Observer Design for Chemical Tubular Reactors Based on System Linearization

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***Abstract*— This paper presents an observer design technique for a class or nonlinear coupled parabolic PDEs using the infinite dimensional approach in Hilbert spaces. In particular, the linear approximate model incorporating the spatially varying coefficients of the set of PDEs is used for designing a Luenberger-like observer in order to achieve exponential convergence of the estimation error dynamics. The proposed observer is applied to a chemical tubular reactor considering only boundary measurements. The observer performance is assessed via numerical simulations.**

Key words: distributed parameter systems, boundary observation, parabolic PDEs, tubular reactor.

I. INTRODUCTION

Distributed parameter systems (DPSs) are a class of important processes in which process variables depend not only on time but also on spatial coordinates. Examples of DPSs can be found in (bio)process monitoring and control, robotics, glass feeders, biomedical engineering and flexible structures [1], [2], [3], [4]. The description of DPSs often takes the form of hyperbolic, parabolic or elliptic partial differential equations (PDEs). Parabolic PDEs represent the dynamics of industrial processes involving convection and diffusion effects. One of the most important examples of such class of systems is the chemical tubular reactor (CTR) with axial dispersion. In order to capture the effects of reactions, diffusion and convection in the reactor, the reactor model is often described by a set of coupled parabolic PDEs.

For the operation and monitoring of processes described by PDEs, the knowledge of system states is of fundamental importance. In most cases it is not possible to have full information of the system states because of economical reasons and/or the fact that not all variables can be measured, that is, installing all the necessary sensors may not be physically possible or their costs may become prohibitive. In such a case, the internal states can be estimated from the measurement of process inputs and outputs. State observers are usually based on the system model with an additional output injection term to improve the convergence of the observation error and they are digitally implemented by a computer for monitoring and/or feedback purposes. Due to the fact that many processes in real world applications can be modeled in terms of PDEs, the synthesis of observers for DPSs has received a growing interest in the last decades. Among the available survey papers, we can cite those by [5], [6], or a more recent textbook [7] where a broad class of estimation techniques for DPSs are presented.

In this work, we are interested in boundary observation of a 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 control problem by applying an exact transformation. The spectrum of the resulting linear operator is computed by solving an eigenvalue problem using techniques for the solution of the heat equation for composite media. Finally, the output injection operator is obtained using the decomposition of the state space induced by the spectral projection operator.

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 [8], [9], [10], [11]. This work investigates an approach for systems that are described by a set of PDEs with spatially varying coefficients, which would model many chemical engineering processes. A case study involving a tubular reactor, wherein the catalytic cracking of gas oil takes place, is used to illustrate our method. The reaction scheme results in a triangular 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 particular, the nonlinear system is linearized around a steady state profile and appropriate state transformations are used to cast the linearized system as a well-posed infinite-dimensional system. In Section III, the dynamics of the tubular reactor (wherein the catalytic cracking of gas oil takes place) is presented. This reaction consists of two series parallel reactions. The mass balance for the reactor results in a set of coupled nonlinear parabolic PDEs. Section IV considers the design of the observer system based on the spectrum decomposition where the triangular structure of the state operator simplifies the computation of its spectrum. Throughout this work, the mathematical notation is standard

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for infinite dimensional systems; see, for instance, [8].

II. Mathematical model description

The dynamics of a one-dimensional tubular reactor with axial convection, dispersion and reaction is given by

$$\theta_t(z,t) = \Gamma_0\theta_{zz}(z,t) - \Upsilon\theta_z(z,t) + F(\theta(z,t)) \quad (1)$$

subject to the following boundary and initial conditions

$$\begin{array}{rcl} \Gamma_0\theta_z(0,t) &=& \Upsilon(\theta(0,t) - u_{in}(t)) \\ \theta_z(l,t) &=& 0 \\ \theta(z,0) &=& \theta_0(z) \end{array} \quad (2)$$

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 domains, respectively. Γ_0 and Υ are n-dimensional diagonal matrices of constant entries that represent the diffusion coefficients and the constant advective velocity respectively. Γ_0 is assumed to be nonsingular and F is a locally Lipschitz continuous nonlinear function from a specific subset of H into H describing the kinetic part of the process (reaction rate equations). 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 $u_{in}(t)$ which produces a convergent state estimate $\hat{\theta}(z,t)$ such that $\lim_{t\to\infty}\theta(z,t) - \hat{\theta}(z,t) = 0$.

The nonlinear system (1)-(2) can be linearized around the steady state profile $(\theta_{ss}(z),u_{ss})$ and the resulting linear system is given by:

$$\tilde{\theta}_t(z,t) = \Gamma_0\tilde{\theta}_{zz}(z,t) - \Upsilon\tilde{\theta}_z(z,t) + K_0(z)\tilde{\theta}(z,t) \quad (3)$$

subject to the following boundary and initial conditions

$$\begin{array}{rcl} \Gamma_0\tilde{\theta}_z(0,t) &=& \Upsilon(\tilde{\theta}(0,t) - \tilde{u}_{in}(t)) \\ \tilde{\theta}_z(l,t) &=& 0 \\ \tilde{\theta}(z,0) &=& \tilde{\theta}_0(z) \end{array} \quad (4)$$

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

Remark 1: It should be emphasized that the formulation developed in this section can be extended to the case where the matrices Γ_0 and Υ are diagonalizable. Indeed, the state transformation can be used to return to the case where the matrices are diagonal. Moreover, in most chemical engineering processes, Γ_0 and Υ are symmetric and then diagonalizable.

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:

$$x(z,t) = T\tilde{\theta}(z,t) = \exp\left(-\frac{1}{2}\Gamma_0^{-1}\Upsilon z\right)\tilde{\theta}(z,t). \quad (5)$$

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:

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

subject to the boundary and initial conditions given by

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

where the matrices $K(z)$ and Γ are given by

$$\begin{array}{rcl} K(z) &=& T[K_0(z) - \frac{1}{4}\Upsilon\Gamma_0^{-1}\Upsilon]T^{-1} \\ \Gamma &=& T\Gamma_0T^{-1}. \end{array} \quad (8)$$

A. Infinite-dimensional formulation

We can formulate the system as an abstract boundary system on the infinite-dimensional space H [8] by considering that $u(t) = \Upsilon\tilde{u}_{in}(t)$ yielding the following state space representation:

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

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

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

B. Reformulation on the extended space

Boundary problems occur frequently in applications, but unfortunately they do not fit into the standard formulation $\Sigma(A, B, C)$ with bounded observation and control operators C and B, respectively. However, for sufficiently smooth control inputs $u(t)$ it is possible to reformulate such problem on an extended state space so that they lead to an associated system in the standard form $\Sigma(A^e, B^e, C^e)$ as described in [8]. Firstly, a new operator $\mathcal{A}$ is defined by

$$\mathcal{A}x = \mathfrak{U}x, \quad (11)$$

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

By using standard results of C_0-semigroup theory (see, e.g., [8] and [12]), 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 $B \in \mathcal{L}(U,H)$ such that for all $u \in U$, $Bu \in D(\mathfrak{U})$ and the following holds:

$$\mathfrak{B}Bu = u. \tag{12}$$

By defining the new input as $\dot{u}(t)$ and a new state

$$x^e(t) = \begin{bmatrix} x_1^e(t) \\ x_2^e(t) \end{bmatrix} = \begin{bmatrix} u(t) \\ x(t) - Bu(t) \end{bmatrix} \tag{13}$$

the system representation can be reformulated on the extended state space $H^e = U \oplus H$ as a well-posed system with bounded input operator and unbounded output operator:

$$\begin{aligned} \dot{x}^e(t) &= A^e x^e(t) + B^e \dot{u}(t) \\ y(t) &= C^e x^e(t) \end{aligned} \tag{14}$$

where

$$A^e = \begin{bmatrix} 0 & 0 \\ \mathfrak{U}B & \mathcal{A} \end{bmatrix} \quad B^e = \begin{bmatrix} I \\ -B \end{bmatrix} \quad C^e = \mathfrak{C}\begin{bmatrix} B & I \end{bmatrix}. \tag{15}$$

Observe that the operator C^e is well-defined on $U \oplus D(\mathfrak{C})$, provided that $D(B) \subset D(\mathfrak{C})$. Hence, the operator A^e generates a C_0-semigroup on H^e given by

$$T^e(t) = \begin{bmatrix} I & 0 \\ \int_0^t T(s)\mathfrak{U}Bxds & T(t) \end{bmatrix} \tag{16}$$

where $T(t)$ is the C_0-semigroup generated by $\mathcal{A}$. Since the performed transformation is an exact transformation, the resulting system (14) is equivalent to the original system in the sense of [8]. As we need to estimate $x(t)$ we must focus on the second state equation of (14) and the measured output $y(t)$ which can be rewritten as

$$\begin{aligned} \dot{x}_2^e(t) &= \mathcal{A}x_2^e(t) + \mathfrak{U}Bu(t) - B\dot{u}(t) \\ y(t) &= \mathfrak{C}x_2^e(t) + \mathfrak{C}Bu(t) \end{aligned} \tag{17}$$

Therefore, the proposed observer is formally given by

$$\begin{aligned} \dot{\hat{x}}_2^e(t) &= \mathcal{A}\hat{x}_2^e(t) + \mathfrak{U}Bu(t) - B\dot{u}(t) + L(\hat{y}(t) - y(t)) \\ \hat{y}(t) &= \mathfrak{C}\hat{x}_2^e(t) + \mathfrak{C}Bu(t). \end{aligned} \tag{18}$$

The convergence of the observer (18) is achieved by finding an bounded operator L which ensures the exponential stability of the corresponding error dynamics. Finally, we can recover the estimation of the original states by using

$$\hat{x}(t) = \hat{x}_2^e(t) + Bu(t). \tag{19}$$

III. Application to a Tubular Reactor

The process considered in this section is the tubular catalytic cracking reactor presented in [13]. This process involves axial dispersion, convection and the following reactions taking place in it:

$$\begin{aligned} &\Theta_1 \xrightarrow{k_1} \Theta_2 \xrightarrow{k_2} \Theta_3 \\ &\Theta_1 \xrightarrow{k_3} \Theta_3 \end{aligned} \tag{20}$$

where Θ_1 represents gas oil, Θ_2 gasoline and Θ_3 other products (e.g. butanes, coke, etc.). Putting aside the reactions related to Θ_3, the dynamics of the system are described by the following parabolic PDEs representing the component balances of Θ_1 and Θ_2 within the reactor:

$$\theta_{1t}(z,t) = \gamma\theta_{1zz}(z,t) - \upsilon\theta_{1z}(z,t) - k_0\theta_1^2(z,t) \tag{21}$$

$$\theta_{2t}(z,t) = \gamma\theta_{2zz}(z,t) - \upsilon\theta_{2z}(z,t) + k_1\theta_1^2(z,t) - k_2\theta_2(z,t) \tag{22}$$

subject to the boundary conditions given by

$$\begin{aligned} \gamma\theta_{1z}(0,t) &= \upsilon(\theta_1(0,t) - u_1(t)) \qquad \theta_{1z}(l,t) = 0 \\ \gamma\theta_{2z}(0,t) &= \upsilon(\theta_2(0,t) - u_2(t)) \qquad \theta_{2z}(l,t) = 0 \end{aligned} \tag{23}$$

for all $t \geq 0$ and all $z \in [0,l]$, where l is the reactor length, and $\theta_1(z,t)$, $\theta_2(z,t)$, γ, υ, $u_1(t)$ and $u_2(t)$ denote the weight fractions of reactant Θ_1 and Θ_2, the axial dispersion coefficient, the superficial velocity, the inlet weight fraction of component A and the inlet weight fraction of component B, respectively. Such model takes the form of (1) by considering

$$\theta(z,t) = \begin{bmatrix} \theta_1(z,t) \\ \theta_2(z,t) \end{bmatrix} \quad \Gamma_0 = \begin{bmatrix} \gamma & 0 \\ 0 & \gamma \end{bmatrix}$$

$$\Upsilon = \begin{bmatrix} \upsilon & 0 \\ 0 & \upsilon \end{bmatrix} \quad F(\theta) = \begin{bmatrix} -k_0\theta_1^2 \\ k_1\theta_1^2 - k_2\theta_2 \end{bmatrix}.$$

The corresponding steady-state equations of the PDEs model defined by (21)-(22) are given by the following ODEs:

$$\gamma\frac{d^2\theta_{1ss}}{dz^2} - \upsilon\frac{d\theta_{1ss}}{dz} - k_0{\theta_1}_{ss}^2 = 0 \tag{24}$$

$$\gamma\frac{d^2\theta_{2ss}}{dz^2} - \upsilon\frac{d\theta_{2ss}}{dz} + k_1{\theta_1}_{ss}^2 - k_2\theta_{2ss} = 0 \tag{25}$$

subject to the boundary conditions

$$\gamma\frac{d\theta_{1ss}}{dz}(0) = \upsilon(\theta_{1ss}(0) - u_{1ss}) \qquad \frac{d\theta_{1ss}}{dz}(l) = 0 \tag{26}$$

$$\gamma\frac{d\theta_{2ss}}{dz}(0) = \upsilon(\theta_{2ss}(0) - u_{2ss}) \qquad \frac{d\theta_{2ss}}{dz}(l) = 0. \tag{27}$$

The adopted numerical values for the process parameters are taken from Table I (see [13]).

Parameters	Numerical Values
l	1 m
k_0	22.9 (h x weight fraction)$^{-1}$
k_1	18.1 (h x weight fraction)$^{-1}$
k_2	1.7 (h)$^{-1}$
γ	0.5 m^2 x h^{-1}
υ	2 m x h^{-1}
$u_1(t)$	0.7 weight fraction
$u_2(t)$	0 weight fraction

TABLE I: Parameters of the process.

The steady state profiles of $\theta_1(z,t)$ and $\theta_2(z,t)$ are shown in Figure 1. They were obtained by solving numerically (24)-(27) considering the parameters given in Table I.

The deviation vector $\tilde{\theta}(z,t) = \theta(z,t) - \theta_{ss}(z)$ is substituted by the new vector variable $x(z,t)$ according to the transformation defined in (5) leading to

$$\begin{bmatrix} x_1(z,t) \\ x_2(z,t) \end{bmatrix} = \begin{bmatrix} \mathrm{e}^{-\frac{\upsilon}{2\gamma}z} & 0 \\ 0 & \mathrm{e}^{-\frac{\upsilon}{2\gamma}z} \end{bmatrix} \begin{bmatrix} \tilde{\theta}_1(z,t) \\ \tilde{\theta}_2(z,t) \end{bmatrix}. \tag{28}$$

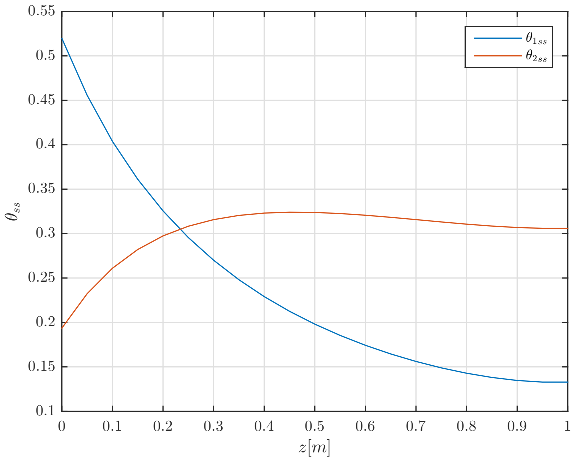

Fig. 1: Steady state profiles.

By applying the procedure described in Section II and assuming that there exists a single input $u_1(t)$ (setting $u_2(t) = 0$), we can formulate the system as an abstract boundary system on the Hilbert space $H = L^2(0,1) \oplus L^2(0,1)$ according to

$$\begin{aligned} \dot{x}(t) &= \mathfrak{U}x(t) \quad x(0) = x_0 \\ \mathfrak{B}x(t) &= u(t) \\ y(t) &= \mathfrak{C}x(t) \end{aligned} \tag{29}$$

where

$$x(\cdot,t) = \left\{ \begin{bmatrix} x_1(\cdot,t) \\ x_2(\cdot,t) \end{bmatrix}, 0 \le z \le l \right\} \in H$$

and the operators $\mathfrak{U} : D(\mathfrak{U}) \to H$, $\mathfrak{B} : D(\mathfrak{B}) \to \mathbb{R}$, $\mathfrak{C} : D(\mathfrak{C}) \to \mathbb{R}^2$ are defined as

$$\mathfrak{U} = \begin{bmatrix} \gamma \frac{d^2}{dz^2} - \hat{k}_1(z) & 0 \\ 2k_1 x_{1ss}(z) & \gamma \frac{d^2}{dz^2} - \hat{k}_2 \end{bmatrix} = \begin{bmatrix} \mathfrak{U}_{11} & 0 \\ \mathfrak{U}_{21} & \mathfrak{U}_{22} \end{bmatrix}$$

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

$$\begin{aligned} \mathfrak{B}x &= \left[-\gamma \tfrac{dx_1}{dz}(0) + \tfrac{\upsilon}{2} x_1(0) \right] \\ \mathfrak{C}x &= \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} \end{aligned} \tag{30}$$

with $\hat{k}_1(z) = \frac{\upsilon^2}{4\gamma} + 2k_0\theta_{1ss}(z)$ and $\hat{k}_2 = \frac{\upsilon^2}{4\gamma} + k_2$.

IV. Observer design

The observer design is based on the procedure described in Section II-B with $\mathcal{A}$ as defined below

$$\mathcal{A}x = \begin{bmatrix} \gamma \frac{d^2}{dz^2} - \hat{k}_1(z) & 0 \\ 2k_1 x_{1ss}(z) & \gamma \frac{d^2}{dz^2} - \hat{k}_2 \end{bmatrix} = \begin{bmatrix} \mathcal{A}_{11} & 0 \\ \mathcal{A}_{21} & \mathcal{A}_{22} \end{bmatrix},$$

$$\begin{aligned} D(\mathcal{A}) &= D(\mathfrak{U}) \cap \ker \mathfrak{B} \\ &= \Big\{ x \in H : x, \frac{dx}{dz} \text{ are a.c.}, \frac{d^2x}{dz^2} \in H \text{ and} \\ &\qquad \Gamma \frac{dx}{dz}(0) - \frac{1}{2}\Upsilon x(0) = 0, \\ &\qquad \Gamma \frac{dx}{dz}(l) + \frac{1}{2}\Upsilon x(l) = 0 \Big\}, \end{aligned} \tag{31}$$

The study of the spectrum of $\mathcal{A}$ allows designing an observer with a specified convergence rate. 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.

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:

- $\mathcal{A}_{22}$ is a linear operator with constant coefficients and its eigenvalues are given by

$$\mu_n = -\gamma w_n^2 - \hat{k}_2, \text{ with } \tan(w_n l) = \frac{4\gamma w_n \upsilon}{4\gamma^2 w_n^2 - \upsilon^2}$$

  and the corresponding eigenfunctions are given by

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

- $\mathcal{A}_{11}$ is a linear operator with reaction coefficient depending on z, consequently the calculation of the spectrum of the operator $\mathcal{A}_{11}$ is a challenging issue. This problem can be carried out by dividing the length of the reactor into a finite number N of segments where it is assumed that at each segment the values of coefficients are constant. The mathematical formulation of this approach can be found in [14]. Hence, the eigenvalues λ_n are given by

$$\lambda_n = -\gamma w_n^2 - \hat{k_1}_n, \text{ with } \tan(w_n l) = \frac{4\gamma w_n \upsilon}{4\gamma^2 w_n^2 - \upsilon^2}$$

  and the corresponding eigenfunctions are given by

$$\chi_n(z) = a_1 \rho_n \sin(w_n z) + \eta_n \sin(w_n z)$$

  where $\rho_1 = 1$; $\rho_n = s_{n,n-1} s_{n-1,n-2} \cdots s_{2,1}$ and

$$\begin{aligned} s_{n,n-1} &= \frac{\sin(w_{n-1} z_n) + \eta_{n-1} \cos(w_{n-1} z_n)}{\sin(w_n z_n) + \eta_n \cos(w_n z_n)} \\ s_{N,N-1} &= \frac{1}{h_N} \frac{\sin(w_{N-1} z_N) + \eta_{N-1} \cos(w_{N-1} z_n)}{\sin(w_N z_N) + \eta_n \cos(w_N z_N)} \\ \eta_1 &= -\frac{\upsilon \sin(w_1 z_1) - 2h_1 w_1 \cos(w_1 z_1)}{\upsilon \cos(w_1 z_1) + 2h_1 w_1 \sin(w_1 z_1)} \\ \eta_i &= \frac{\text{num}_i}{\text{den}_i} \end{aligned}$$

with

$$\begin{aligned}\text{num}_i &= \cos(w_i z_i)(\sin(w_{i-1} z_i) + \eta_{i-1}\cos(w_{i-1} z_i)) \\ &\quad - \sin(w_i z_i)(\cos(w_{i-1} z_i) - \eta_i \sin(w_{i-1} z_i)) \\ \text{den}_i &= \sin(w_i z_i)(\sin(w_{i-1} z_i) + \eta_{i-1}\cos(w_{i-1} z_i)) \\ &\quad + \cos(w_i z_i)(\cos(w_{i-1} z_i) - \eta_i \sin(w_{i-1} z_i)).\end{aligned}$$

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

The operator $\mathcal{A}$ is triangular and therefore 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:

$$\sigma(\mathcal{A}) = \begin{cases} \sigma_{2n+1} = \lambda_n, & \forall n \geq 0 \\ \sigma_{2n} = \mu_n, & \forall n \geq 1, \end{cases} \tag{32}$$

with the corresponding eigenvectors given by

$$\begin{aligned}\phi_{2n+1} &= \begin{bmatrix} \chi_n \\ (\lambda_n I - A_{22})^{-1} A_{21} \chi_n \end{bmatrix} \\ \phi_{2n} &= \begin{bmatrix} 0 \\ \psi_n \end{bmatrix}.\end{aligned} \tag{33}$$

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

$$\begin{aligned}\Psi_{2n+1} &= \begin{bmatrix} \chi_n \\ 0 \end{bmatrix} \\ \Psi_{2n} &= \begin{bmatrix} (\mu_n I - A_{11})^{-1} A_{21} \psi_n \\ \psi_n \end{bmatrix}\end{aligned} \tag{34}$$

where

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

Hence, the first five eigenvalues of the operators $\mathcal{A}_{11}$ and $\mathcal{A}_{22}$ are as follows

$$\begin{aligned}\lambda = \{&-2.39 \times 10^{-5}, \ -1.34 \times 10^{-4}, \ -4.46 \times 10^{-4}, \\ &-1.12 \times 10^{-3}, \ -2.35 \times 10^{-3}\} \\ \mu = \{&-2.04 \times 10^{-6}, \ -1.096 \times 10^{-5}, \ -5.68 \times 10^{-5}, \\ - \quad &2.08 \times 10^{-4}, \ -5.78 \times 10^{-4}\}.\end{aligned}$$

B. Luenberger-observer

In order to design a dynamical observer of the form (18), we must guarantee the β-exponential detectability of the pair ($\mathcal{A}$,$\mathfrak{C}$), where $\mathfrak{C}$ should be interpreted as a bounded linear functional on H which approaches the action of the Dirac delta distribution. Assuming a decay rate for the state estimation error $\beta = -2.5 \times 10^{-6}$, which provides faster convergence than the one of the states, the spectrum of $\sigma(\mathcal{A})$ is the union of two parts, $\overline{\sigma}_\beta^+(\mathcal{A})$ and $\sigma_\beta^-(\mathcal{A})$, such that a rectifiable, closed, simple curve C_β can be drawn so as to enclose an open set containing $\overline{\sigma}_\beta^+(\mathcal{A})$ in its interior and $\sigma_\beta^-(\mathcal{A})$ in its exterior. The operator, P_{C_β}, defined by

$$P_{\mathsf{C}_\beta} x = \frac{1}{2\pi j} \int_{\mathsf{C}_\beta} (\lambda I - \mathcal{A})^{-1} x d\lambda \tag{35}$$

is the spectral projection operator that induces a decomposition of the state space as well as the operators according to

$$\begin{aligned} H &= H_\beta^+ \oplus H_\beta^- \\ P_{\mathsf{C}_\beta} x &= \sum_{\sigma(\mathcal{A}) \in \sigma(\mathcal{A})_\beta^+} \langle x, \Psi_n \rangle \phi_n \\ \mathcal{A}_\beta^+ x &= \mathcal{A} P_{\mathsf{C}_\beta} x = \sum_{\sigma(\mathcal{A}) \in \sigma(A)_\beta^+} \sigma_n(\mathcal{A}) \langle x, \Psi_n \rangle \phi_n \\ \mathfrak{C}_\beta^+ x &= \mathfrak{C} P_{\mathsf{C}_\beta} x = \sum_{\sigma(A) \in \sigma(A)_\beta^+} \langle x, \Psi_n \rangle \mathfrak{C} \phi_n. \end{aligned} \tag{36}$$

The system $\Sigma(\mathcal{A}, - ,\mathfrak{C})$ is β-exponentially detectable by $L = i_\beta L_0$, where L_0 is such that $\mathcal{A}_\beta^+ + L_0 \mathfrak{C}_\beta^+$ is β-exponentially stable and i_β is the injection operator from H_β^+ to H as shown in [8]. To guarantee the well-posedness of our formulation with bounded operators, the operator $\mathfrak{C}$ is redefined as

$$\mathfrak{C} x = \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} \simeq \begin{bmatrix} \int_0^1 1_{[0,\epsilon]} x_1(z,t) dz \\ \int_0^1 1_{[0,\epsilon]} x_2(z,t) dz \end{bmatrix} \tag{37}$$

where

$$1_{[0,\epsilon]} = \begin{cases} \frac{1}{\epsilon}, & 0 \leq z \leq \epsilon, \\ 0, & \text{elsewhere}, \end{cases}$$

for a sufficiently small ϵ. Considering that $\epsilon = 0.01$, we obtain

$$\begin{aligned} (\mathcal{A}_\beta^+, - , \mathfrak{C}_\beta^+) &= \left(\mu_2, - , \begin{bmatrix} 0 \\ \int_0^\epsilon 1_{[0,\epsilon]} \psi_1(z) dz \end{bmatrix} \right) \\ &= \left(-2.04 \times 10^{-6}, -, \begin{bmatrix} 0 \\ 0.91 \end{bmatrix} \right) \end{aligned} \tag{38}$$

and $L_0 = [0 \ \ -5.05 \times 10^{-7}]$. Notice that L_0 is such that $\mathcal{A}_\beta^+ + L_0 \mathfrak{C}_\beta^+$ is β-exponentially stable. Thus,

$$Ly = i_\beta L_0 y = \begin{bmatrix} 0 \\ \psi_1(z) \end{bmatrix} [0 \ \ -5.05 \times 10^{-7}] y. \tag{39}$$

The observer system has been simulated considering the parameters of the system given in Table I with the initial profiles for the observer system as $\hat{\theta}_1 = \hat{\theta}_2 = 0$. The numerical simulation of PDE systems can be achieved using the method of lines and the MATMOL library [15]. Figures 2 and 3 show the evolution of the actual states θ_1, θ_2 (red lines) and the estimated states $\hat{\theta}_1$, $\hat{\theta}_2$ (blue lines) related to the proposed observer.

V. Concluding Remarks

In this paper, a Luenberger-type 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 a given steady-state profile is considered, which results in a linear DPS with spatially-varying coefficients. The observer output injection operator is thereby initially determined by making use of the boundary conditions for the stability of a triangular operator having Sturm-Liouville operators in its diagonal.

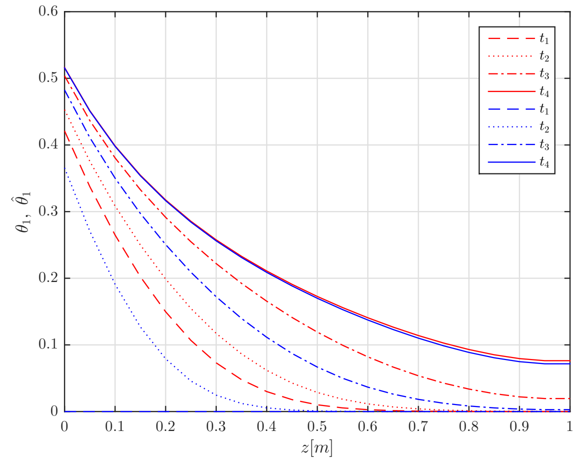

Fig. 2: Time evolution of the spatial profile of θ_1 and $\hat{\theta}_1$ at time instants $t_1 = 0$, $t_2 = 61.5s$, $t_3 = 320.7s$, $t_4 = 644.7s$.

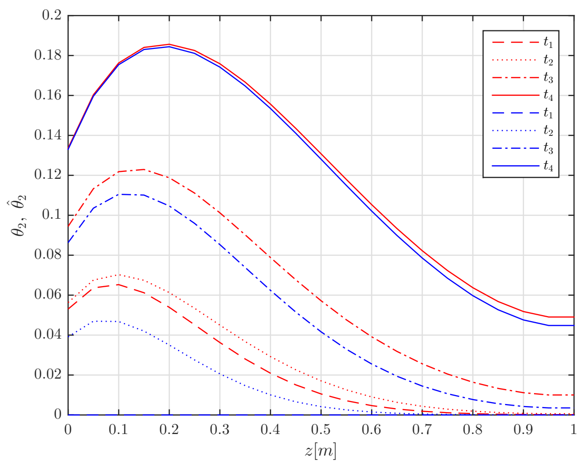

Fig. 3: Time evolution of the spatial profile of θ_2 and $\hat{\theta}_2$ at time instants $t_1 = 0$, $t_2 = 61.5s$, $t_3 = 320.7s$, $t_4 = 644.7s$.

Subsequently, the output injection operator is designed by using spectrum decomposition conditions ensuring a certain convergence decay rate for the estimation error dynamics. The proposed observer was applied to a tubular catalytic cracking 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.

Moreover, in view of the promising numerical results obtained in the application (see e.g. Figures 2 and 3), an interesting open problem is the extension of the method described in this paper to a more general class of coupled parabolic PDEs with not necessarily triangular structure. This problem is currently under investigation by the authors. Thus, the proposed study is a point of departure to design observers based on the spectrum for more general state operators.

References

[1] W. Ray, “Some recent applications of distributed parameter systems theorya survey,” *Automatica*, vol. 14, no. 3, pp. 281–287, 1978.

[2] D. Dochain, “Contribution to the analysis and control of distributed parameter systems with application to (bio)chemical processes and robotics,” Thèse d’Aggrégation de l’Enseignement Supérieur, UCL, Belgium, 1994.

[3] M. S. de Queiroz, D. M. Dawson, M. Agarwal, and F. Zhang, “Adaptive nonlinear boundary control of a flexible link robot arm,” *IEEE Transactions on Robotics and Automation*, vol. 15, no. 4, pp. 779–787, 1999.

[4] D. L. Russell, “Distributed parameter systems: An overview,” *Encyclopedia of Life Support Systems (EOLSS): Control Systems, Robotics And Automation*, 2003.

[5] N. Fujii, “Feedback stabilization of distributed parameter systems by a functional observer,” *SIAM Journal on Control and Optimization*, vol. 18, no. 2, pp. 108–120, 1980.

[6] A. Vande Wouwer and M. Zeitz, “State estimation in distributed parameter systems,” *Control Systems, Robotics and Automation–Volume XIV: Nonlinear, Distributed, and Time Delay Systems-III*, p. 92, 2009.

[7] H. T. Banks and K. Kunisch, *Estimation techniques for distributed parameter systems*. Springer Science & Business Media, 2012.

[8] R. F. Curtain and H. Zwart, *An introduction to infinite-dimensional linear systems theory*. Springer Science & Business Media, 2012, vol. 21.

[9] H. O. Fattorini, “Boundary control systems,” *SIAM Journal on Control*, vol. 6, no. 3, pp. 349–385, 1968.

[10] Z. Emirsjlow and S. Townley, “From pdes with boundary control to the abstract state equation with an unbounded input operator: a tutorial,” *European Journal of Control*, vol. 6, no. 1, pp. 27–49, 2000.

[11] A. Smyshlyaev and M. Krstic, “Backstepping observers for a class of parabolic pdes,” *Systems & Control Letters*, vol. 54, no. 7, pp. 613–625, 2005.

[12] C. Delattre, D. Dochain, and J. Winkin, “Sturm-liouville systems are riesz-spectral systems,” *International Journal of Applied Mathematics and Computer Science*, vol. 13, pp. 481–484, 2003.

[13] L. Mohammadi, I. Aksikas, S. Dubljevic, and J. F. Forbes, “Lq-boundary control of a diffusion-convection-reaction system,” *International Journal of Control*, vol. 85, no. 2, pp. 171–181, 2012.

[14] F. de Monte, “An analytic approach to the unsteady heat conduction processes in one-dimensional composite media,” *International Journal of Heat and Mass Transfer*, vol. 45, no. 6, pp. 1333–1343, 2002.

[15] A. Vande Wouwer, P. Saucez, and C. Vilas, *Simulation of ode/pde Models With Matlab, Octave and Scilab*. Springer, 2014.