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Spectral Dissipativity Observer for a Class of Tubular Reactors

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Abstract— **The problem of designing a globally convergent observer for a class of tubular chemical reactors is addressed. The proposed approach combines dissipativity and modal detectability notions for distributed systems in the light of the particular tubular reactor properties due to the interplay between convective-diffusive transport and nonlinear reaction. The result is a nonlinear single-sensor observer with distributed modal measurement injection, and a global convergence condition in terms of the convection-to-diffusion Peclet number, the dominant frequency of the non-innovated dynamics, the maximum reaction rate slope, and the sensor location. The proposed design is illustrated for a representative example with non-monotonic reaction rate through simulations.**

I. Introduction

The last decades were marked by an intensive research activity in distributed parameter systems (DPS) theory ([1], [2], [3], [4], [5] and references therein), with the early-lumping (EL) and late-lumping (LL) approaches. In the EL approach lumped parameter systems (LPS) approximations of the original model equations are employed for control and observer design. The use of the EL approach enables the application of well-established design methods (see e.g. [6], [5]), but make difficult the exploitation of intrinsic structural and dynamic properties reflected in the DPS model. On the other hand, the LL approach refer to methods based directly on the distributed model and therefore enables designs on the basis of intrinsic information contained in the original model equations, but leads to higher technical complexity due to the infinite-dimensional features of the related framework.

In the light of practical applications the observer design should: (i) contain a sensor location criterium, (ii) provide solvability conditions with physical meaning, and (iii) enable the assurance of a suitable compromise between convergence speed and robustness. These design characteristics have been achieved for lumped parameter systems (LPS) [7], [8] and DPS [9]. The idea is to set a data-assimilation scheme so that the resulting estimation error dynamics are made of two dissipative subsystems, one that is linear, dynamical and driven by standard measurement injection, and one that is nonlinear, static and (eventually) subjected also to measurement injection. The estimation error convergence is ensured by adequately matching the dissipative properties of both subsystems, or equivalently, choosing a suitable two-way energy exchange mechanism, within Popov's well-known absolute stability framework (see e.g. [10],[11]). This approach has been applied to biochemical ([12]) and chemical ([8]) continuous lumped reactors with non-isotonic kinetic rates, in the understanding that this kind of kinetics represent a difficult observer and control design problem, because of the lack of local observability around the concentration which maximizes the reaction rate. The approach has already been extended to tubular reactors via variational LL techniques [9] considering point-injections for a single species isothermic process. The main features are: (i) explicit physical solvability conditions, (ii) rigorous mathematical basis for a practical gain adjustment in the sense of a compromise between convergence speed and robustness issues, and (iii) only basic knowledge of advanced calculus is required. Nevertheless, the results do not provide explicit criteria for sensor location.

The linear observer design case without reaction has been satisfactorily solved in the middle 70's and 80's [13], [14], [15]. The bilinear case with boundary innovation mechanism has been satisfactorily treated in [16]. The nonlinear problem considering chemical reaction has been tackled with a diversity of approaches, among them are: Kalman filters [17], [6], orthogonal collocation truncations [18], [19], modal truncation-based dissipativity [20], Riccatti approaches based on spectral factorizations [21], open-loop (asymptotic) observers [22] and approximate inertial manifolds (see e.g. [23], [5]).

In this work, we propose an alternative approach based on the results for linear parabolic systems ([13],[15]) in combination with our results on observer design for lumped (continuous or batch) reactors ([12], [8]) and our previous variational approach to tubular reactor state estimators [9]. These results are combined in an energy interchange framework, enabling the solution of the nonlinear problem via linear design methods. *The present work thus provides a basis for extensions to the more complicated cases of the dissipativity-based design framework* [7]. For this purpose, the scope is circumscribed to a rather simple single-reaction axial tubular reactor class which captures the fundamental transport, reaction, and measurement mechanisms which underlie an ample class of tubular reactors. The reactor case example has one spatial (axial) dimension and includes the basic dynamical mechanisms inherent to tubular reactor problems: diffusion, convection and nonlinear (possibly non-monotonic) reaction kinetic rate.

The main result is an innovation gain condition in conjunction with a criterion for sensor location, ensuring the global observer convergence. Such condition involves the di-

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mensionless Peclet number (convection-to-diffusion quotient measure) as well as the reaction frequency. The proposed approach is illustrated and tested through numerical simulations with a case example with non-monotonic kinetics. The global convergence feature is verified and, as expected, the measurement injection speeds up the error dynamics with respect to the natural ones. Furthermore, the results provide insight on how to establish a practical compromise between convergence speed and robustness issues.

The paper is organized as follows. In Section 2 the observation problem is formulated. The observer design is presented in Section 3. Its application to a representative case example with non-monotonic reaction rate is presented in Section 4. Section 5 concludes the paper.

II. Observation problem

Consider an (open or packed) isothermal tubular reactor with diffusion/dispersion, convection, nonlinear single species kinetics over the axial spatial domain $[0,1]$, and a single domain measurement $y(t)$ located in the domain $\xi \in (0,1)$. The spatial concentration profile is governed by the partial differential equation:

$$\begin{array}{ll} \frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - \pi_e \frac{\partial c}{\partial x} - r(c), & x \in (0,1) \\ \frac{\partial c}{\partial x} = \pi_e \left(c - c_e(t)\right), & x = 0 \\ \frac{\partial c}{\partial x} = 0, & x = 1 \\ c(x,0) = c_0(x), & x \in (0,1) \\ y(t) = c(\xi,t) & \end{array}, \tag{1}$$

where

$$\pi_e = \frac{t_D}{t_C} = \frac{Lv}{D}, \quad t_D = \frac{L^2}{D}, \quad t_C = \frac{L}{v}, \quad v = \frac{q}{A}.$$

c is the dimensionless reaction concentration (referred to pure reactant), x is the dimensionless axial position referred to the reactor length L, t is the dimensionless time referred to Einstein's diffusion time t_D, D is the diffusion/dispersion coefficient, π_e is Peclet's number, or equivalently the diffusion(t_D)-to-convection(t_C) characteristic time quotient, v is the axial flow velocity, meaning the volumetric flow rate(q)-to-area(A) quotient, and $r(c)$ is the (monotonic or non-monotonic) reaction rate function. Typically, the Peclet number ranges over $[10^4, 10^6]$ for open tubes and over $[10, 10^3]$ for packed beds ([24]).

Given a dominant frequency and the related set of high frequency harmonics, our *reactor observation problem* consists in designing a globally convergent observer on the basis of a suitably located concentration measurement $y(t) = c(\xi,t)$. We are interested in: (i) performing the estimation task with a low dimensional measurement injection scheme, in the sense that only a set of slow (linear) modes is speeded up while the rapid-stable modes are left in open-loop estimation mode, and (ii) drawing a global convergence condition in terms of parameters associated with convection, diffusion, reaction and sensor location. The proposed design is illustrated with a representative example through simulations for low and high convection-to-diffusion regimes. It must be pointed out, that the tackling of this problem is a step towards the consideration of the more complex non-isothermal multi-species tubular reactor case.

III. Observer Design

A. Linear estimation without reaction

The observer problem for linear distributed systems has been satisfactorily resolved: Gressang and Lamont [13] considered regional sensors mean value measurements, and Curtain [15] employed point sensors. Following the latter approach (for a reactor without chemical reaction, i.e. $r = 0$), introducing the measurement operator $C_\xi = \delta(x - \xi)$, (δ being the Dirac-distribution), one obtains the following observer:

$$\begin{array}{ll} \frac{\partial \hat{c}}{\partial t} = \frac{\partial^2 \hat{c}}{\partial x^2} - \pi_e \frac{\partial \hat{c}}{\partial x} - L(x)[C_\xi \hat{c} - y(t)], & x \in (0,1) \\ \frac{\partial \hat{c}}{\partial x} = \pi_e \left(c - c_e(t)\right) - L(0)[C_\xi \hat{c} - y(t)], & x = 0 \\ \frac{\partial \hat{c}}{\partial x} = -L(1)[C_\xi \hat{c} - y(t)], & x = 1 \\ \hat{c}(x,0) = \hat{c}_0(x), & x \in (0,1), \end{array} \tag{2}$$

with finite-dimensional measurement injection mechanism

$$L(x) = L_0 \sum_{n=0}^{N} \phi_n(x), \tag{3}$$

where L_0 is an *adjustable scalar gain function*, and $\phi_i(x)$ the i-th (real) eigenfunction of the convective-diffusive linear operator (cp. [1], [3])

$$A = \frac{d^2}{dx^2} - \pi_e \frac{d}{dx}, \text{ where } A\phi_i = \lambda_i \phi_i \tag{4}$$

(λ_i is the i-th eigenvalue). The operator A is defined in the underlying Hilbert space $\mathcal{Z} = \mathcal{L}^2([0,1])$ with domain $\mathcal{D}(A)$. Note that $-A$ is a Sturm-Liouville operator, has a completely disconnected (pure point) spectrum $\sigma(A) = \sigma_p(A)$ (see [3]) and is a Riesz spectral operator (see [25]). The eigenvalues λ_i of A are all real, negative and diverge to $-\infty$, so that A generates an exponentially stable C_0-semigroup.

The sensor location ξ is chosen so that ξ is not a root of any of the N-eigenfunction set $\{\phi_1, \ldots, \phi_N\}$, this is

$$\phi_i(\xi) \neq 0, \quad i = 1, \ldots, N, \tag{5}$$

where N is chosen such that the corresponding dominant frequency λ_{N+1} of the non-observable modes ensures a prescribed convergence velocity. This means that the first N eigenfunctions are involved in the measurement injection scheme.

Set $r = 0$ in (1), subtract it from (2), and obtain the linear estimation error dynamics

$$\begin{array}{ll} \frac{\partial \tilde{c}}{\partial t} = (A - LC_\xi)\,\tilde{c}, & x \in (0,1) \\ \frac{\partial \tilde{c}}{\partial x} = (\pi_e - L(0))\,\tilde{c}, & x = 0 \\ \frac{\partial \tilde{c}}{\partial x} = -L(1)\tilde{c}, & x = 1 \\ \tilde{c}(x,0) = \tilde{c}_0(x), & x \in [0,1] \end{array} \tag{6}$$

where $\tilde{c}(x,t) = \hat{c}(x,t) - c(x,t)$, A is the linear convective-diffusive spatial differential operator (4), L is the innovation injection (3) and C_ξ is the measurement operator.

Introduce a storage functional $\mathcal{S}(\tilde{c})$ defined by the weighted squared concentration error norm[1]

$$\mathcal{S}(\tilde{c}) \triangleq \frac{1}{2}\langle \tilde{c}, P\tilde{c}\rangle = \frac{1}{2}||z||_P\,, \text{ with } P(x) = e^{-\pi_e x}, \quad (7)$$

with $P(x)$ being the positive weight so that the operator (PA) is self-adjoint. Denote by A_L the innovated linear diffusive-convective operator $A - LC_\xi$, and write the time-derivative

$$\frac{d\mathcal{S}}{dt} = \frac{1}{2}\langle \tilde{c}, (A_L^* P + PA_L), \tilde{c}\rangle = \langle \tilde{c}, PA_L\tilde{c}\rangle\,. \quad (8)$$

Express the operator PA_L in a spectral form

$$PA_L z = \sum_{i=1}^{\infty} \bar{\lambda}_i \langle z, \phi_i\rangle \phi_i, \quad (9)$$

where the $\bar{\lambda}_i$ are the eigenvalues manipulated by the innovation mechanism. Next, conclude from the spectral decomposition (9) and the definition of $L(x)$ (3) that

$$\frac{d\mathcal{S}}{dt} \leq \bar{\lambda}^+ \langle P\tilde{c}, \tilde{c}\rangle = \bar{\lambda}^+ \mathcal{S}, \quad (10)$$

where $\bar{\lambda}^+$ is the dominant eigenvalue[2] of the innovated convective-diffusive linear operator $A - LC_\xi$. Thus, the exponential dissipation for $\bar{\lambda}^+ < 0$ follows ([7], [26]). The innovation effect can therefore be interpreted as an injection of dissipative terms into the estimation error dynamics, ensuring the global dissipation, with a prescribed rate $\epsilon > 0$, of the energy stored in the error state. As mentioned before this has to be ensured by meeting the sensor location criterion (5) [15], this is $\phi_i(\xi) \neq 0$ for all $i \leq N$ such that $\lambda_{N+1} < -\epsilon$. Thus, the corresponding innovation gain L_0 (3) is then determined by

$$L_0 \geq \lambda_1 + \epsilon. \quad (11)$$

Finally, from the application of Lyapunov's second method ([27]) the exponential convergence of the observer is concluded.

B. Nonlinear observer construction

Motivated by the known solutions for linear systems ([13],[15]) let us consider a candidate observer for the reactor system (1) with chemical reaction ($r \neq 0$), given by a copy of the system itself with adjustable-gain (L) for distributed injection of the measurement at position ξ, over the first N (to be determined) dominant eigenfunctions of the convective-diffusive linear operator:

$$\begin{aligned}
&\frac{\partial \hat{c}}{\partial t} = \frac{\partial^2 \hat{c}}{\partial x^2} - \pi_e \frac{\partial \hat{c}}{\partial x} - r(\hat{c}) - L(x)[C_\xi \hat{c} - y(t)]\,, x \in (0,1)\\
&\frac{\partial \hat{c}}{\partial x} = \pi_e(\hat{c} - c_e(t)) - L(0)[C_\xi \hat{c} - y(t)]\,, \quad x = 0\\
&\frac{\partial \hat{c}}{\partial x} = -L(1)[C_\xi \hat{c} - y(t)]\,, \quad x = 1\\
&\hat{c}(x,0) = \hat{c}_0(x), \quad x \in (0,1),
\end{aligned} \quad (12)$$

where the distributed innovation $L(x)$ is defined by (3). The nonlinearity due to chemical reaction will be handled with a sector condition, which characterizes the corresponding regions of energy production or consumption. This will enable the observer design within the preceding dissipativity interpretation of the linear modal estimation framework ([13],[15]), by separating the error dynamics into a linear dynamic (convective-diffusive) subsystem and a non-linear static (reactive) one. This approach has been recently applied in a continious stirred tank reactor study ([8]) and a tubular reactor study via a non-spectral approach ([9]) and is tackled in the next paragraph.

C. Error Dynamics

From the subtraction of (12) from (1) the dynamics of the estimation error $\tilde{c}(x,t) = \hat{c}(x,t) - c(x,t)$ follows:

$$\begin{aligned}
&\frac{\partial \tilde{c}}{\partial t} = (A - LC_\xi)\,\tilde{c} - \rho\,(c;\tilde{c})\,, x \in (0,1)\\
&\frac{\partial \tilde{c}}{\partial x} = (\pi_e - L(0))\,\tilde{c}, \; x = 0\\
&\frac{\partial \tilde{c}}{\partial x} = -L(1)\tilde{c}, \; x = 1\\
&\rho\,(c;\tilde{c}) \triangleq r\,(c + \tilde{c}) - r\,(c)\\
&\tilde{c}(x,0) = \tilde{c}_0(x), \; x \in [0,1],
\end{aligned} \quad (13)$$

with $\tilde{c}$ and ρ denoting the concentration and reaction rate estimation errors, respectively. Recall the definitions of the spatial linear operator A (4), the finite-dimensional distributed innovation $L(x)$ (3) and the measurement operator $C_\xi = \delta(x - \xi)$. Following the dissipativity framework, let us write the error dynamics (13) in negative feedback interconnection form

$$\begin{aligned}
&\dot{\tilde{c}} = (A - LC_\xi)\tilde{c} + \nu, \; \tilde{c}(0) = \tilde{c}_0\\
&\nu = -\rho\,(c;\tilde{c})\;,
\end{aligned} \quad (14)$$

with two subsystems: (i) one linear dynamical subsystem $\Sigma_L(A+LC)$ with the convection, diffusion and measurement injection mechanisms, and forced by the exogenous input ν, and (ii) a nonlinear static (time-varying) subsystem $\nu = -\rho(c;\tilde{c})$ which, driven by the estimation error, generates the reaction rate error. The dissipative method is based upon the concept of performing a suitable abstract energy release, in the sense that: (i) zero energy content means zero estimation error, (ii) the energy dissipation sets the prescribed convergence rate, and (iii) an adequate compromise between robustness and reconstruction speed amounts to appropriately performing the energy dissipation task in the two system interconnection. For this aim, the energy interchange property of each subsystem will be characterized in terms of the

[1]Note that since $P(x)$ is continuous and positive it attains positive maximum and minimum values over the compact interval $[0,1]$ and the P-norm is thus equivalent to the standard L^2-norm.

[2]Due to the Sturm-Liouville property of $-A$ this corresponds to the first eigenvalue, this is $\bar{\lambda}^+ = \bar{\lambda}_1$.

output injection gain L, the sensor location, and the conic bounds of the nonlinear (possibly non-monotonic) reaction rate. Then the overall energy dissipation in the two subsystem interconnection will be ensured.

D. Dissipation shaping

To design the innovation in such a way that the two-subsystem interconnection (13) is strictly dissipative ([26], [7]) consider the quadratic storage candidate functional $\mathcal{S}(\tilde{c}) = 1/2\,\langle \tilde{c}, P\tilde{c}\rangle$ defined above (7) with weighting function $P = e^{-\pi_e x}$, so that $(PA)^* = PA$, write the time derivative is

$$\frac{d\mathcal{S}}{dt} = \langle P(A - LC_\xi)\tilde{c}, \tilde{c}\rangle + \langle P\nu(c;\tilde{c}), \tilde{c}\rangle\,. \tag{15}$$

Observe that the energy interchange property of the linear subsystem has been determined in (10), say

$$\langle P(A - LC_\xi)\tilde{c}, \tilde{c}\rangle \leq \bar{\lambda}^+ \mathcal{S}, \tag{16}$$

where $\bar{\lambda}^+$ is the dominant eigenvalue of the innovated linear operator $A - LC_\xi$. From a recent study on continuous chemical (LPS) reactor [8], the sector condition for the reaction rate estimation error $\rho(c;\tilde{c})$ has been determined (via an application of the mean value theorem), yielding

$$K_1\tilde{c}^2 \leq \rho\,(c;\tilde{c})\,\tilde{c} \leq K_2\tilde{c}^2, \tag{17}$$

where K_1 and K_2 represent the minimum and maximum values of the reaction rate derivative $r'(c)$, respectively. It must be pointed out that the bounds K_1 and K_2 depend on the reaction rate function and not on the specific reactor configuration (continuous, batch or tubular), and correspond to an extreme case drawn from mass conservation arguments.[3] In the distributed case this is a pointwise condition which, by the exponential weighted integration in the second term of (15) yields an bound for the maximal energy content of the reactive subsystem:

$$\langle P\nu, \tilde{c}\rangle = -\langle P\rho(c;\tilde{c}), \tilde{c}\rangle = -\int_0^1 P\rho(c;\tilde{c})\tilde{c} \leq -K_1\mathcal{S}, \tag{18}$$

meaning that the energy exchange property of the nonlinear part is completely bounded by the lower bound of the reaction rate's slope. Summarizing, we obtain that from (16) and (18)

$$\frac{d\mathcal{S}}{dt} \leq \left(\bar{\lambda}^+ - K_1\right)\mathcal{S}, \tag{19}$$

meaning that the presence of the nonlinearity increases (or diminishes) the dissipation or equivalently the convergence rate, if the reaction is monotonic (or non-monotonic).[4] In virtue of (19) we obtain the following result:

The strict dissipation with adjustable rate $\epsilon > 0$ of the linear (transport)–nonlinear (reaction) interconnection can be ensured by placing the dominant eigenvalues $\bar{\lambda}^+$ of the convective-diffusive linear subsystem, by the innovation gain L_0 such that[5]

$$\bar{\lambda}^+ - K_1 \leq -\epsilon, \tag{20}$$

which is a task that can be executed with existing procedures [13], [15]. For this aim the following conditions must be met:

(I) *The N dominant modes of the convective-diffusive linear operator A (4), with N such that $\lambda_{N+1} - K_1 \leq -\epsilon \leq \lambda_N - K_1$, are observable.*

(II) *The innovation gain L_0 (3) is chosen such that (20) holds.*[5]

The first condition ensures that all dominant (slow) eigenvalues $\lambda_i, \quad i \leq N$ can be arbitrarily located, provided a sensor location criterion is met. The second condition on the innovation gain L_0 ensures that the slow eigenvalues are located so that all the eigenvalues of the innovated linear operator $A - L(x)C(x,\xi)$ are sufficiently small. This in turn ensures the exponential dissipation and the exponential observer convergence. The main condition is therefore condition (I), which *amounts to ensuring the exponential output-feedback stabilizability with prescribed rate in the linear case* (5) [15]. Thus, the global estimator convergence assurance amounts to finding a joint gain–sensor location condition so that the (stabilizing or destabilizing) speed modification effect of the non-linear reaction rate is compensated with respect to a prescribed exponential dissipation.

E. Global Convergence

The preceding results are summarized in the next proposition.

Proposition 1: The observer (12) is globally exponentially convergent with a prescribed exponential rate ϵ if:

(i) The innovation dimension N is chosen so that

$$\lambda_{N+1} \leq K_1 - \epsilon, \tag{21}$$

(ii) The sensor location ξ is in no root of the N eigenfunctions $\phi_n(x)$, i.e.

$$\phi_n(\xi) \neq 0 \quad \forall \quad n \leq N, \tag{22}$$

(iii) The gain L_0 is chosen so that

$$\lambda^+ - L_0 - K_1 \leq -\epsilon, \tag{23}$$

with $\lambda^+ = \lambda_1$ the dominant eigenvalue[6] of the linear convective-diffusive operator A (4) and K_1 the minimum value of the reaction rate's slope $r'(c)$ (17).

Note that in the case of a monotonic (or non-monotonic) reaction rate K_1 is nonnegative (or negative). Monotonic reactions rates therefore improve dissipation (convergence rate) as (20) is satisfied even for $L_0 = 0$. In contrast, in the non-monotonic case, globally thinking, there are divergence effects at play, due to the inhibition feature in the chemical reaction.

Next the proposed approach is applied to a subclass of tubular reactors with non-monotonic kinetics.

[3] In a practical application this task has to be performed in correspondence to the actual process operation mode conditions (initial condition estimations, optimal inlet concentration, etc.).

[4] A non-monotonic rate is characterized by the presence of an antitonic branch with negative slope.

[5] Compare with the condition (11) on L_0 in the linear case.

[6] Remember the Sturm-Liouville property of the linear diffusive-convective operator A.

IV. A Case Study

A. Problem statement and characterization

In the chemical reactor engineering field, it is known that continuous reactors (LPS) with non-monotonic kinetic rates rise, due to lack of observability, observer and control design difficulties, a problem recently addressed via the dissipativity approach ([8],[9]). The observability problem is due to the problem that, given the actual reaction rates value it is not possible to establish if the concentration is in the isotonic or antitonic branch of the function.

Let us consider our reactor (1) observation problem with the non-monotonic (Langmuir-Hinshelwood) kinetics employed in our previous LPS [8] and DPS [9] studies:

$$r(c) = \frac{kc}{(1+\sigma c)^2},\ t_R = \frac{1}{k} \tag{24}$$

where $k > 0$ $[1/s]$ is the reaction frequency factor, t_R its corresponding characteristic reaction time, and σ is the auto-inhibition constant, the rate error function $\rho(c;\tilde{c})$ in (14) encompasses the sector $[-\frac{k}{27}, k]$, implying that (cp. with (17)) [8]

$$-\frac{k}{27}\,||\tilde{c}||_P^2 \le \rho(c;\tilde{c})\tilde{c} \le k\,||\tilde{c}||_P^2\,. \tag{25}$$

On the other hand, the eigenvalues λ_i of A (4) are $\lambda_i = -\pi_e^2/4 - \omega_i^2$, with the eigenfrequencies ω_i corresponding to the (symmetric) solutions of the implicit equation $4\omega_i\pi_e\cos(\omega_i) = \sin(\omega_i)\left[\pi_e^2 - 4\omega_i^2\right]$. It can be easily verified that for $\pi_e \ge \pi$ it holds:

$$\lambda_n \le -\frac{\pi_e^2}{4} - (n-1)^2\pi^2, \quad \lambda_1 \le -\frac{\pi_e^2+\pi^2}{4}. \tag{26}$$

Correspondingly, the innovation dimension N is determined according to (21). The observer gain L_0 is then determined so that (23) is satisfied. The functioning is ensured by sensor location in base of the knowledge of the first N eigenfunctions $\phi_i, i = 1,\dots,N$ of A: $\phi_i(x) = \Omega_i e^{\pi_e/2x}\left[2\omega_i/\pi_e\cos(\omega_i x) + \sin(\omega_i x)\right]$, $\Omega_i \in \mathbb{R}$. These eigenfunctions define a non-orthogonal Riesz basis (cp. [28]). The fulfillment of the given conditions (21-23) in turn implies the strict dissipativity of the two-subsystem interconnection and thus the exponential convergence of the estimation error $\tilde{c}(x,t)$.

Summarizing, the above conditions: (i) establish that the measurement innovation injection must be chosen according with the Peclet (π_e) and reaction frequency (k) value, (ii) show the key interplay between sensor location and observer design, and (iii) constitute the basis of a sensor-location dependent gain tuning procedure in the sense of a practical compromise between reconstruction speed-up and robustness issues.

B. Implementation and Simulation study

To illustrate the observer performance in a concrete example, the reactor (1) was regarded with the (diffusion-dominated) Peclet-inhibition-reaction frequency triplet $(\pi_e, \sigma, k) = (10, 3, 20)$ and the initial concentration profile $c_0(x) = 0.3$ (on the isotonic branch). The observer was set with the deviated initial profile $\hat{c}_0(x) = 0.4$ (on the antitonic branch). Innovation is imposed on the first 4 eigenmodes of the linear subsystem. The sensor is located in $\xi = 0.5$ and the corresponding behavior is illustrated in Fig. 1, in comparison to the natural system response (i.e. for $L_0 = 0$). The simulations have been carried out with a standard finite-difference algorithm. Keeping in mind that the reactor time is scaled with respect to the diffusion time, the corresponding estimation behavior is interpreted as follows: (i) the natural convergence behavior is wave-like from the entrance towards the output while the measurement injection smoothes this up and down stream by diffusing the sensor information from the sensor location, and (ii) practical profile convergence of around 2% is attained with a rate about 40% faster than the natural ones.

From the preceding implementation results, the following comments are in order:
(i) The proposed convergence conditions of Proposition 1 is a point of departure for a gain tuning procedure, in the understanding of a compromise between convergence speed up and robustness against model-uncertainties and measurement noise.
(ii) The strict dissipativity itself implies a practical (input-to-state) stability property (see e.g. [8]), in the sense of estimation error convergence to a tube around the zero solution (in the presence of some uncertainties). This issue has been numerically tested for representative reaction parameter error of $(-5\%, +10\%)$ bias in (σ, k) and measurement noise: $\hat{y}(t) = c(\xi,t) + 0.01sin(300t)$. The results, presented in Fig. 2, show:(a) the convergence acceleration is maintained and (b) the predicted deviation is remarkably improved.

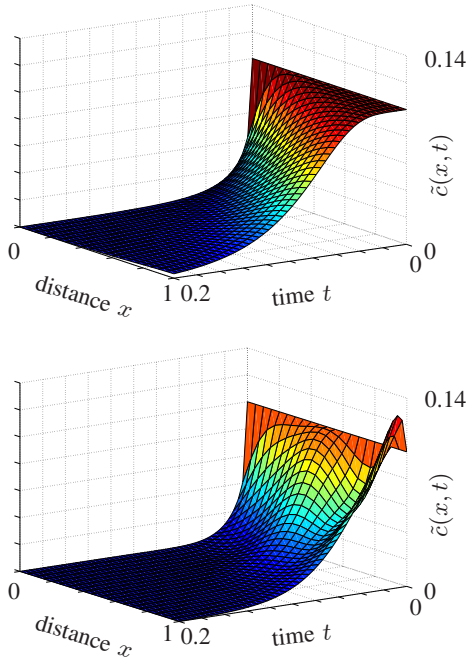

Fig. 1. Estimation error profile evolution. Above: natural response, below: with measurement innovation.

(iii) The observer performance can be enhanced applying various simultaneous measurements ensuring that at least one of the p sensors in $\xi_i,\ i = 1, \ldots, p$ yields $\phi_j(\xi_i) \neq 0$ for $j = 1, \ldots, N$ (compare [15]).

V. Conclusions

The problem of designing a globally convergent observer for a class of tubular reactors with domain measurement has been tackled with a spectral dissipativity approach. The data-assimilation scheme was designed so that the estimation error dynamics were given by a two-dissipative system interconnection: one linear distributed dynamical system with convective and diffusive mechanisms, and one nonlinear lumped static system with the (monotonic or non-monotonic) reaction kinetics. The convergence conditions were drawn on the basis of Lyapunov's second method. The interplay between observer design and sensor location has been identified and interpreted, and sufficient conditions for the observer existence have been drawn based on earlier works on linear DPS observer design by different authors. The considered reactor class covers monotonic as well as non-monotonic reactions and the different implications on the corresponding stability properties and conditions have been delimited and discussed. The proposed approach was illustrated through simulations with a representative tubular reactor with non-monotonic reaction.

Acknowledgements

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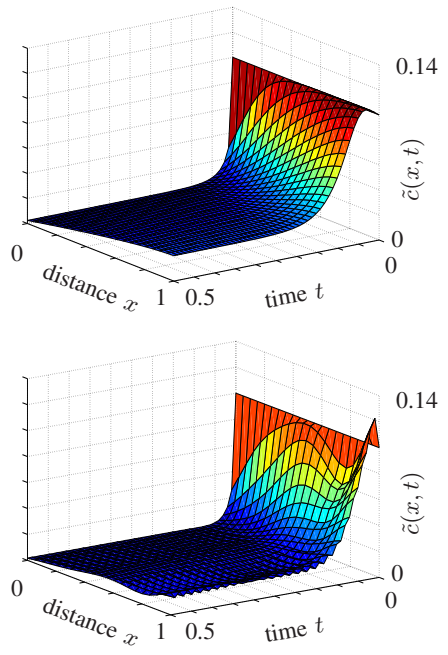

Fig. 2. Estimation error profile evolution for a $(-5\%, +10\%)$ bias in (σ, k). Above: natural response, below: with measurement innovation.

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