

# Dissipativity-based Globally Convergent Observer Design for a Class of Tubular Reactors

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**Abstract:** The problem of designing a globally convergent observer for a class of tubular reactors with boundary measurements is addressed. The problem is tackled by extending a dissipativity theory-based observer design for nonlinear finite-dimensional systems, which has been recently applied to a class of continuous stirred tank reactors. The underlying idea of the proposed observer approach consists in designing the tubular reactor data-assimilation scheme so that the estimation error dynamics are given by a two-dissipative system interconnection: one linear distributed dynamical system with the convective and diffusive mechanisms, and one nonlinear lumped static system with the reaction kinetics. The approach is applied to a tubular reactor with non-monotonic kinetics and boundary measurements, and the associated sufficient solvability condition was identified and interpreted in terms of dissipativity and dimensionless numbers with physical meaning.

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## 1. INTRODUCTION

The last decades were marked by a rapid and intensive development of control theory for infinite-dimensional (distributed parameter) systems (DPS) (see e.g. Gilles [1973], Franke [1987], Curtain and Zwart [1995], Vande Wouwer and Zeitz [2002], Christofides [2001] and references therein). There are two main approaches: the so called early-lumping (EL) and late-lumping (LL). The first one (EL) refers to a model truncation via Galerkin-approximation, orthogonal collocation, approximative inertial manifolds, and others. This approach yields in general a set of coupled ordinary differential equation (ODEs) or "lumped parameter systems" (LPS). The main advantage of EL approaches is the possibility of applying well-known design methods from well-established LPS theory (see e.g. Christofides [2001]). The main disadvantage of the EL approaches is the difficulty of exploiting the intrinsic structural dynamical properties of the system reflected in the DPS model, for design purposes. The LL approach refers to methods which confront the distributed system feature and its main advantage is the possibility of performing the observer design on the basis of information contained in the original model equations. Nevertheless, most of these approaches need certain knowledge about semigroup theory and thus are hard to be used in a control engineering framework.

Recently, a dissipativity-based approach to observer design for LPSs has been proposed e.g. by Arcaj and Kokotovic [2001] and Moreno [2005]. 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 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. Popov [1964]). This approach has been applied to design globally convergent observers for biochemical (Schaum and Moreno [2006]) and chemical (Schaum, Moreno, Diaz-Salgado and Alvarez [2007]) continuous lumped reactors with non-monotonic 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 problem of designing observers and control for the regarded system class has been addressed by several authors. Alvarez, Romagnoli and Stephanopoulos [1981] used orthogonal collocation to obtain a truncated model for which a variable measurement structure was implemented. Boubaker, Babary and Ksouri [1998] tackled the observation problem of a nonlinear plug-flow reactor also by an orthogonal collocation method yielding a LPS for which a variable structure estimator was then designed. Similar problems have been tackled (e.g. in Hagen and Mezic [2003]), by applying a storage functional on the original system's equations and prior introducing a modal representation, designing the observer by solving a Linear Matrix Inequality (LMI). One of the main advantages of this contribution is the ensurance of a dominated observer (control) spill-over. Curtain, Demetriou and Ito [2003]

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developed a distributed observer design based on spectral factorizations, ensuring a solution of a Riccati equation based on which a compensator (observer-based controller) was designed.

In this work, a first step towards the extension to distributed biochemical and chemical process systems of the afore mentioned dissipativity observer design for continuous lumped chemical reactors is taken. For this purpose, the scope is circumscribed to a rather simple single-reaction axial tubular reactor class which captures the fundamental convection, diffusion, reaction, and measurement mechanisms of an ample class of tubular reactors. The reactor case example has one spatial (axial) dimension, two boundary measurements, and includes the basic mechanisms at play: diffusion, convection and nonlinear (possibly non-monotonic) reaction kinetic rate. This consideration must be regarded in the understanding that such reactor class includes some cases of practical interest, and above all represents an inductive methodological step that must be addressed and resolved before considering more complex reactors (multiple reactions and species, axial and radial space distributions, and domain measurements).

First, the reactor model is represented as a two-system interconnection: one linear distributed dynamical exponentially stable subsystem with the combined diffusion-convection mechanism, and one nonlinear, static subsystem with the nonlinear kinetics. Then, an observer with two boundary measurement injections is set and the resulting error dynamics is analyzed via Lyapunov energy method, yielding a sufficient condition for the existence of a globally convergent observer. Such condition involves two dimensionless numbers: the Peclet number (convection-to-diffusion proportion) and a Damköhler-like number (convection-to-reaction quotient). 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.

The present paper is organized as follows. The system model is presented in Section 2. The proposed observer design is presented in Section 3 and tested by numerical simulations. Finally Section 4 concludes the paper.

## 2. OBSERVATION PROBLEM

Consider an (open or packed) isothermal tubular reactor with diffusion/dispersion, convection, nonlinear single species kinetics over the axial spatial domain  $[0, 1]$ . The evolution of the concentration spatial profile is described by the following partial differential equation:

$$\begin{aligned} \frac{\partial c}{\partial t} &= \frac{\partial^2 c}{\partial x^2} - \pi \frac{\partial c}{\partial x} - r(c), \quad 0 < x < 1, \quad t > 0 \\ x = 0 : \quad \frac{\partial c}{\partial x} - \pi c &= -\pi c_e(t), \quad t \geq 0 \\ x = 1 : \quad \frac{\partial c}{\partial x} &= 0, \quad t \geq 0 \\ t = 0 : \quad c(x, 0) &= c_0(x), \quad 0 \leq x \leq 1 \\ y(t) &= [c(0, t) \quad c(1, t)]^T = [y_e(t) \quad y_f(t)]^T, \end{aligned} \quad (1)$$

where

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

$c$  is the dimensionless reaction concentration (say, referred to pure reactant),  $x$  is the dimensionless axial position referred to the reactor length  $L$ ,  $y_e$  (or  $y_f$ ) is the entrance (or exit) boundary concentration measurement,  $\tau$  is the actual time,  $t$  is the dimensionless time referred to Einstein's diffusion time  $t_D$ ,  $D$  is the diffusion/dispersion coefficient,  $\pi$  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 (Fogler [1999]).

Our observation problem consists in designing a globally convergent observer to reconstruct the composition profile on the basis of two boundary measurements. The problem will be addressed via the dissipativity focus we employed before in the consideration of lumped continuous stirred reactors (Schaum, Moreno, Diaz-Salgado and Alvarez [2007]).

It must be pointed out that the proposed approach for system (1) can be extended in the future to non-isothermal reactors and multi-species kinetics, with the possibility of suitably located domain measurements.

## 3. OBSERVER DESIGN

### 3.1 Principal considerations

Let us consider the following observer for system (1):

$$\begin{aligned} \frac{\partial \hat{c}}{\partial t} &= \frac{\partial^2 \hat{c}}{\partial x^2} - \pi \frac{\partial \hat{c}}{\partial x} - r(\hat{c}), \quad 0 < x < 1, \quad t > 0 \\ x = 0 : \quad \frac{\partial \hat{c}}{\partial x} - \pi \hat{c} &= -\pi c_e(t) + k_0(\hat{y}_e(t) - y_e(t)), \quad t \geq 0 \\ x = 1 : \quad \frac{\partial \hat{c}}{\partial x} &= k_1(\hat{y}_f(t) - y_f(t)), \quad t \geq 0 \\ t = 0 : \quad \hat{c}(x, 0) &= \hat{c}_0(x), \quad 0 \leq x \leq 1 \\ y(t) &= [\hat{c}(0, t) \quad \hat{c}(1, t)]^T = [\hat{y}_e(t) \quad \hat{y}_f(t)]^T, \end{aligned} \quad (2)$$

with two measurement injections: one in the entrance ( $x = 0$ ) and one in the exit ( $x = 1$ ), and two adjustable gains ( $k_0$  and  $k_1$ ), one per measurement. From the subtraction of (2) from (1) the estimation error dynamics follows:

$$\begin{aligned} \frac{\partial \tilde{c}}{\partial t} &= \frac{\partial^2 \tilde{c}}{\partial x^2} - \pi \frac{\partial \tilde{c}}{\partial x} + \nu(x, t), \quad 0 < x < 1, \quad t > 0 \\ x = 0 : \quad \frac{\partial \tilde{c}}{\partial x} - \pi \tilde{c} &= k_0(\hat{y}_e(t) - y_e(t)), \quad t \geq 0 \\ x = 1 : \quad \frac{\partial \tilde{c}}{\partial x} &= k_1(\hat{y}_f(t) - y_f(t)), \quad t \geq 0 \\ t = 0 : \quad \tilde{c}(x, 0) &= \tilde{c}_0(x), \quad 0 \leq x \leq 1 \\ \nu(x, t) &\triangleq -[r(c + \tilde{c}) - r(c)] \triangleq -\rho(\tilde{c}, t), \end{aligned} \quad (3)$$

where  $\tilde{c}(x, t) = \hat{c}(x, t) - c(x, t)$  is the observation error. Note that this system can be represented in the Hilbert space  $\mathcal{Z} = L_2([0, 1], \mathbb{R})$ , defining an adequate operator in the framework of abstract differential equations. Thus, system (3) is a nonlinear boundary control system in  $\mathcal{Z}$ , whose linear part generates an exponentially stable  $C_0$ -semigroup. For the purpose at hand, it suffices to keep

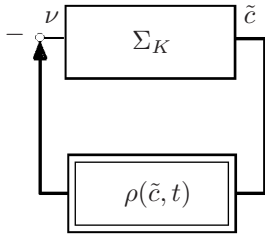


Fig. 1. Illustration of the structure of the observation error. in mind that the developments take place in the Hilbert space  $\mathcal{Z} = L_2([0, l], \mathbb{R})$ .

Let us regard the observation error dynamics as a two-subsystem interconnection: (i) one linear dynamical subsystem

$$\begin{aligned} \frac{\partial \tilde{c}}{\partial t} &= \frac{\partial^2 \tilde{c}}{\partial x^2} - \pi \frac{\partial \tilde{c}}{\partial x} + \nu(x, t), \quad 0 < x < 1, \quad t > 0 \\ x = 0 : \frac{\partial \tilde{c}}{\partial x} - \pi \tilde{c} &= k_0(\hat{y}_e(t) - y_e(t)), \quad t \geq 0 \\ x = 1 : \frac{\partial \tilde{c}}{\partial x} &= k_1(\hat{y}_f(t) - y_f(t)), \quad t \geq 0 \\ t = 0 : \tilde{c}(x, 0) &= \hat{c}_0(x), \quad 0 \leq x \leq 1 \end{aligned} \quad (4)$$

with the convection, diffusion and measurement injection mechanisms, and the reaction rate spatio-temporal function  $\nu(x, t)$  as exogenous distributed input, and (ii) one nonlinear static subsystem

$$-\nu(x, t) \triangleq \rho(\tilde{c}(x, t), t) \quad (5)$$

which, driven by the concentration error profile  $\tilde{c}(x, t)$  generates the reaction rate error profile ( $\rho$ ). In other words, system (3) is seen as the negative interconnection of a linear system  $\Sigma_K : \nu \xrightarrow{k_0, k_1} \tilde{c}$ , that maps the distributed source function  $\rho(\tilde{c})$  (in a way modified by the output injection  $K\hat{y}$ ) to  $\tilde{c}(x, t)$ , with a static time-varying nonlinearity  $\nu = -\rho(\tilde{c}, t)$ . The system structure of this is illustrated in Figure 1. From an abstract energy perspective, the nonlinear part supplies energy to the linear part, and vice versa. On basis of an energy exchange framework the methodological steps of the proposed approach are stated next:

- *Sector condition for  $\rho(\tilde{c}(x, t), t)$* : Find bounds of the energy supply from the nonlinear part ( $\rho$ ) to the linear part ( $\Sigma_K$ ) by drawing a sector type dissipativity condition for  $\rho(\tilde{c}(x, t), t)$ .
- *Strict dissipativity of  $\Sigma_K$* : Then, a Lyapunov energy dissipativity condition for  $\Sigma_K$  is employed, so that the negative interconnection of  $\Sigma_K$  with  $\rho(\tilde{c}(x, t), t)$  is strictly dissipative.

This pursuit will be carried out in a concrete storage functional based framework, with direct implications of the stability of the error's zero solution by means of Lyapunov's second method (see e.g. Zubov [1964], Gilles [1973], Franke [1987]).

### 3.2 Sector condition for $\rho(\tilde{c}(x, t), t)$

From the application of the mean value theorem, the reaction rate error function satisfies the following expression:

$$\rho(\tilde{c}, t) = r(c + \tilde{c}) - r(c) = r'(c + \eta\tilde{c})\tilde{c}, \quad \eta \in (0, 1).$$

Thus, the range of  $\rho(\tilde{c}, t)$  is completely included in the sector determined by the maximum and minimum of the reaction rates gradient

$$K_1 \leq r'(c + \eta\tilde{c}) \leq K_2, \quad K_1, K_2 \in \mathbb{R}, \quad (6)$$

and  $\rho(\tilde{c}, t) \in [K_1, K_2]$  (Khalil [2002]), this is

$$(K_1\tilde{c} - \rho)(\rho - K_2\tilde{c}) \geq 0 \quad (7)$$

or equivalently

$$K_1\tilde{c}^2 \leq \rho(\tilde{c}, t)\tilde{c} \leq K_2\tilde{c}^2. \quad (8)$$

Inequality (7) represents a (pointwise) dissipativity condition in  $\mathcal{Z}$  (cp. Moreno [2005]). From integration over the spatial domain  $[0, 1]$  and the definition of inner product in  $\mathcal{Z}^2$ , this can be interpreted as a distributed dissipativity inequality. Note that for  $K_1 \geq 0$  the non-linearity is passive and a sufficient condition for the stability of the (negative) interconnection of  $\Sigma_K$  with  $\rho$  is the exponential stability of the linear dynamical subsystem  $\Sigma_K$ . Therefore the more interesting case is given for  $K_1 < 0$ , as in this case the exponential stability of  $\Sigma_K$  is (generally speaking) not sufficient for a stability assessment for its interconnection with  $\rho$ . This issue is analyzed next.

### 3.3 Strict dissipativity of $\Sigma_K$

Here the idea is to choose  $k_0, k_1$  in (3), so that the dissipativeness of the linear convective-diffusive subsystem  $\Sigma_K$  is ensured (in an appropriate manner). For this aim, introduce a quadratic storage functional candidate  $\mathcal{S}(\tilde{c})$  defined by the weighted squared concentration error norm

$$\mathcal{S}(\tilde{c}) \triangleq \langle \tilde{c}, P\tilde{c} \rangle, \quad (9)$$

with a positive weight function  $P(x) > 0$  to be determined. If one can show that, with respect to  $\mathcal{S}(\tilde{c})$ , the linear part enables us to choose the gain pair  $(k_0, k_1)$  so that the energy stored in the concentration profile error is (strictly) dissipated, in virtue of the conic form of the chosen storage functional, the (exponential) stability of  $\tilde{c} = 0$  can be concluded. For this aim, we have to show that:

$$\exists P > 0, \epsilon > 0, k_0, k_1 : \frac{d\mathcal{S}(\tilde{c})}{dt} \leq -\epsilon\mathcal{S}(\tilde{c}). \quad (10)$$

If this condition is met,  $\mathcal{S}$  is a Lyapunov functional, and the exponential stability of  $\tilde{c} = 0$  follows by Lyapunov's second method (see e.g. Zubov [1964], Gilles [1973], Franke [1987]).

Thus, the key step is to find  $P > 0, \epsilon > 0$  and an observer gain pair  $(k_0, k_1)$  so that the convection-diffusion-reaction interconnection  $(\Sigma_K, -\rho(\tilde{c}, t))$  meets the negative dissipation rate inequality (10). There are different approaches to achieve this. Here, the task will be pursued via a natural concept of absolute stability concepts for the interconnection in combination with strict dissipation with respect to the quadratic storage functional  $\mathcal{S}(\tilde{c})$ .

Next, conditions for the (adjustable) gains  $k_0, k_1$  are drawn so that the linear convective-diffusive dynamical subsystem  $\Sigma_K : \nu \xrightarrow{k_0, k_1} \tilde{c}$  meets dissipativity condition (10) that allows the required stability assessment of the interconnection with  $\nu = -\rho(\tilde{c})$ . In the next proposition

<sup>2</sup> The used inner product is the conventional one in  $\mathcal{Z} = L_2$ , i.e.  $\langle a, b \rangle = \int_0^l abd x, \quad a, b \in \mathcal{Z}$ .

are stated sufficient conditions on the observer gains to achieve this.

*Proposition 1. (Proof in the Appendix)*

There is an observer gain pair  $(k_0, k_1)$  which makes the reactor observer (2) globally exponentially convergent if the Peclet number  $\pi$  (convection-to-diffusion measure) and the lower bound (possibly negative)  $K_1$  (6) of the reaction rate derivative meet the following condition:

$$\frac{\pi^2}{4} + 2K_1 > 0. \quad (11)$$

A particular solution for the gain pair is

$$(k_0, k_1) = \left(-\frac{3}{4}, \frac{1}{4}\right)\pi \quad (12)$$

which ensures that the dissipativity inequality (10) is satisfied with  $\epsilon = \pi^2/4 + 2K_1$ .

According to equation (12): (i) the convergence condition is always met by reactors with monotonic kinetics, as  $K_1 \geq 0$  (passive case), and (ii) the fulfillment of the convergence condition by a reactor with non-monotonic kinetics ( $K_1 < 0$ ) requires that the lower bound  $K_1 < 0$  of the reaction rate derivative, in the antitonic branch, is smaller than one eight of the square Peclet number. Moreover for the gain choice (12) represents a limiting case, and the point of departure to perform the gain tuning procedure in the light of an adequate estimator functioning with a suitable compromise between reconstruction rate and robustness. Actually from the proof results that the gain pair has to be chosen such that

$$\pi - \sqrt{\pi^2 + 8K_1 - 4\epsilon} \leq 4k_1 \leq \pi + \sqrt{\pi^2 + 8K_1 - 4\epsilon} \quad (13)$$

$$k_0 = k_1 - \pi$$

The following section illustrates the methodology for a representative case with non-monotonic reaction rate.

## 4. A CASE STUDY

### 4.1 Problem specification

In the chemical reactor engineering field, it is known that continuous reactors with non-monotonic kinetic rates rise difficult observer and control problems, because there is a lack of local observability around a steady-state with maximum reaction rate, and of global observability (Schaum and Moreno [2007]). This is caused by the lack of concentration distinguishability in the sense 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. Given that the observation problem for continuous reactors has been recently addressed via the dissipativity approach, (Schaum and Moreno [2006], Schaum, Moreno, Diaz-Salgado and Alvarez [2007]), and that the scope of the present study is the extension of such approach to the tubular reactor case, let us consider our reactor (1) observation problem with non-monotonic (Haldane-type) kinetics

$$r(c) = \frac{kc}{(1 + \sigma c)^2}, \quad t_R = \frac{1}{k} \quad (14)$$

where  $k > 0$  [1/s] is the reaction frequency factor,  $t_R$  its corresponding characteristic reaction time, and  $\sigma > 0$  is the auto-inhibition constant. It must be pointed out that

this kinetics rate underlies an important class of industrial (bio)chemical processes. From the above mentioned continuous reactor dissipativity-based observation study (Schaum, Moreno, Diaz-Salgado and Alvarez [2007]), we know that the rate error function  $\rho(\tilde{c}, t)$  encompasses the sector  $[-k, \frac{k}{27}]$ . Consequently, following the above result (A.11) the absolute stability of the linear part with respect to non-linearities in  $[K_1, K_2]$  follows if

$$\pi > 2\sqrt{2k} \quad (15)$$

implying that the observer gains must meet the conditions (13). This in turn implies that the strictly negative dissipation rate inequality (10) is met, and that the storage functional  $\mathcal{S}(\tilde{c})$  is a Lyapunov functional. It follows that  $\exists M > 0 : \mathcal{S} \leq Me^{-\epsilon t}$ , and  $\|\tilde{c}(x, t)\| \rightarrow 0$  exponentially fast. From continuity arguments (note that  $\tilde{c}(x, t)$  has to be at least twice differentiable in  $x$ ), it follows that the error profile  $\tilde{c}(x, t)$  vanishes exponentially. Thus the exponential convergence of the estimate to the actual value for each point of the tubular reactor is concluded.

Summarizing, the fulfillment of the inequalities (15) ensures the global exponential stabilizability of the two-subsystem interconnection  $(\Sigma_K, \rho)$ . The condition says that the destabilization potential of the chemical reaction must be dominated by the convection-diffusion mechanism. The condition pair (??), (??):(i) establishes that the boundary linear measurement innovation injection must be chosen according with the Peclet ( $\pi$ ) and reaction rate ( $k$ ) value, and (ii) constitutes the basis of a gain tuning procedure.

### 4.2 Simulation study

In a first simulation, the reactor (1) was regarded with the Peclet-inhibition-reaction rate triplet  $(\pi, \sigma, k) = (10, 3, 4)$  and the initial concentration profile  $c_0(x) = 0$ . The observer was set with the derived initial profile  $\hat{c}_0(x) = 1$ , and the application of the gain condition (A.10) yielded the gain pair  $(k_0, k_1) = (-7.5, 2.5)$ . Keeping in mind that the reactor time is scaled with respect to the diffusion time, the corresponding estimation behavior is presented in Figure 2, showing that: (i) as expected, the close-to-boundary regions converge quickly, (ii) there is a convergence speeding diffusion-like propagation of innovation (i.e. information contained in the measurement and not in the model) from the boundary towards the center, and (iii) practical profile convergence within a 98% setting is attained with a rate about eight times faster than the natural reactor dynamics. For comparison a different scenario was tested: the Peclet-inhibition-reaction rate triplet was set to  $(\pi, \sigma, k) = (1000, 3, 400)$ , while the initial profiles were kept equal ( $c_0(x) = 0, \hat{c}_0(x) = 1$ ). The optimal (with respect to observer convergence speed) observer gain conditions yielded  $(k_0, k_1) = (-750, 250)$ . The corresponding estimation error evolution is presented in Figure 3, showing: (i) quick close-to-boundary convergence, (ii) a convergence speeding wave (convection)-like axial propagation of innovation, and (iii) convergence rate about twenty times faster than the natural one.

### 4.3 Concluding Remarks

From the preceding implementation results, the following comments are in order:

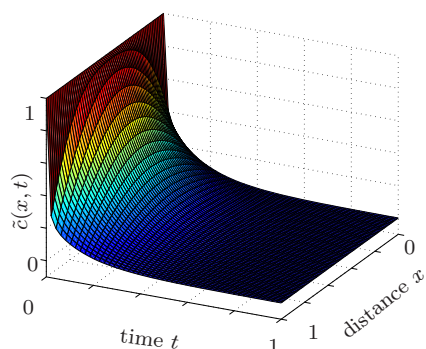


Fig. 2. I

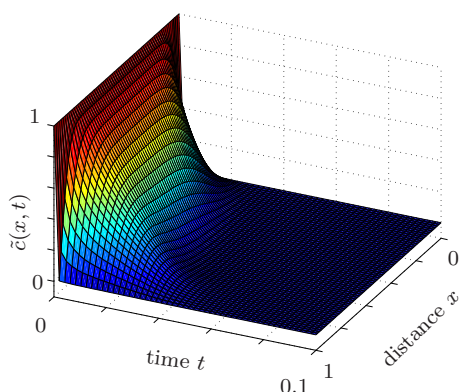


Fig. 3. Observer error profile evolution: scenario 2.

- Due to the Lyapunov-like approach, there is a given "a-priori" robustness of the observer convergence with respect to additive proportional errors of the type  $\delta(\hat{c}) = \beta\hat{c}$ , which grows with the Peclet number  $\pi$ . This means that high superficial velocities and/or low diffusion coefficients favor robustness. In other words, a "plug-flow like" reactor exhibits the best robustness property.
- The observer performance can be improved by further incorporating suitably located domain measurements and/or improved data assimilation mechanisms.
- It is known from LPS theory that the system's detectability is a necessary condition for observer design. In particular, this means that the observer error converges to zero for all the so called bad exogenous inputs (here the inflow concentration  $c_e(t)$ ) which may cause indistinguishable concentration profiles. These results suggest that the reactor's detectability property and the sensor location issue can be addressed as a detectability assessment problem.

## 5. CONCLUSIONS

The problem of designing a globally convergent observer for a class of tubular reactors with boundary measurements has been addressed. The problem has been solved by applying a dissipativity theory based observer design. 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 reaction kinetics. The convergence conditions were drawn via Lyapunov's second method, and endowed with physical meaning. The underlying tradeoff between profile reconstruction rate and

robustness was identified. The proposed approach was illustrated with a representative example through simulations.

The proposed study is a point of departure to design reduced order observers and to perform optimal sensor location assessments.

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## REFERENCES

- J. Alvarez, J.A. Romagnoli, G. Stephanopoulos, Variable measurement structures for the control of a tubular reactor, *Chem. Eng. Sci.* (36)10, p. 1695-1712, 1981.
- I. Aksikas, J.J. Winkin, D. Dochain, Optimal LQ-feedback regulation of a nonisothermal plug flow reactor model by spectral factorization, *IEEE Trans. on Autom. Contr.* (52)7, p. 1179-1193, 2007.
- M. Arcak, P. Kokotovic, Nonlinear Observers: a circle criterion design and robustness analysis, *Automatica* (37), p. 1923-1930, 2001.
- O. Boubaker, J.P. Babary, M. Ksouri, Variable structure estimation and control of nonlinear distributed parameter bioreactors, *IEEE*, 1998.
- P.D. Christofides, Nonlinear and robust control of PDE systems, *Systems & Control: Foundations & Applications*, Birkhäuser, 2001.
- R. Curtain, H. Zwart, An Introduction to infinite-dimensional linear systems theory, *Springer Verlag*, 1995.
- R. Curtain, M.A. Demetriou, M.A., K. Ito, Adaptive compensators for perturbed positive real infinite-dimensional systems, *Int. J. Appl. Math. Comput. Sci.*, (13)4, p. 441-452, 2003.
- J. Diaz Salgado, A. Schaum, J. Alvarez, J.A. Moreno, Interlaced estimator-control design for continuous exothermic reactors with non-monotonic kinetics, *Prepr. of the 8th IFAC Symp. DYCOPS*, V. 3, p. 43-48, 2007.
- H.S. Fogler, Elements of Chemical Reaction Engineering, third edition, *Prentice Hall*, 1999.
- D. Franke, Systeme mit örtlich verteilten Parametern (Eine Einführung in die Modellbildung, Analyse und Regelung), *Springer-Verlag*, 1987.
- E.D. Gilles, Systeme mit verteilten Parametern (Einführung in die Regelungstheorie) *R. Oldenburg Verlag*, 1973.
- G. Hagen, I. Mezic, Spillover stabilization in finite-dimensional control and observer design for dissipative evolution equations, *SIAM J. Control Optim.* (42)2, p. 746-768, 2003.
- H.K. Khalil, Nonlinear Systems, *Prentice Hall, Upsaddle River, New Jersey, 3rd Edition*, 2002.
- J.A. Moreno, Approximate Observer Error Linearization by Dissipativity Methods, *Control and Observer Design for Nonlinear Finite and Infinite Dimensional Systems*, Springer Berlin Heidelberg New York, 2005.
- V.M. Popov, A problem in the theory of absolute stability of controllable systems, *Avtom. Telemekh.*, (9), p. 1257-1262, 1964.

- A. Schaum, J.A. Moreno, Dissipativity-based observer design for a class of biochemical reactors, *CONCIBE 2006*, p. 2006.
- A. Schaum, J.A. Moreno, Dynamical analysis of global observability properties for a class of biological reactors, *Prepr. of the 10th IFAC Symposium CAB*, V.1, p. 209-214, 2007.
- A. Schaum, J.A. Moreno, J. Diaz-Salgado, J. Alvarez, Dissipativity-based observer and feedback control design for a class of chemical reactors, *Prepr. of the 8th IFAC Symposium DYCOFS*, V.4, pp. 73-78, 2007.
- A. Smyshlyaev, M. Krstic, Backstepping observers for a class of parabolic PDEs, *System and Control Letters*, 54, p. 613-625, 2005.
- A. Vande Wouwer, M. Zeitz, State estimation in distributed parameter systems, *Encyclopedia of Life Support Systems*, <http://www.eolss.net>, 2002.
- V.I. Zubov, Methods of A.M. Lyapunov and their application, *P. Nordhoff LTD - Groningen - The Netherlands*, 1964.

## 6. APPENDIX A.

*Proof of Proposition 1:* Take the time derivative of  $\mathcal{S}(\tilde{c})$  (9), this is

$$\frac{d\mathcal{S}(\tilde{c})}{dt} = 2 \int_0^1 \left( \frac{\partial^2 \tilde{c}}{\partial x^2} - \pi \frac{\partial \tilde{c}}{\partial x} + \nu \right) P \tilde{c} dx \quad (\text{A.1})$$

By the divergence theorem we have that

$$2 \int_0^1 \frac{\partial^2 \tilde{c}}{\partial x^2} P \tilde{c} dx = \left[ 2P \frac{\partial \tilde{c}}{\partial x} \tilde{c} \right]_0^1 - \int_0^1 \left\{ \frac{dP}{dx} \frac{\partial[\tilde{c}^2]}{\partial x} + 2P \left[ \frac{\partial \tilde{c}}{\partial x} \right]^2 \right\} dx. \quad (\text{A.2})$$

Consider the boundary conditions in (4) and obtain

$$\left[ 2P(x) \frac{\partial \tilde{c}}{\partial x} \tilde{c} \right]_0^1 = 2P(1)k_1 \tilde{c}^2(x) - 2P(0)[k_0 + \pi] \tilde{c}^2(0).$$

Introduce the auxiliary function  $K(x)$  such that

$$K(0) = k_0 + \pi, \text{ and } K(1) = k_1.$$

By means of  $K(x)$  rewrite the boundary term

$$\left[ 2P(x) \frac{\partial \tilde{c}}{\partial x} \tilde{c} \right]_0^1 = \left[ 2P(x)K(x)\tilde{c}^2 \right]_0^1.$$

The last term can be expressed as an integral by

$$\left[ 2P(x)K(x)\tilde{c}^2 \right]_0^1 = \int_0^1 \frac{\partial}{\partial x} \left[ 2P(x)K(x)\tilde{c}^2 \right] dx. \quad (\text{A.3})$$

Substituting (A.3) into (A.2) yields

$$2 \int_0^1 \frac{\partial^2 \tilde{c}}{\partial x^2} P \tilde{c} dx = \int_0^1 \left\{ 2PK \frac{\partial[\tilde{c}^2]}{\partial x} + 2 \left( \frac{dP}{dx} K + P \frac{dK}{dx} \right) \tilde{c}^2 - \frac{dP}{dx} \frac{\partial[\tilde{c}^2]}{\partial x} - 2P \left[ \frac{\partial \tilde{c}}{\partial x} \right]^2 \right\} dx. \quad (\text{A.4})$$

For the sake of simplicity choose  $K$  constant, implying that

$$k_1 = k_0 + \pi, \text{ and } \frac{dK}{dx} = 0, \quad (\text{A.5})$$

so that (A.4) becomes

$$2 \int_0^1 \frac{\partial^2 \tilde{c}}{\partial x^2} P \tilde{c} dx = \int_0^1 \left\{ \left[ 2PK - \frac{dP}{dx} \right] \frac{\partial[\tilde{c}^2]}{\partial x} + 2 \frac{dP}{dx} K \tilde{c}^2 - 2P \left[ \frac{\partial \tilde{c}}{\partial x} \right]^2 \right\} dx. \quad (\text{A.6})$$

Now recall the sector condition on  $\nu = -\rho$  (8) to obtain

$$2 \int_0^1 P \nu \tilde{c} dx = -2 \int_0^1 P \rho \tilde{c} dx \leq -2K_1 \int_0^1 P \tilde{c}^2 dx. \quad (\text{A.7})$$

Substitute this into (A.1) and obtain finally

$$\frac{d\mathcal{S}(\tilde{c})}{dt} \leq \int_0^1 \left\{ \left[ (2K - \pi)P - \frac{dP}{dx} \right] \frac{\partial[\tilde{c}^2]}{\partial x} + \left[ 2 \frac{dP}{dx} K - 2PK_1 \right] \tilde{c}^2 \right\} dx.$$

Conclude that the dissipation inequality (10) is met if the following two conditions are satisfied

$$\frac{dP}{dx} - (2K - \pi)P = 0 \quad (\text{A.8})$$

$$2 \frac{dP}{dx} K - 2K_1 P \leq -\epsilon P, \quad \epsilon > 0. \quad (\text{A.9})$$

The solution of the differential equation (A.8) yields

$$P(x) = e^{(2K-\pi)x},$$

and the substitution of this expression into the differential inequality (A.9) yields the algebraic inequality

$$[(4K - 2\pi)K - 2K_1 + \epsilon] P \leq 0.$$

Thus, the corresponding gain possibilities are given by

$$K = \frac{1}{4} \left[ \pi \pm \sqrt{\pi^2 + 8K_1 - 4\epsilon} \right]. \quad (\text{A.10})$$

The existence of a real solution for the observer gain function  $K$  is ensured if the following condition is met

$$0 < \frac{\pi^2}{4} + 2K_1. \quad (\text{A.11})$$

Keeping in mind (A.5), a possible choice of the observer gain is

$$\begin{aligned} k_0 &= -\frac{3\pi}{4} \\ k_1 &= \frac{\pi}{4}, \end{aligned} \quad (\text{A.12})$$

implying that (10) is satisfied with

$$\epsilon = \frac{\pi^2}{4} + 2K_1. \quad (\text{A.13})$$

This ends the proof.  $\square$