamma\overline{\psi}(1) - \upsilon\overline{\psi}(0) = 0 \tag{31}$$

$$\sum_{k=1}^{\infty} kh^{k-1}\overline{\psi}(k) = 0. \tag{32}$$

Let $\overline{\psi}(0) = c$, from the recursive formula (30), we calculate $\overline{\psi}(1)$, $\overline{\psi}(2), ...,$ $\overline{\psi}(n_T)$, where n_T is decided by the convergence of the eigenvalue. Substituting $\overline{\psi}(1)...\overline{\psi}(n_T)$ into (32), we have

$$c[f^{(n_T)}(\mu)] = 0 \tag{33}$$

where $f^{(n_T)}(\mu)$ is a polynomial of μ corresponding to n_T. For nontrivial solutions of eigenfunctions, we have $c \neq 0$, and $f^{(n_T)}(\mu) = 0$, whose solutions are

$$\mu = \mu_i^{(n_T)}, \quad \text{where } i = 1, 2, ... \tag{34}$$

$\mu_i^{(n_T)}$ is the ith estimated eigenvalue corresponding to n_T, and n_T is decided by the following equation

$$|\mu_i^{(n_T)} - \mu_i^{(n_T-1)}| \leq \epsilon \tag{35}$$

where $\mu_i^{(n_T-1)}$ is the i-th estimated eigenvalue corresponding to $n_T - 1$ and ϵ is a small value we set. If (35), then $\mu_i^{(n_T)}$ is the ith eigenvalue μ_i. Substituting μ_i into $\overline{\psi}(0)$, $\overline{\psi}(2), ...,$ $\overline{\psi}(n_T)$ and using (32), we obtain

$$\psi_i(z) = \sum_{k=0}^{\infty} z^k\overline{\psi}_{\mu_i}(k) \tag{36}$$

where $\overline{\psi}_{\mu_i}(k)$ is $\overline{\psi}(k)$ whose μ is substituted by μ_i, and $\psi_i(z)$ is the eigenfunction corresponding to the eigenvalue μ_i.

The first four eigenvalues of $\mathcal{A}_{11}$ and $\mathcal{A}_{22}$ are as follows

$$\lambda = \{-0.0451, \ -0.2415, \ -0.7393, \ -1.5628\}$$
$$\mu = \{-0.0919, \ -0.8845, \ -1.2949 \ -13.2906\}.$$

B. Eigenvalues and eigenfunctions of the operator $\mathcal{A}$

The linear operator $\mathcal{A}$ is a Riesz-spectral operator and due to be triangular, its eigenvalues consist of the union of eigenvalues of $\mathcal{A}_{11}$ and $\mathcal{A}_{22}$, i.e., $\sigma(\mathcal{A}) = \sigma(\mathcal{A}_{11}) \cup \sigma(\mathcal{A}_{22})$, where:

$$\sigma(\mathcal{A}) = \begin{cases} \sigma_{2n+1} = \lambda_n, & \forall n \geq 0 \\ \sigma_{2n} = \mu_n, & \forall n \geq 1, \end{cases} \tag{37}$$

with the corresponding eigenvectors given by

$$\Phi_{2n+1} = \begin{bmatrix} \chi_n \\ (\lambda_n I - A_{22})^{-1}A_{21}\chi_n \end{bmatrix}, \quad \Phi_{2n} = \begin{bmatrix} 0 \\ \psi_n \end{bmatrix}. \tag{38}$$

The corresponding biorthonormal eigenfunctions can be found by solving the eigenvalue problem for the adjoint operator $\mathcal{A}^*$ and are given by

$$\Psi_{2n+1} = \begin{bmatrix} \chi_n \\ 0 \end{bmatrix}, \quad \Psi_{2n} = \begin{bmatrix} (\mu_n I - A_{11})^{-1}A_{21}\psi_n \\ \psi_n \end{bmatrix} \tag{39}$$

where

$$\begin{aligned} (\mu_n I - A_{11})^{-1}A_{21}\psi_n &= \textstyle\sum_{m=0}^{\infty} \frac{1}{\mu_n - \lambda_m}\langle A_{21}\psi_n, \chi_m\rangle\chi_m, \\ (\lambda_n I - A_{22})^{-1}A_{21}\chi_n &= \textstyle\sum_{m=0}^{\infty} \frac{1}{\lambda_n - \mu_m}\langle A_{21}\chi_n, \psi_m\rangle\psi_m. \end{aligned}$$

VI. Kalmam filter

Let us consider the optimal state estimation described in section III for the system given $\Sigma(\mathcal{A}, \ \mathfrak{C})$ and the observer system (13) with $V = I$. By arguments similar to those used in [7], it can be shown that the operator $\mathfrak{C}$ is $\mathcal{A}$-bounded. More precisely, it can be shown that

$$\mathfrak{C}x = x(0) = \langle (I - \mathcal{A})x, \sum_{n=1}^{\infty}\frac{1}{1-\sigma_n}\Phi_n(0)\Psi_n\rangle. \tag{40}$$

Since $\mathcal{A}$ is a Riesz-spectral operator where ϕ_n is the set of eigenvectors of $\mathcal{A}$ and Ψ_n is the set of eigenvectors of $\mathcal{A}^*$. The Riccati Equation (16) with $x_1 = \Psi_n$ and $x_2 = \Psi_m$ becomes

$$\langle \hat{\Pi}\Psi_n, \mathcal{A}^*\Psi_m\rangle + \langle \mathcal{A}^*\Psi_n, \hat{\Pi}\Psi_m\rangle - \langle \hat{\Pi}\Psi_n, \mathfrak{C}^*V^{-1}\mathfrak{C}\hat{\Pi}\Psi_m\rangle = 0. \tag{41}$$

If we assume that the solution has the self-adjoint form $\hat{\Pi}x = \sum_{n,m}\hat{\Pi}_{nm}\langle x, \Phi_m\rangle\Phi_n$, the following holds

$$\hat{\Pi}_{nm} = \langle \Psi_n, \hat{\Pi}\Psi_m\rangle = \hat{\Pi}_{mn} = \langle \Psi_m, \hat{\Pi}\Psi_n\rangle. \tag{42}$$

Using the fact that σ_n is an eigenvalue of the operator A^* and Ψ_n is the corresponding eigenvector, one has

$$\begin{aligned}\langle \hat{\Pi}\Psi_n, A^*\Psi_m\rangle + \langle A^*\Psi_n, \hat{\Pi}\Psi_m\rangle &= \langle \hat{\Pi}\Psi_n, \sigma_m\Psi_m\rangle + \langle \sigma_n\Psi_n, \hat{\Pi}\Psi_m\rangle \\ &= (\sigma_m + \sigma_n)\hat{\Pi}_{nm}.\end{aligned} \tag{43}$$

Furthermore regarding the last term of (41)

$$\begin{aligned}\langle \hat{\Pi}\Psi_n, \mathfrak{C}^*V^{-1}\mathfrak{C}\hat{\Pi}\Psi_m\rangle &= \langle \hat{\Pi}\Psi_n, \textstyle\sum_k \langle \mathfrak{C}^*V^{-1}\mathfrak{C}\hat{\Pi}\Psi_m, \Phi_k\rangle \Psi_k\rangle \\ &= \textstyle\sum_k \langle \mathfrak{C}^*V^{-1}\mathfrak{C}\hat{\Pi}\Psi_m, \Phi_k\rangle \langle \hat{\Pi}\Psi_n, \Psi_k\rangle \\ &= \textstyle\sum_k \langle \hat{\Pi}\Psi_m, \mathfrak{C}^*V^{-1}\mathfrak{C}\Phi_k\rangle \hat{\Pi}_{nk} \\ &= \textstyle\sum_k \langle \hat{\Pi}\Psi_m, \sum_l \langle \mathfrak{C}^*V^{-1}\mathfrak{C}\Phi_k, \Phi_l\rangle \Psi_l\rangle \hat{\Pi}_{nk} \\ &= \textstyle\sum_{k,l} \langle \mathfrak{C}^*V^{-1}\mathfrak{C}\Phi_k, \Phi_l\rangle \langle \hat{\Pi}\Psi_m, \Psi_l\rangle \hat{\Pi}_{nk} \\ &= \textstyle\sum_{k,l} \mathfrak{C}_{kl}\hat{\Pi}_{ml}\hat{\Pi}_{nk}.\end{aligned} \tag{44}$$

Then Equation (41) becomes a system of infinite number of coupled scalar equations

$$(\sigma_n + \sigma_m)\hat{\Pi}_{nm} - \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \mathfrak{C}_{lk}\hat{\Pi}_{lm}\hat{\Pi}_{kn} = 0, \tag{45}$$

where $\mathfrak{C}_{lk} = \langle \mathfrak{C}^*V^{-1}\mathfrak{C}\Phi_k, \Phi_l\rangle$. Once the parameters Π_{mn} of the operator Π are calculated, the output injection operator can be computed. Equation (45) 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 output injection operator given by

$$\mathcal{L}y = -\hat{\Pi}\mathfrak{C}^*V^{-1}y = -\sum_{n,m}^{N} \hat{\Pi}_{nm}\langle \mathfrak{C}^*V^{-1}y, \Psi_m\rangle \Psi_n. \tag{46}$$

A. Numerical results

A computation of the parameters of $\hat{\Pi}$ was carried by using $N = 15$ modes, $V = I$ and the parameters of the system given in Table I. The observer system has been simulated considering the parameters given in Table I with the initial profiles for the observer system as $\hat{L} = \hat{C} = 0$. Figures 2 and 3 show the evolution of the actual states L, C (red lines) and the estimated states $\hat{L}$, $\hat{C}$ (blue lines) related to the proposed observer.

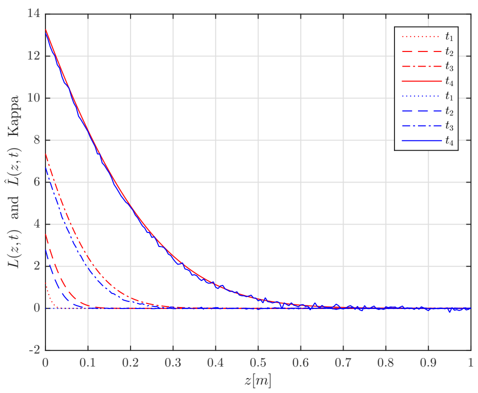

Fig. 2. Time evolution of the spatial profile of $L(z,t)$ and $\hat{L}(z,t)$ at time instants $t_1 = 0,\ t_2 = 0.09\ min,\ t_3 = 0.4491\ min,\ t_4 = 1.7991\ min.$

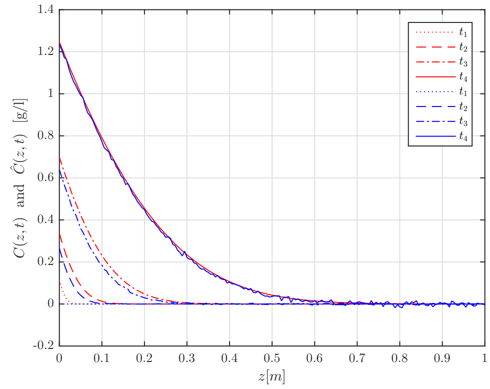

Fig. 3. Time evolution of the spatial profile of $C(z,t)$ and $\hat{C}(z,t)$ at time instants $t_1 = 0,\ t_2 = 0.09\ min,\ t_3 = 0.4491\ min,\ t_4 = 1.7991\ min$

VII. Conclusion

In this paper, an optimal state observer is presented for a certain class of nonlinear coupled parabolic PDEs considering only boundary measurements. To this end, a linear approximate model of the system around the steady-state profile is considered, which results in a linear DPS with spatially-varying coefficients. The observer output injection operator is determined by solving the infinite-dimensional Riccati equation making use of the properties associated to Riesz-spectral operators. The proposed observer was applied to a tubular bleaching reactor and the observer performance was studied via numerical simulations. It has been observed that the formulated observer has provided an accurate estimation of the states of the original plant.

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