State Estimators for a Class of Isothermal Tubular Reactors

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Abstract

This work presents two state estimators for a class of isothermal tubular reactors involving sequential reactions for which the kinetics depends on the reactants concentrations only. These conceptions are performed by describing the model as infinite-dimensional state-space system, with bounded observation. It is shown that the given observers ensure asymptotic state estimator with exponentially decay error, when measurements (a) of both the reactant and product concentrations and (b) of only the product concentration, are available at the reactor output. Simulation results are also presented showing the effectiveness of the proposed observers.

Keywords: Distributed parameter systems, state estimators, perturbed systems, tubular reactor, C_0-semigroup.

1. Introduction

Although tubular reactors have been largely used in (bio)process industry for several decades, system analysis and design of state observers has taken an increasing importance over the past decades (see [1], [2], [3], [4], [5], [6], [7], [8] and the references within).

For the system control, the exact and full knowledge of system's states is important. However, in the mathematical model of the tubular reactors, the states depend on spatial variable and that makes it not possible to have full information of the system's states due to the fact that installing necessary sensors for measurements may not be physically possible or the costs may become excessive. In such a case, the states can be estimated using state estimators (observers).

The motivation of this paper is to investigate this issue and provide an observer, that ensures asymptotic state estimator with exponentially decay error, for the basic dynamical model of isothermal axial dispersion reactors involving sequential reactions for which the kinetics only depends on the reactants concentrations involved in the following chemical reaction:

$$C_1 \rightarrow bC_2 \tag{1}$$

where C_1 is the reactant, C_2 the product, and $b > 0$ is the stoichiometric coefficient of the reaction. The dynamics of the process in a tubular reactor with axial dispersion are given, for all time $t \geq 0$ and for all $z \in [0, L]$ where L is the reactor length, by mass balance equations (see [4]):

$$\begin{aligned} \frac{\partial x_1}{\partial t} &= D_a \frac{\partial^2 x_1}{\partial z^2} - \upsilon \frac{\partial x_1}{\partial z} - r(x_1, x_2), \\ \frac{\partial x_2}{\partial t} &= D_a \frac{\partial^2 x_2}{\partial z^2} - \upsilon \frac{\partial x_2}{\partial z} + br(x_1, x_2) \end{aligned} \tag{2}$$

with the boundary conditions:

$$\begin{aligned} &D_a \frac{\partial x_1}{\partial z}(z=0,t) - \upsilon x_1(z=0,t) = -\upsilon x_{in}(t), \\ &D_a \frac{\partial x_2}{\partial z}(z=0,t) - \upsilon x_2(z=0,t) = 0, \\ &D_a \frac{\partial x_{i=1,2}}{\partial z}(z=L,t) = 0, \end{aligned} \tag{3}$$

and the initial conditions:

$$x_1(z, t=0) = x_1^0, \quad x_2(z, t=0) = x_2^0 \tag{4}$$

where $x_1(z,t), x_2(z,t), x_{in}(z,t), \upsilon, D_a$ and r are the concentrations of C_1 and C_2 (mol/l), the influent reactant concentration (mol/l) and the fluid superficial velocity (m/s), the axial dispersion coefficient (m^2/s), and the reactant rate $(mol/l\,s)$. We assume that the kinetics depend only on the reactant concentration x_1 and we consider a reaction rate model of the form $r = k_0 x_1$, where

k_0 is the kinetic constant (s^{-1}). x_1^0, x_2^0 are the initial states. The purpose of this work is to reconstruct the state variables initially unknown, when measurements may occur at the reactor output only, in the case (a) both reactant concentration and product concentration are measured and (b) only the product concentration is available for measurements.

2.State-space system framework

Let consider the Hilbert space $H = L^2[0,L] \times L^2[0,L]$, endowed with the usual inner product defined by

$$\langle z_1, z_2 \rangle = \langle x_1, x_2 \rangle_{L^2} + \langle y_1, y_2 \rangle_{L^2},$$

for all $z_1 = (x_1, y_1)^T$ and $z_2 = (x_2, y_2)^T$ in H, *and the induced norm defined by*

$$\|(x_1, x_2)^T\| = \sqrt{\|x_1\|_{L^2}^2 + \|x_2\|_{L^2}^2},$$

for all $(x_1, x_2)^T \in H$, *where*

$$\langle f, g \rangle_{L^2} = \int_0^L f(z) g(z) dz \text{ and } \|f\|_2 = \sqrt{\langle f, f \rangle_{L^2}}.$$

In the dynamic model (2)-(4), x_{in} is considered as the control at $z = 0$. In order to facilitate our study we have to carry out some transformations. If we extract the boundary controlled part, the basic model given by (2)-(3) and the unknown initial condition (4), when expended with an output equation, is given a description in terms of a linear differential equation on H, viz., for all positive t and all initial conditions $x_0 := (x_1^0, x_2^0)^T$ in H, (see [4] and the references within),

$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ y(t) = Cx(t), x(0) = x_0 \end{cases} \qquad (5)$$

where, $\dot{x}$ stands for the time derivative of the state $x(t) = (x_1(.,t), x_2(.,t))^T$, and the linear operator A is defined by

$$Ax = \begin{pmatrix} D_1 \frac{d^2.}{dz^2} - \upsilon \frac{d.}{dz} - k_0 & 0 \\ bk_0 & D_2 \frac{d^2.}{dz^2} - \upsilon \frac{d.}{dz} \end{pmatrix} \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix}$$

on its domain

$$D(A) = \left\{ \begin{array}{l} x = (x_1, x_2)^T \in H : x, \frac{dx}{dz} \in H \text{ are absolutely} \\ \text{continuous}, \frac{d^2x}{dz^2} \in H, D_a \frac{dx_i}{dz}(0) - \upsilon x_i(0) = 0, \\ \frac{dx_i}{dz}(L) = 0, \text{ for } i = 1,2 \end{array} \right\}$$

The operator $A := \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}$ is the infinitesimal generator of a C_0-semigroup $(T_A(t))_{t \geq 0}$ on H, exponentially stable (see [4]), i.e., there exists constant $M > 0$ such that,

$$\|T_A(t)\| \leq M \exp(-\frac{\upsilon^2}{4D_a} t), \quad \forall t \geq 0$$

The control operator B is a bounded linear operator from IR^2 to H, which is defined by $B = \begin{pmatrix} \upsilon \\ 0 \end{pmatrix} \delta(.)$, where $\delta(z)$ is the Dirac delta distribution. The control $u(t) = x_{in}(t)$, and the output trajectory C is a bounded linear operator.

The following Theorem will be needed in the sequel for the state observer conceptions.

Theorem 2.1 ([9], p., 109) Let A be the infinitesimal generator of a C_0-semigroup $(T_A(t))_{t \geq 0}$ and D is linear bounded operator on H. The operator $A + D$ is the infinitesimal generator of a C_0-semigroup $(T_{A+D}(t))_{t \geq 0}$ which is the unique solution of the equation

$$T_{A+D}(t)x_0 = T(t)x_0 + \int_0^T T(t-s) D T_{A+D}(s) x_0 ds,$$

For all $x_0 \in H$. If in addition, $\|T_A(t)\| \leq Me^{\omega t}$, then

$$\|T_{A+D}(t)\| \leq Me^{(\omega + M\|D\|)t}.$$

2.1 State observer

Hereafter we consider measurements of the state vector $x(t)$ are available at the reactor output only. In this case, the output function $y(.)$ is defined as follows: we consider a (very small) finite interval at the reactor output $[1-\omega, 1]$ such that:

$$y(t) = (Cx)(t) := \int_0^1 \chi_{[1-\omega,1]}(a)x(a,t)da, \quad \forall t \in IR^+ \quad (6)$$

Where, $\chi_{[1-\omega,1]}(a) = 1$ if $a \in [1-\omega,1]$ and $\chi_{[1-\omega,1]}(a) = 0$ elsewhere, with $0 < \omega < 1$ is a small number. The observer operator $C : H \to IR^2$ is linear bounded. For all $x, y \in H \times IR^2$,

$$\langle Cx, y\rangle_{IR^2} = \langle \int_0^1 \chi_{[1-\omega,1]}(a)x(a,.)da, y\rangle_{IR^2} = \int_0^1 \langle x(a,.), \chi_{[1-\omega,1]}(a)y\rangle_{IR^2} da$$

The adjoint operator C^* of C is defined for all $(z,t) \in [0,1] \times IR^+$ by:

$$(C^* y)(z) = \chi_{[1-\omega,1]}(z)y$$

For all $x \in H$,

$$\|C^* Cx\|^2 = \int_0^1 (\chi_{[1-\omega]}(z)(\int_0^1 \chi_{[1-\omega,1]}(a)x(a,.)da))^2 dz \le \omega \|\chi_{[1-\omega,1]}\|^2 \|x\|^2 = \omega^2 \|x\|^2$$

Then,

$$\|C^* C\| \le \omega$$

A candidate observer for the system (2)-(4), is obtained as the output of the following dynamic system

$$\begin{aligned} \frac{\partial \hat{x}_1}{\partial t} &= D_a \frac{\partial^2 \hat{x}_1}{\partial z^2} - \upsilon \frac{\partial \hat{x}_1}{\partial z} - k_0 \hat{x}_1 + \upsilon \delta x_{in}(t) + gC_1^*(C_1 x_1 - C_1 \hat{x}_1) \\ \frac{\partial \hat{x}_2}{\partial t} &= D_a \frac{\partial^2 \hat{x}_2}{\partial z^2} - \upsilon \frac{\partial \hat{x}_2}{\partial z} + bk_0 \hat{x}_1 + gC_2^*(C_2 x_2 - C_2 \hat{x}_2) \end{aligned} \quad (7)$$

with the boundary conditions:

$$\begin{aligned} &D_a \frac{\partial \hat{x}_1}{\partial z}(z=0,t) - \upsilon \hat{x}_1(z=0,t) = -\upsilon x_{in}(t), \\ &D_a \frac{\partial^2 \hat{x}_2}{\partial z^2}(z=0,t) - \upsilon \hat{x}_2(z=0,t) = 0, \\ &D_a \frac{\partial \hat{x}_{i=1,2}}{\partial z}(z=L,t) = 0, \end{aligned} \quad (8)$$

and the initial conditions:

$$\hat{x}_1(z,t=0) = \hat{x}_1^0, \quad \hat{x}_2(z,t=0) = \hat{x}_2^0 \quad (9)$$

with $C = (C_1 \quad C_2)^T$ defined by (6) and g is a positive number.
The system (7)-(9) can be written on its compact form

$$\begin{cases} \dot{\hat{x}}(t) = A\hat{x}(t) + Bu(t) + GC^* C(x(t) - \hat{x}(t)) \\ \hat{y}(t) = C\hat{x}(t), \quad \hat{x}(0) = \hat{x}_0 \end{cases} \quad (10)$$

where, $x(t) = (x_1(.,t), x_2(.,t))^T$ is the state variable of (5) and $\hat{x}(t) = (\hat{x}_1(.,t), \hat{x}_2(.,t))^T$. The linear operator G is the observer gain, satisfying $G = gI$ with I is the identity operator of the Hilbert H.

The initial state $(x_1(0), x_2(0))^T$ of (5) is unknown while the initial state $(\hat{x}_1(0), \hat{x}_2(0))^T$ of the observer can be assigned arbitrarily. Thus, the estimation error is still an unknown quantity even if we know $(\hat{x}_1(0), \hat{x}_2(0))^T$.

2.2. Full-order observer

In this section a full-order observer, when both the reactant concentration and the product concentration are available for measurements at the reactor output, is provided as an asymptotic state estimator with exponentially decay error.

Proposition 2.1: Given the isothermal axial-dispersion reactor basic dynamical model (2)-(4). Suppose that there exists a bounded linear operator $G = gI$, where G is a positif number, such that $g < \frac{\upsilon^2}{8D_a \omega}$, the dynamic system (7)-(9) is an exponential observer for the system (2)-(4).

Proof 2.1 Let consider the linear operator $G = gI$, where g is a positive number. The operator $GC^* C$ is a bounded linear operator on H, such that $\|GC^* C\| \le g\omega$.

On the other hand, the C_0-semigroup $(T_A(t))_{t\ge 0}$ on H, is exponentially stable, such that

$$\|T_A(t)\| \le M \exp(-\frac{\upsilon^2}{4D_a} t), \quad \forall t \ge 0$$

Thus,

$$\frac{\log\|T_A(t)\|}{t} \le \frac{\log M}{t} - \frac{\upsilon^2}{4D_a}, \quad \forall t \ge 0$$

There exists a time t_M such that, $\frac{\log M}{t} \leq \frac{\upsilon^2}{4D_a}$, for all $t \geq t_M$ (since $\frac{\log M}{t}$ converges to zero).

It follows,

$$\|T_A(t)\| \leq \exp(-\frac{\upsilon^2}{8D_a}), \qquad \forall t \geq t_M$$

Now, by the Theorem 2.1, the linear operator $A - GC^*C$ is the infinitesimal generator of a C_0-semigroup $(T_{A-GC^*C}(t))_{t\geq 0}$ satisfying, for all $t \geq t_M$:

$$\begin{aligned} \|T_{A-GC^*C}(t)\| &\leq \exp((-\frac{\upsilon^2}{8D_a} + \|GC^*C\|)t) \\ &\leq \exp((-\frac{\upsilon^2}{8D_a} + g\omega)t) \end{aligned}$$

Let consider the dynamics (5) and (10), the evolution of the estimation error $e(t) = \hat{x}(t) - x(t)$, given by

$$\begin{cases} \dot{e}(t) = (A - GC^*C)e(t) \\ e(0) = \hat{x}_0 - x_0 \end{cases}$$

admits a unique mild solution on the interval $[0,+\infty[$ given by: $e(t) = T_{A-GC^*C}(t)e(0)$, for all $e(0) \in H$ and $t \geq 0$ (see [10]).

Hence,

$$\|e(t)\| \leq \|T_{A-GC^*C}(t)\| \|e(0)\|, \quad \forall t \geq 0$$

It follows, if $g \leq \frac{\upsilon^2}{8D_a\omega}$, the estimation error converges exponentially to zero.

That means that the dynamic system (7)-(9) is an exponential observer for the system (2)-(4). More precisely the reconstruction error $\hat{x}(t) - x(t)$ satisfies, for all $t \geq t_M$

$$\|\hat{x}(t) - x(t)\| \leq \|\hat{x}(0) - x(0)\| \exp((-\frac{\upsilon^2}{8D_a} + g\omega)t)$$

The above proposition presents a "full-order" observer when both reactant concentration and product concentration are measured at the reactor output. In most cases it is not possible to have access to measure the reactant concentration, in such a case the states can be estimated using a "reduced-order" observer based on measurements at the reactor output of the product concentration only.

2.3. Reduced-order observer

In this section, we will present an observer in the case where only the product concentration is available for measurements. Let consider the dynamic

$$\begin{aligned} \frac{\partial \hat{x}_1}{\partial t} &= D_a \frac{\partial^2 \hat{x}_1}{\partial z^2} - \upsilon \frac{\partial \hat{x}_1}{\partial z} - k_0 \hat{x}_1 \\ &\quad + \upsilon \delta x_{in}(t), \\ \frac{\partial \hat{x}_2}{\partial t} &= D_a \frac{\partial^2 \hat{x}_2}{\partial z^2} - \upsilon \frac{\partial \hat{x}_2}{\partial z} + bk_0 \hat{x}_1 \\ &\quad + gC_2^*(C_2 x_2 - C_2 \hat{x}_2) \end{aligned} \tag{11}$$

with the boundary and initial conditions (8)-(9).

Proposition 2.2 Given the isothermal axial-dispersion reactor basic dynamical model (2)-(4). Suppose that there exists a bounded linear operator $G = gI$ with g is a positif number, such that $g \leq \frac{\upsilon^2}{8D_a\omega}$, then the dynamic system (11) and (8)-(9) is an exponential observer for the system (2)-(4).

Proof 2.2 It is proved in the previous section that there exists a time t_M such that the C_0-semigroup $(T_A(t))_{t\geq 0}$ satisfies for all $t \geq t_M$,

$$\|T_A(t)\| \leq M \exp(-\frac{\upsilon^2}{8D_a}t).$$

Thus, for all $t \geq t_M$

$$\begin{aligned} \|T_{A_1}(t)\| &\leq esp(-\frac{\upsilon^2}{8D_a}t) \\ \|T_{A_2}(t)\| &\leq \exp(-\frac{\upsilon^2}{8D_a}t), \end{aligned}$$

where $(T_{A_1}(t))_{t\geq 0}$ and $(T_{A_2}(t))_{t\geq 0}$ are the C_0-semigroup generated respectively by A_1 and A_2.

Let consider the linear operator

$$G := \begin{pmatrix} G_1 & 0 \\ 0 & G_2 \end{pmatrix} = gI,$$

where g is a positive number, and $C = \begin{pmatrix} 0 & C_2 \end{pmatrix}^T$.

The operator GC^*C is a bounded linear operator on H, such that

$$\|G_2 C_2^* C_2\| \leq g\omega.$$

By the Theorem 2.1, the linear operator $A_2 - G_2 C_2^* C_2$ is the infinitesimal generator of a C_0-semigroup $(T_{A_2 - G_2 C_2^* C_2}(t))_{t\geq 0}$

satisfying, for all $t \geq t_M$

$$\left\| T_{A_2 - G_2 C_2^* C_2}(t) \right\| \leq \exp((-\frac{\upsilon^2}{8D_a} + g\omega)t)$$

Let now consider the dynamics (5) and (10), the evolution of the estimation error $e(t) = \hat{x}(t) - x(t)$, given by

$$\begin{cases} \dot{e}_1(t) = A_1 e_1(t), & e_1(0) = \hat{x}_1(0) - \hat{x}_1(0) \\ \dot{e}_2(t) = (A_2 - gC_2^* C_2) e_2(t), & e_2(0) = \hat{x}_2(0) - x_2(0) \end{cases}$$

Admits a unique mild solution on the interval $[0, +\infty[$ given for all $(e_1(0), e_2(0))^T \in H$ by: $(e_1(t), e_2(t))^T = (T_A(t) e_1(0), T_{A-GCC}(t) e_2(0))^T$, For all $t \geq 0$. That implies,

$$\begin{aligned} \|e_1(t)\| &\leq \|T_A(t)\| \|e_1(0)\| \\ \|e_2(t)\| &\leq \left\| T_{A_2 - G_2 C_2^* C_2}(t) \right\| \|e_2(0)\| \end{aligned}$$

Hence, for all $t \geq t_M$

$$\begin{aligned} \|\hat{x}_1(t) - x_1(t)\| &\leq \|\hat{x}_1(0) - x_1(0)\| \exp(-\frac{\upsilon^2}{4D_a} t) \\ \|\hat{x}_2(t) - x_2(t)\| &\leq \|\hat{x}_2(0) - x(0)\| \exp((-\frac{\upsilon^2}{8D_a} + g\omega)t) \end{aligned}$$

It follows that, if $g \leq \frac{\upsilon^2}{8D_a \omega}$, the estimation errors converge exponentially to zero, and that mains that the dynamic system (11) and (8)-(9) is an exponential observer for the system (2)-(4).

Commentaire 2.1 In this section, we have described two different exponential observers for the isothermal Axial-Dispersion reactor basic dynamical model. The first one (eq. (7)-(9)) improves the convergence rate of the concentration error by reintroducing a measurement of both the reactant and product concentrations. The second one (eq. (11) and (8)-(9)) shows that an exponential observer can be constructed even if the reactant concentration is not measured. The Proposition 2.2 provides a simple conception of observer but less effective than that given by Proposition 2.1, since the dynamic of the state error on the reactant concentration remains dependent on the system's dynamic.

2.4. Simulation result

In order to test the performance of the proposed observers, numerical simulations will be given with the following set of parameter values (see [7,6]): $D_a = 0.167\, m^2/s$, $\upsilon = 0.025\, m/s$, $L = 1m$, $k_0 = 10^6 s^{-1}$, $x_{in} = 0.02$, $b = 2\, mol/l$.

The measurements are taken on the length interval $[3*L/4, L]$ i.e., $\omega = 3*L/4$, and the process model has been arbitrary initialized with the constant profiles $x_1(0,z) = 1, x_2(0,z) = 0, \hat{x}_1(0,z) = 0$, and $\hat{x}_2(0,z) = 1$. In order to response to the assumptions of the Propositions 2.1 and 2.2, we set $g = \frac{\upsilon^2}{16D_a \omega}$ for the observer design parameter.

Figure 1. shows the time evolution of the estimation error $e = (e_1, e_2)^T$ related to the exponential observer (7)-(9).

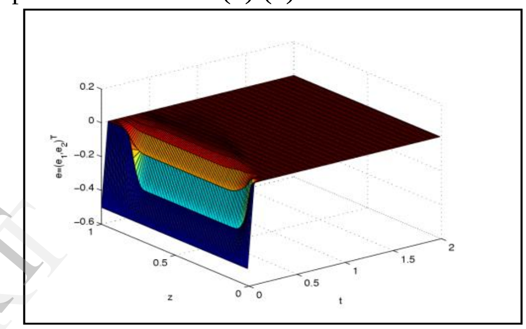
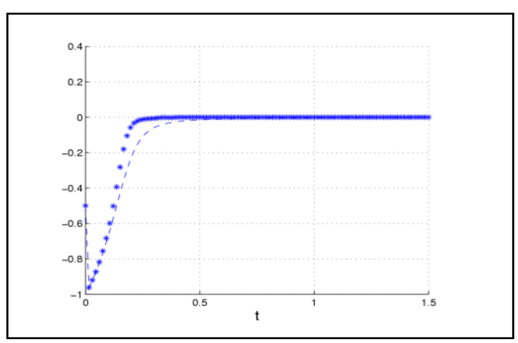
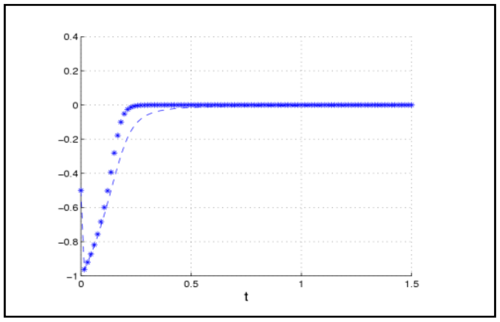


Figure1: Evolution in time and space of the estimation error $e = (e_1, e_2)^T$.

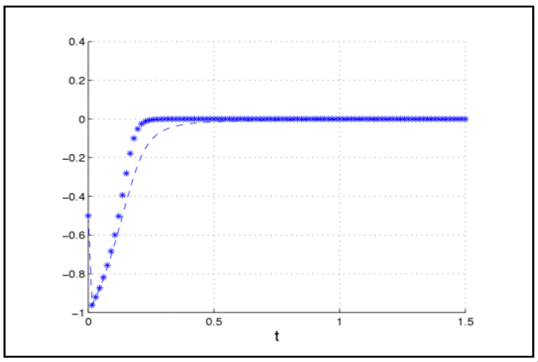
Figures (a), (b) and (c) show respectively the time evolution of the estimation error at the positions 3*L/4, 2*L/4 and L/4, for the case where only the product concentration is measured (the plot '- -') i.e the exponential observer (11) and (8)-(9), and for the case where both the reactant and the product concentrations are measured with the exponential observer (7)-(9).



(a) Estimation error at z=0.9L



(b) Estimation error at z=0.5L



(c) Estimation error at 0.1L

It is seen as expected that the product concentration error related to the exponential observer (7)-(9) is faster than the one related to the exponential observer (11) and (8)-(9).

3. Conclusions and prospects

In this paper we present two observers to estimate the state variables initially unknown of isothermal tubular reactor models, namely axial dispersion reactors involving sequential reactions for which the kinetics only depends on the reactants concentrations involved in the reaction. The proposed observers are based on measurements available at the reactor output only, and performed by a simulation study in which the parameters can be tuned by the user to satisfy specific needs in terms of convergence rate. It is shown in the theoretical setting and in the simulations that the "Full-order" observer is effective relatively to the convergence time. However, the "Reduced-order" observer is more satisfactory since it answers to difficulties of the reactant concentration measurements for a wide range of (bio)-chemical reactor.

9. Knowlegments

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