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A Robust Extended State Observer for the Estimation of Concentration and Kinetics in a CSTR

Abstract: This paper presents a state estimation structure for a Continuous Stirred Tank Reactor (CSTR), by means of an Asymptotic Observer jointly with a disturbance high order sliding mode-based estimator. The proposed estimation scheme allows the asymptotic reconstruction of the concentration inside the reactor based on the measures of the temperature inside the reactor and the temperature inside the jacket, in presence of changes in the global coefficient of heat transfer UA, the Arrhenius constant k_0 and the activation energy E. Additionally, the structure is able to estimate UA and the kinetics term $k_0 e^{-\frac{E}{RT}}$. The properties of the proposed scheme are proved mathematically and verified through numerical simulations.

Keywords: state estimator, state observer, sliding modes, nonlinear observers

1 Introduction

The continuous stirred-tank reactor (CSTR) is one of the most studied operation units due its wide application in several processes (Bequette 2002). In addition, it is a representative case of the so-called reaction systems. Those systems are a class of nonlinear dynamical systems that is widely used in areas such as chemical engineering and biotechnology. For these chemical processes, it is well known that nonlinear state observers, parameter and unknown inputs estimators have been becoming of great interest due to they allow to reduce the quantity of installed sensors in a plant, since they only require some variables measurements and a dynamic model of the process (Walcott, Corless, and Zak 1987; Bequette 2002). The main uses for those methods are the design of observer-based controllers, monitoring schemes, the synthesis of fault detection and isolation methods, among other applications in a reliable and affordable way (Dochain 2003a).

In a chemical process, there are dynamic changes as a result from the normal operation of the plant, the aging of the materials, the conduct obstruction, the physical changes of the components and the changes on the properties of the reagents entering to the reactor. These changes make some parameters of the process to be modified, particularly those related to the reaction kinetics and the heat transfer. As a result, the process model used by a state observer become outdated. However, most of the observation methods are based on models that assume the parameters to be set to a perfectly known fixed value, while in the real system these parameters are unknown and only approximations can be obtained, moreover some of them are changing permanently. This issue makes the estimated variables to deviate from their actual values leading to undesirable situations as low performance controllers, insufficient quality products and operation regimes with unacceptable safety levels.

Considering the mentioned uncertainties related to the mathematical model and limited availability of online sensors, the proposal of robust observation schemes for this class of systems is of fundamental importance (Bastin and Dochain 1990; Soroush 1998). There are several solutions to the observer design problem for these systems as the exposed in (Bastin and Dochain 1990), including the use of the extended Kalman and Luenberger observers (Dochain and Vanrolleghem 2001), adaptive observers (Bastin and Dochain 1990; Dochain 2003b; Farza et al. 2009), the asymptotic observers which allow the estimation of some variables independently from the knowledge of the reaction kinetics (Bastin and Dochain 1990; Dochain, Perrier, and Ydstie 1992;

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Dochain and Vanrolleghem 2001; Moreno and Dochain 2005), Luenberger-asymptotic observers (Hulhoven, Vande Wouwer, and Bogaerts 2006), interval observers (Gouzé, Rapaport, and Hadj-Sadok 2000), dissipative observers (Moreno 2008) and observer based estimators (OBE) for the case of parameter estimation (Oliveira, Ferreira, and Feyo de Azevedo 2002; Perrier et al. 2000).

On the other hand, an important class of nonlinear observers are the sliding mode observers (SMO) (Utkin 1992; S. V. Drakunov 1992; Boukhobza and Barbot 1998; Barbot, Boukhobza and Djemai 1996; Spurgeon 2008) which have the main features of the sliding mode (SM) algorithms. Those algorithms are proposed with the idea to drive the dynamics of a system to a sliding manifold, that is an integral manifold with finite reaching time (Drakunov and Utkin 1992), exhibiting very interesting features such as work with reduced observation error dynamics, the possibility of obtain a step by step design, robustness and insensitivity under parameter variations and external disturbances, and finite time stability (Utkin 1992; Drakunov and Utkin 1995). In addition, the last feature can be extended to uniform finite-time stability (Cruz-Zavala, Moreno, and Fridman 2010) or fixed-time stability (Polyakov 2012), allowing the controllers and estimators to converge with a settling-time independent to the initial conditions. For a SMO design case, the chattering reduces to a numerical problem (Slotine, Hedrick, and Misawa 1986; Utkin 1992). Hence, some SMO have attractive properties similar to those of the Kalman filter (i.e. noise resilience) but with simpler implementation (Drakunov 1983). For chemical processes the SMO have been applied for several cases, some examples are shown in (Wang, Peng, and Huang Wang, Shiou Peng, and Ping Huang 1997; Drakunov and Law 2007; Martínez-Guerra, Aguilar, and Poznyak 2004; Moreno and Mendoza 2014) including joint schemes for parameter estimation based on the OBE design (Botero and Alvarez 2011; Giraldo, Botero, and Sánchez-Torres 2011; Botero et al. 2014).

As an extension of the mentioned approaches, the aim of this paper is to present a nonlinear estimation structure for a CSTR. In the previous works, asymptotic observers are used to estimate a variable, usually a concentration, by compensating the effect of the uncertainty caused by the kinetics. An estimate of the kinetics can be helpful to know the process traceability; however, in some cases this effect of the kinetics is only eliminated but the kinetics itself is not estimated. In addition, the initial formulation of the asymptotic observer does not take into account the parametric change in the global coefficient of heat transfer, which can cause variations in the routine operation of the process. On the other hand, adaptive or SM observers are used to estimate the kinetics under the assumption of the concentration or the global coefficient of heat transfer availability. Consequently, a state estimation structure for a CSTR is proposed here, by means of an asymptotic observer jointly with a second order sliding mode-based estimator. By noting that the asymptotic observers use a state transformation in order to avoid using the kinetic model and this transformation results to be the regular form (Luk'yanov and Utkin 1981) it is presented a novel asymptotic observer that allows to obtain an estimate of the concentration compensating the effect of two uncertainty sources, namely the kinetics and the global coefficient of heat transfer. This structure is obtained by taking advantage of the regular form nesting properties. In addition, based on the observer presented in (Davila, Fridman, and Levant 2005), the kinetics and the global coefficient of heat transfer are estimated with a second order SMO based on the generalized super twisting algorithm (GSTA) (Cruz-Zavala, Moreno, and Fridman 2010), a fixed-time stable extension of the well known super twisting algorithm (Levant 1993). The whole estimation scheme allows the exact and exponentially fast reconstruction of the concentration, the reaction kinetics term and the global coefficient of heat transfer.

In the following, the Section 2 presents the mathematical model of the CSTR. The estimation structure is presented in Section 3. The Section 4 presents results of numerical simulation. Finally, the conclusions of this paper are presented in the Section 5.

2 Mathematical model for the CSTR

This work uses a CSTR model, which is widespread in the process industry and its complexity has been evidenced (Bequette 2002). In this case, it is assumed that the model has three state variables, which are: concentration C_A, temperature inside the reactor T and temperature inside the jacket T_j. It is also assumed that the tank level is perfectly controlled. With these assumptions, the model is still valid for lots of common situations in chemical processes and bioprocesses (Bequette 2002; Dochain 2003a). Inside the reactor, there is produced an exothermic reaction of the form $A \rightarrow B$. The model equations, which are obtained from mass and energy balances at the reactive mass and at the flow inside the jacket, are:

$$\dot{C}_A = \frac{F}{V}\left(C_{in} - C_A\right) - \kappa C_A$$

$$\dot{T} = \frac{F}{V}\left(T_{in} - T\right) - \frac{\Delta H}{\rho C_p}\kappa C_A + \frac{\Lambda}{\rho C_p V}\left(T_j - T\right) \qquad (1)$$

$$\dot{T}_j = \frac{F_{jf}}{V_j}\left(T_{jf} - T_j\right) - \frac{\Lambda}{\rho_j C_{pj} V_j}\left(T_j - T\right).$$

Here, C_A is the concentration of reactive inside the reactor, T is the temperature inside the reactor, T_j is the temperature inside the jacket, F is the flow into the reactor, which is always positive and usually constant due to the continuous operation of the reactor, V is the volume of the reaction mass, C_{in} is the reactive input concentration, T_{in} is the inlet temperature of the reactant, ΔH is the heat of reaction, ρ is the density of the mixture in the reactor, C_p is the heat capacity of food, F_{jf} is the feeding flow, V_j is the jacket volume, T_{jf} is the inlet temperature to the jacket, ρ_j is the density of jacket flow and, C_{pj} is the heat capacity of the jacket flow. The term $\kappa = k_0 e^{-\frac{E}{RT}}$ represents the kinetics, where k_0 is the Arrhenius kinetic constant, E is the activation energy and R is the universal gas constant. Finally, the parameter $\Lambda = UA$ is the global coefficient of heat transfer, where U is the overall coefficient of heat transfer and A is the heat transfer area (Bequette 2002).

It is assumed that the temperatures T and T_j are available for continuous measurement. The problem consists in the estimation of the concentration C_A, the reaction kinetics κ and the global coefficient of heat transfer Λ.

3 Observation scheme

In this section, with the continuous measurements of the temperatures T and T_j, an observer for the variables C_A, κ and Λ is designed.

3.1 CSTR extended model

Taking into account that in (1) the concentration C_A is the unmeasured state variable, κ is an unknown function and, Λ is an unknown, possibly, time-varying parameter, the plant model (1) is extended to the following system:

$$\dot{C}_A = \frac{F}{V}\left(C_{in} - C_A\right) - \kappa C_A$$

$$\dot{T} = \frac{F}{V}\left(T_{in} - T\right) - \frac{\Delta H}{\rho C_p}\kappa C_A + \frac{\Lambda}{\rho C_p V}\left(T_j - T\right)$$

$$\dot{T}_j = \frac{F_{jf}}{V_j}\left(T_{jf} - T_j\right) - \frac{\Lambda}{\rho_j C_{pj} V_j}\left(T_j - T\right) \qquad (2)$$

$$\dot{\kappa} = f_\kappa$$

$$\dot{\Lambda} = f_\Lambda,$$

where f_κ and f_Λ are unknown but bounded functions with $|f_\kappa| \le \delta_\kappa$ and $|f_\Lambda| \le \delta_\Lambda$, and $\delta_\kappa, \delta_\Lambda > 0$ are known constants.

3.2 On the regular form and asymptotic observers

Consider the following system:

$$\dot{x}_1 = a_{11}x_1 + a_{12}x_2 + b_1 f(t)$$

$$\dot{x}_2 = a_{21}x_1 + a_{22}x_2 + b_2 f(t) \qquad (3)$$

$$y = x_2,$$

where $x_1, x_2 \in \mathbb{R}$ are state variables, y is the measured output, $f(t) \in \mathbb{R}$ is an unknown input depending on the time $t \in \mathbb{R}_+$ and $a_{11}, a_{12}, a_{21}, a_{22}, b_1, b_2 \in \mathbb{R}$ are the system parameters.

Here, the main objective is to find a state transformation such that the input $f(t)$ does not appear in the first equation of (3). The transformed system, if existing, is called the regular form of (3) with respect to $f(t)$ (Luk'yanov and Utkin 1981). With this aim, define $z_1 = x_1 - \frac{b_1}{b_2}x_2$ and $z_2 = x_2$; with this transformation the system (3) reduces to:

$$\dot{z}_1 = \bar{a}_{11}z_1 + \bar{a}_{12}z_2$$

$$\dot{z}_2 = \bar{a}_{21}z_1 + \bar{a}_{22}z_2 + b_2 f(t), \qquad (4)$$

with $\quad \bar{a}_{11} = a_{11} - \frac{a_{21}b_1}{b_2}, \quad \bar{a}_{12} = -a_{21}\left(\frac{b_1}{b_2}\right)^2 + (a_{11} - a_{22})\frac{b_1}{b_2} + a_{12},$ $\bar{a}_{21} = a_{21}$ and $\bar{a}_{22} = a_{22} + \frac{b_1}{b_2}a_{21}$.

The expression (4), in addition to be a suitable representation of the system (3) for control design as shown in (Luk'yanov and Utkin 1981), is also very useful for observer design. To illustrate the observer design case, consider the system (3). Here, the main objective is to design an state observer to estimate the unmeasured variable x_1 considering x_2 to be available for continuous measurements and $f(t)$ as an unknown input. Transforming the system (3) to the regular form with respect to the unknown input $f(t)$ (4), the following observer is presented:

$$\dot{\hat{z}}_1 = \bar{a}_{11}\hat{z}_1 + \bar{a}_{12}z_2$$

$$\hat{x}_1 = \hat{z}_1 + \frac{b_1}{b_2}x_2. \qquad (5)$$

The observer (5) is commonly known as the asymptotic observer (Bastin and Dochain 1990; Dochain, Perrier, and Ydstie 1992) and its main characteristic is its independence and therefore its robustness against the unknown input $f(t)$.

Defining the error variable $\tilde{z}_1 = z_1 - \hat{z}_1$, it follows

$$\dot{\tilde{z}}_1 = \bar{a}_{11}\tilde{z}_1,$$

where it is noted that the convergence of the observer depends on the parameter $\bar{a}_{11}$ which is not tunable.

This procedure can be extended to the following third order system:

$$\dot{x}_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + b_{11}f_1(t)$$

$$\dot{x}_2 = a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + b_{21}f_1(t) + b_{22}f_2(t)$$

$$\dot{x}_3 = a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + b_{32}f_2(t) \tag{6}$$

$$y_1 = x_2$$

$$y_2 = x_3,$$

where $x_1, x_2, x_3 \in \mathbb{R}$ are state variables, y_1 and y_2 are the measured outputs, $f_1(t), f_2(t) \in \mathbb{R}$ are unknown inputs depending on the time $t \in \mathbb{R}_+$ and $a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{23}, a_{31}, a_{32}, a_{33}, b_{11}, b_{21}, b_{22}, b_{32} \in \mathbb{R}$ are the system parameters.

To obtain the regular form with respect to the inputs $f_1(t)$ and $f_2(t)$, define the new nested variables $z_1 = x_1 - \frac{b_{11}}{b_{21}}x_2 + \frac{b_{11}b_{22}}{b_{21}b_{32}}x_3$, $z_2 = x_2$ and $z_3 = x_3$. Using this transformation the system (6) becomes:

$$\dot{z}_1 = \bar{a}_{11}z_1 + \bar{a}_{12}z_2 + \bar{a}_{13}z_3$$

$$\dot{z}_2 = \bar{a}_{21}z_1 + \bar{a}_{22}z_2 + \bar{a}_{23}z_3 + b_{21}f_1(t) + b_{22}f_2(t) \tag{7}$$

$$\dot{z}_3 = \bar{a}_{31}z_1 + \bar{a}_{32}z_2 + \bar{a}_{33}z_3 + b_{32}f_2(t),$$

where $\bar{a}_{11} = a_{11} - \frac{b_{11}}{b_{21}}a_{21} + \frac{b_{11}b_{22}}{b_{21}b_{32}}a_{31}$, $\bar{a}_{12} = \frac{b_{11}}{b_{21}}\left(a_{11} - \frac{b_{11}}{b_{21}}a_{21} + \frac{b_{11}b_{22}}{b_{21}b_{32}}a_{31}\right) + a_{12} - \frac{b_{11}}{b_{21}}a_{22} + \frac{b_{11}b_{22}}{b_{21}b_{32}}a_{32}$, $\bar{a}_{13} = a_{13} - \frac{b_{11}}{b_{21}}a_{23} + \frac{b_{11}b_{22}}{b_{21}b_{32}}a_{33} - \frac{b_{11}b_{22}}{b_{21}b_{32}}(a_{11} - \frac{b_{11}}{b_{21}}a_{21} + \frac{b_{11}b_{22}}{b_{21}b_{32}}a_{31})$, $\bar{a}_{21} = a_{21}$, $\bar{a}_{22} = a_{22} + \frac{b_{11}}{b_{21}}a_{21}$, $\bar{a}_{23} = a_{23} - \frac{b_{11}b_{22}}{b_{21}b_{32}}a_{21}$, $\bar{a}_{31} = a_{31}$, $\bar{a}_{32} = a_{32} + \frac{b_{11}}{b_{21}}a_{31}$, $\bar{a}_{33} = a_{33} - \frac{b_{11}b_{22}}{b_{21}b_{32}}a_{31}$.

Using the transformed system (7), an observer for the system (6) to estimate the unmeasured variable x_1, can be designed similarly to the observer (5), in the following form:

$$\dot{\hat{z}}_1 = \bar{a}_{11}\hat{z}_1 + \bar{a}_{12}z_2 + \bar{a}_{13}z_3$$

$$\hat{x}_1 = \hat{z}_1 + \frac{b_{11}}{b_{21}}x_2 - \frac{b_{11}b_{22}}{b_{21}b_{32}}x_3. \tag{8}$$

The proposed observer (8) can be considered as an extension of the observer (5). Its main characteristic is its invariance with respect to the unknown inputs inputs $f_1(t)$ and $f_2(t)$.

3.3 A regular form for the CSTR

In this subsection the main objective is to design an observer that does not depend on the kinetics κ and global coefficient of heat transfer Λ. Taking advantage that for system (1) κ appears in the first and second equations, as $f_1(t)$ in (6), and Λ appears in the second

and third equations, as $f_2(t)$ in (6), the procedure exposed in (6)-(8) is applied. The variable z is defined as

$$z = C_A - \frac{\rho C_p}{\Delta H}\left(T + \frac{\rho_j C_{pj} V_j}{\rho C_p V}T_j\right), \tag{9}$$

it can be considered as a transformation of the concentration C_A.

The dynamics of (9) is given by

$$\dot{z} = \frac{F}{V}\left(C_{in} - z - \frac{\rho C_p}{\Delta H}\left(T + \frac{\rho_j C_{pj} V_j}{\rho C_p V}T_j\right)\right) - \frac{\rho C_p F}{V \Delta H}(T_{in} - T)$$
$$- \frac{\rho_j C_{pj} F_{jf}}{V \Delta H}(T_{jf} - T_j), \tag{10}$$

where is observed the independence with respect to the unknown variables κ and Λ, as exposed in (8), while the others variables remain untransformed. Thus, the system (1) is yields to regular form with respect to the unknown variables κ and Λ.

3.4 Observer structure

Using (2), (9) and (10), the following observer is proposed:

$$\hat{C}_A = \hat{z} + \frac{\rho C_p}{\Delta H}\left(\hat{T} + \frac{\rho_j C_{pj} V_j}{\rho C_p V}\hat{T}_j\right)$$

$$\dot{\hat{z}} = \frac{F}{V}\left(C_{in} - \hat{C}_A\right) - \frac{\rho C_p F}{V \Delta H}\left(T_{in} - \hat{T}\right) - \frac{\rho_j C_{pj} F_{jf}}{V \Delta H}\left(T_{jf} - \hat{T}_j\right)$$

$$\dot{\hat{T}} = \frac{F}{V}\left(T_{in} - \hat{T}\right) - \frac{\Delta H}{\rho C_p}\hat{\kappa}\hat{C}_A + \frac{\hat{\Lambda}}{\rho C_p V}\left(\hat{T}_j - \hat{T}\right) + k_{11}\phi_1(\tilde{T})$$

$$\dot{\hat{T}}_j = \frac{F_{jf}}{V_j}\left(T_{jf} - \hat{T}_j\right) - \frac{\hat{\Lambda}}{\rho_j C_{pj} V_j}\left(\hat{T}_j - \hat{T}\right) + k_{12}\phi_1(\tilde{T}_j)$$

$$\dot{\hat{\kappa}} = -k_{21}\frac{\rho C_p}{\Delta H \delta_1}\phi_2(\tilde{T})$$

$$\dot{\hat{\Lambda}} = k_{22}\frac{\rho_j C_{pj} V_j}{\delta_2}\phi_2(\tilde{T}_j)$$

$$\dot{\hat{\kappa}}_f = \frac{1}{\tau_1}\left(\hat{\kappa} - \hat{\kappa}_f\right)$$

$$\dot{\hat{\Lambda}}_f = \frac{1}{\tau_2}\left(\hat{\Lambda} - \hat{\Lambda}_f\right), \tag{11}$$

where $\hat{C}_A$, $\hat{z}$, $\hat{T}$, $\hat{T}_j$, $\hat{\kappa}$ and $\hat{\Lambda}$ are the estimates of C_A, z, T, T_j, κ and Λ, respectively. The observer input injections are given by $\phi_1(\cdot) = \lfloor\cdot\rceil^{\frac{1}{2}} + \mu\lfloor\cdot\rceil^{\frac{3}{2}}$ and $\phi_2(\cdot) = \frac{1}{2}\lfloor\cdot\rceil^0 + 2\mu\cdot + \frac{3}{2}\mu^2\lfloor\cdot\rceil^2$ with the gain $\mu \geq 0$. The function $\lfloor\cdot\rceil^\alpha = |\cdot|^\alpha \text{sign}(\cdot)$ is defined for $\alpha \geq 0$, where $\text{sign}(x) = 1$ for $x > 0$,

$\mathrm{sign}(x) = -1$ for $x < 0$ and $\mathrm{sign}(0) \in [-1, 1]$; $\tilde{T} = T - \hat{T}$ and $\tilde{T}_j = T_j - \hat{T}_j$ are the observation error variables; $\hat{\kappa}_f$ and $\hat{\Lambda}_f$ are the filtered variables of $\hat{\kappa}$ and $\hat{\Lambda}$, respectively; k_{11}, k_{12}, k_{21} and k_{22} are the observer positive gains. The parameters τ_1 and τ_2 are the time constants of the filters. Finally, δ_1 and δ_2 are positive observer parameters which will be chosen thereafter.

The filters for $\hat{\kappa}$ and $\hat{\Lambda}$, are added in order to reduce the noise effect on the variables estimation, taking advantage of the large time constants which are usually present on chemical processes.

3.5 Convergence analysis

Define the observation error variables $\tilde{z} = z - \hat{z}$, variables $\tilde{z} = z - \hat{z}$, $\tilde{C}_A = C_A - \hat{C}_A$, $\tilde{\kappa} = \kappa - \hat{\kappa}$ and $\tilde{\Lambda} = \Lambda - \hat{\Lambda}$. Then, from (2), (9), (10) and (11), it follows

$$\tilde{C}_A = \tilde{z} + \frac{\rho C_p}{\Delta H}\left(\tilde{T} + \frac{\rho_j C_{pj} V_j}{\rho C_p V}\tilde{T}_j\right)$$

$$\dot{\tilde{z}} = -\frac{F}{V}\tilde{z} + \left(\frac{\rho C_{pj} F_{jf}}{V\Delta H} - \frac{F\rho_j C_{pj} V_j}{V^2 \Delta H}\right)\tilde{T}_j$$

$$\dot{\tilde{T}} = -\frac{F}{V}\tilde{T} - \frac{\Delta H}{\rho C_p}\hat{C}_A\tilde{\kappa} - \frac{\Delta H}{\rho C_p}\tilde{C}_A\kappa + \frac{\Lambda}{\rho C_p V}\left(T_j - T\right)$$

$$\quad - \frac{\hat{\Lambda}}{\rho C_p V}\left(\hat{T}_j - \hat{T}\right) - k_{11}\phi_1(\tilde{T})$$

$$\dot{\tilde{T}}_j = -\frac{F_{jf}}{V_j}\tilde{T}_j - \frac{\tilde{\Lambda}}{\rho_j C_{pj} V_j}\left(\hat{T}_j - \hat{T}\right) - \frac{\Lambda}{\rho_j C_{pj} V_j}\left(\tilde{T}_j - \tilde{T}\right) - k_{12}\phi_1(\tilde{T}_j)$$

$$\dot{\hat{\kappa}} = f_\kappa + k_{21}\frac{\rho C_p}{\Delta H \delta_1}\phi_2(\tilde{T})$$

$$\dot{\hat{\Lambda}} = f_\Lambda - k_{22}\frac{\rho_j C_{pj} V_j}{\delta_2}\phi_2(\tilde{T}_j)$$

$$\tag{12}$$

Define now the new variables q_1 and q_2 as

$$q_1 = -\frac{\Delta H}{\rho C_p}\hat{C}_A\tilde{\kappa} - \frac{\Delta H}{\rho C_p}\tilde{C}_A\kappa + \frac{\Lambda}{\rho C_p V}\left(T_j - T\right) - \frac{\hat{\Lambda}}{\rho C_p V}\left(\hat{T}_j - \hat{T}\right)$$

$$\tag{13}$$

$$q_2 = -\frac{\tilde{\Lambda}}{\rho_j C_{pj} V_j}\left(\hat{T}_j - \hat{T}\right) - \frac{\Lambda}{\rho_j C_{pj} V_j}\left(\tilde{T}_j - \tilde{T}\right).$$

$$\tag{14}$$

Then, the system (12) yields

$$\tilde{C}_A = \tilde{z} + \frac{\rho C_p}{\Delta H}\left(\tilde{T} + \frac{\rho_j C_{pj} V_j}{\rho C_p V}\tilde{T}_j\right)$$

$$\dot{\tilde{z}} = -\frac{F}{V}\tilde{z} + \left(\frac{\rho C_{pj} F_{jf}}{V\Delta H} - \frac{F\rho_j C_{pj} V_j}{V^2 \Delta H}\right)\tilde{T}_j$$

$$\dot{\tilde{T}} = -\frac{F}{V}\tilde{T} + q_1 - k_{11}\phi_1(\tilde{T})$$

$$\tag{15}$$

$$\dot{\tilde{T}}_j = -\frac{F_{jf}}{V_j}\tilde{T}_j + q_2 - k_{12}\phi_1(\tilde{T}_j)$$

$$\dot{q}_1 = -k_{21}\theta_1\phi_2(\tilde{T}) + \Delta_{q_1}$$

$$\dot{q}_2 = -k_{22}\theta_2\phi_2(\tilde{T}_j) + \Delta_{q_2},$$

where $\theta_1 = \frac{\hat{T} - \hat{T}_j}{\delta_1}$ and $\theta_2 = \frac{\hat{C}_A}{\delta_2}$. The terms

$$\Delta_{q_1} = -\frac{\Delta H}{\rho C_p}\hat{C}_A f_\kappa - \frac{\Delta H}{\rho C_p}\dot{\hat{C}}_A\tilde{\kappa}$$

$$\quad + \frac{d}{dt}\left[-\frac{\Delta H}{\rho C_p}\tilde{C}_A\kappa + \frac{\Lambda}{\rho C_p V}\left(T_j - T\right) - \frac{\hat{\Lambda}}{\rho C_p V}\left(\hat{T}_j - \hat{T}\right)\right] \text{ and}$$

$$\Delta_{q_2} = -\frac{f_\Lambda}{\rho_j C_{pj} V_j}\left(\hat{T}_j - \hat{T}\right) - \frac{\tilde{\Lambda}}{\rho_j C_{pj} V_j}\left(\dot{\hat{T}}_j - \dot{\hat{T}}\right)$$

$$\quad - \frac{d}{dt}\left[\frac{\Lambda}{\rho_j C_{pj} V_j}\left(\tilde{T}_j - \tilde{T}\right)\right],$$

are considered in (15) as unknown but bounded disturbances with $|\Delta_{q_1}| \le \delta_{q_1}$ and $\Delta_{q_2} \le \delta_{q_2}$, and $\delta_{q_1}, \delta_{q_2} > 0$ are known positive constants.

If the observer gains k_{11}, k_{12}, k_{21} and k_{22} are chosen as

$$\mathcal{K} = \left\{(k_{11}, k_{12}, k_{21}, k_{22}) \in \mathbb{R}^4 \,|\, < 0 \; k_{11} \le 2\sqrt{\delta_{q_1}}, \; 0 \right.$$

$$< k_{12} \le 2\sqrt{\delta_{q_2}}, k_{21} > \frac{k_{11}^2}{4} + \frac{4\delta_{q_1}^2}{k_{11}^2}, k_{22} > \frac{k_{12}^2}{4} + \frac{4\delta_{q_2}^2}{k_{12}^2}\right\}$$

$$\cup \left\{(k_{11}, k_{12}, k_{21}, k_{22}) \in \mathbb{R}^4 \,|\, k_{11} > 2\sqrt{\delta_{q_1}}, \; k_{12}\right.$$

$$\left. > 2\sqrt{\delta_{q_2}}, k_{21} > 2\delta_{q_1}, k_{22} > 2\delta_{q_1}\right\},$$

and the parameters δ_1 and δ_2 are selected such that $\theta_1 = \frac{\hat{T} - \hat{T}_j}{\delta_1} > 1$ and $\theta_2 = \frac{\hat{C}_A}{\delta_2} > 1$, then a sliding mode appears in the system (15) on the manifold $(\tilde{T}, \tilde{T}_j, q_1, q_2) = (0, 0, 0, 0)$ in a fixed time $t_q > 0$ (Cruz-Zavala, Moreno, and Fridman 2010).

From (14), it follows that $\tilde{\Lambda}(t) = 0$ for $t > t_q$, and from (13) to (15), the motion of the system (12) is constrained to the sliding manifold $(\tilde{T}, \tilde{T}_j, q_1, \tilde{\Lambda}) = (0, 0, 0, 0)$, which means $(\hat{T}, \hat{T}_j, q_1, \hat{\Lambda}) = (T, T_j, 0, \Lambda)$. In this manifold, the dynamics of (12) is described by the reduced order system

$$\dot{\tilde{z}} = -\frac{F}{V}\tilde{z}$$

$$\tilde{C}_A = \tilde{z} \qquad (16)$$

$$\tilde{\kappa} = -\frac{\kappa}{\hat{C}_A}\tilde{z}.$$

Therefore, from the model hypothesis $F > 0$, the observer error pair $\left(\tilde{C}_A, \tilde{\kappa}\right)$ converges exponentially to $(0, 0)$. Finally, taking into account that $\dot{\hat{\kappa}}_f = \frac{1}{\tau_1}\left(\hat{\kappa} - \hat{\kappa}_f\right)$ and $\dot{\hat{\Lambda}}_f = \frac{1}{\tau_2}\left(\hat{\Lambda} - \hat{\Lambda}_f\right)$ are linear first order low-pass filters for the estimates of κ and Λ, respectively, the convergence analysis is completed.

4 Numerical simulation results

In this section, the numerical simulations results of the proposed estimation scheme applied to a CSTR, are presented. All simulations presented here were conducted using the Euler integration method, with a fundamental step size of 2×10^{-3} [min]. The CSTR parameters are shown on Table 1.

It can be noticed that, the proposed observer (11) does not use the information relative to the function κ (i.e. the parameters E, k_0 and R) nor the parameter Λ. To verify the robustness of the proposed observer, plant parameter variations were introduced in the simulation, see Table 2. Under normal operating conditions, this sort of variation is very common, and consequently, the simulation results (see Figures 1–6) show that the observer is able to deal with what happens in reality. Is worth to notice that this variation is unknown for the proposed estimation scheme.
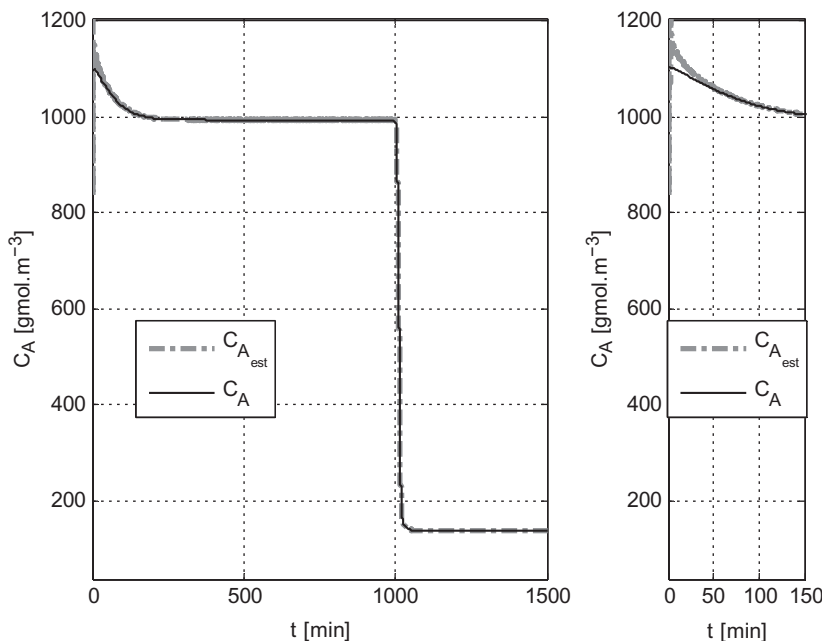
Table 1: Nominal parameters of the CSTR.

Parameter	Values [Unit]	Parameter	Values [Unit]
F	0.1605 [$m^3 min^{-1}$]	C_p	$3,571.3$ [$J \cdot kg^{-1}$]
V	2.4069 [m^3]	U	2.5552×10^4 [$J \cdot (min \cdot m^2 \cdot K)^{-1}$]
C_{in}	$2,114.5$ [$gmol.m^3$]	A	8.1755 [m^2]
k_0	2.8267×10^{11} [min^{-1}]	F_{jf}	0.3376 [$m^3 \cdot min^{-1}$]
E	75361.14 [$J \cdot gmol^{-1}$]	V_j	0.24069 [m^3]
R	8.3174 [$J \cdot gmol^{-1} K^{-1}$]	T_{jf}	279 [K]
T_{in}	295.22 [K°]	ρ_j	1000 [$kg \cdot m^3$]
ΔH	-9.0712×10^4 [$J \cdot g\, mol^{-1}$]	C_{pj}	3728.87 [$J \cdot kg^{-1}$]
ρ	1000 [$kg \cdot m^{-3}$]		

Table 2: CSTR parametric variations.

Parameter	Variation time	Variation magnitude
Λ	1,000 min	90%-negative step

The initial conditions for the CSTR were selected to: $C_A(0) = 1105.2102$ [$gmol \cdot m^{-3}$], $T_j(0) = 283.1049$ [K] and $T(0) = 310.7727$ [K]; and for the observer to: $z(0) = 1.4571 \times 10^4$, $\hat{T}(0) = 300$ [K], $\hat{T}_j(0) = 290$ [K], $\hat{\kappa}(0) = \hat{\kappa}_f(0) = 0$ [min^{-1}] and $\hat{\Lambda}(0) = \hat{\Lambda}_f(0) = 2.2 \times 10^5$ [$J \cdot (min \cdot K)^{-1}$]. Furthermore, the parameter values for the observer were adjusted to: $k_{11} = 1$, $k_{12} = 1 \times 10^1$, $k_{21} = 5$, $k_{22} = 1 \times 10^{-1}$, $\delta_1 = 1 \times 10^2$, $\delta_2 = 1$, $\mu = 1$ and $\tau_1 = \tau_2 = \frac{1}{5}$ [min].

In the following, this section is divided into two parts. In the first part, there is assumed that the temperature measurements are noiseless; and in the second part
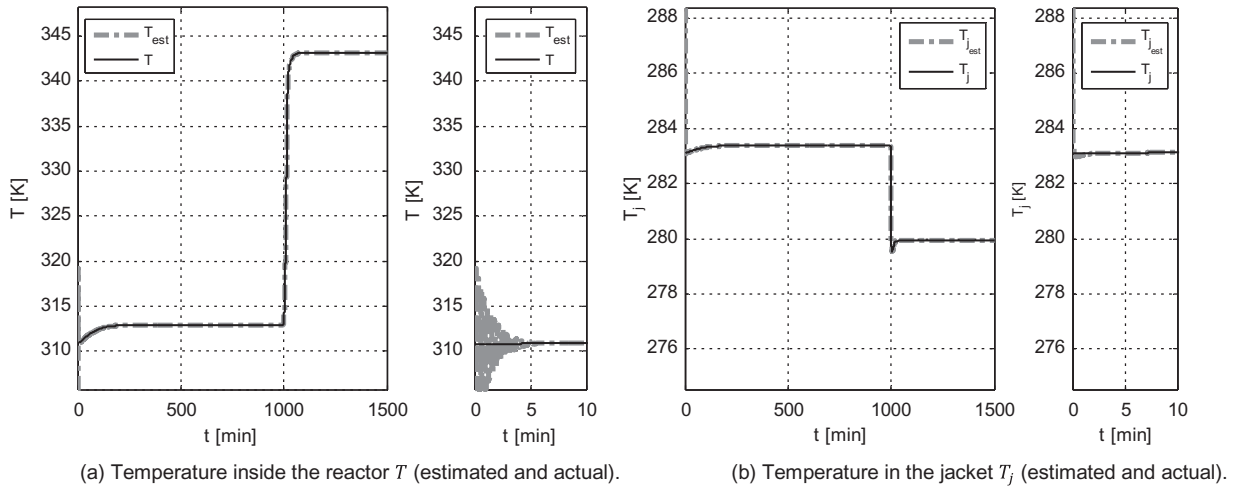

Figure 1: Concentration of the reactive inside the reactor C_A (estimated and actual).

(a) Temperature inside the reactor T (estimated and actual).

(b) Temperature in the jacket T_j (estimated and actual).

Figure 2: Temperature inside the reactor T and temperature in the jacket T_j (estimated and actual).

(a) Reaction kinetics κ (estimated and actual).

(b) Global coefficient of heat transfer Λ (estimated and actual).
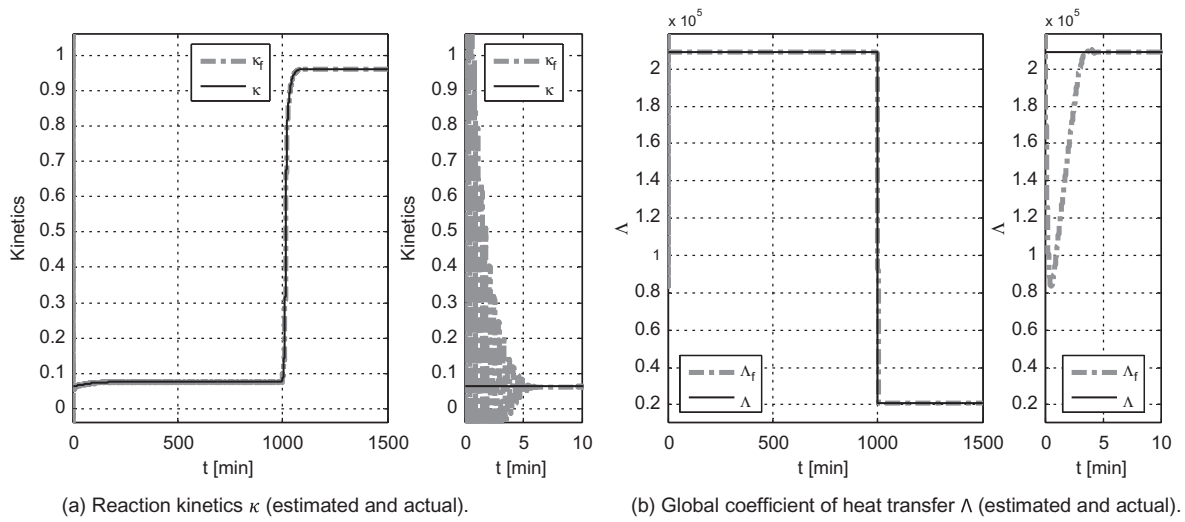
Figure 3: Reaction kinetics kinetics κ and global coefficient of heat transfer Λ (estimated and actual).
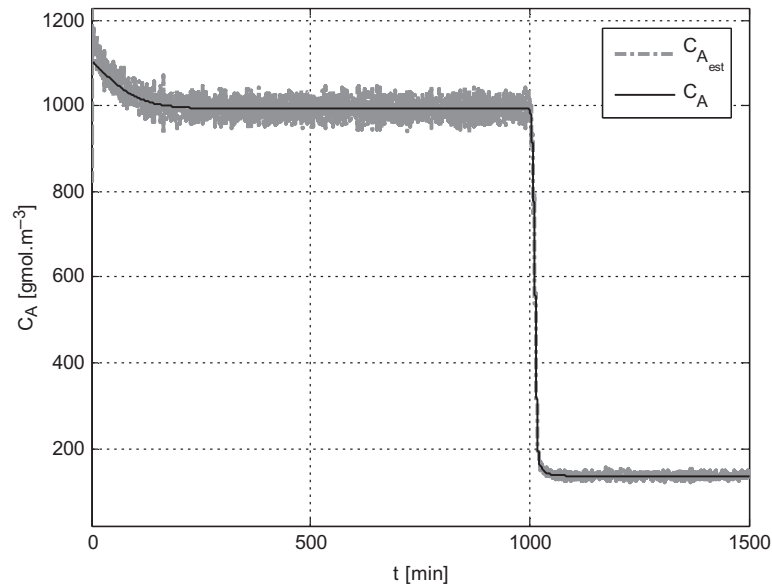

Figure 4: Concentration of the reactive inside the reactor C_A (estimated and actual). Noisy measurements.

(a) Temperature inside the reactor T (measured, estimated and actual). Noisy measurements.

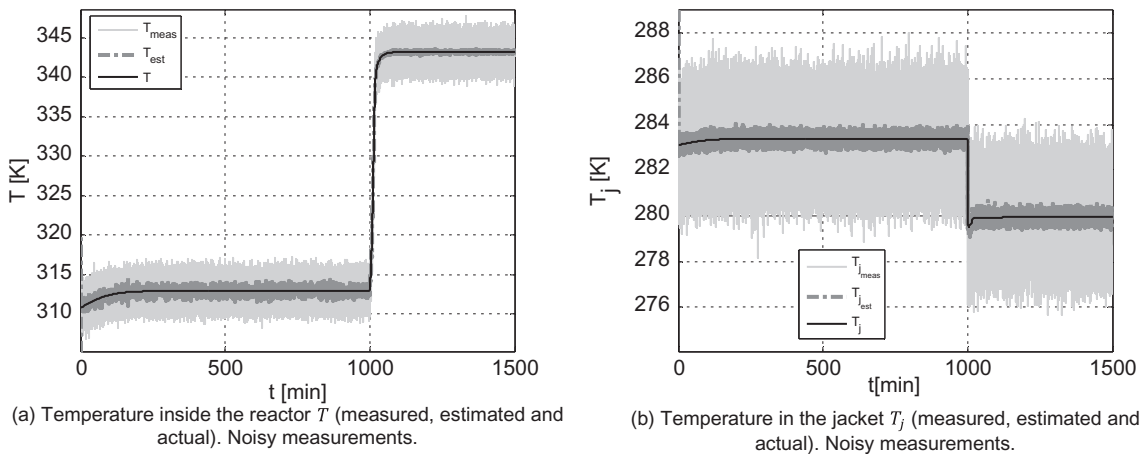(b) Temperature in the jacket T_j (measured, estimated and actual). Noisy measurements.

Figure 5: Temperature inside the reactor T and temperature in the jacket T_j (measured, estimated and actual). Noisy measurements.
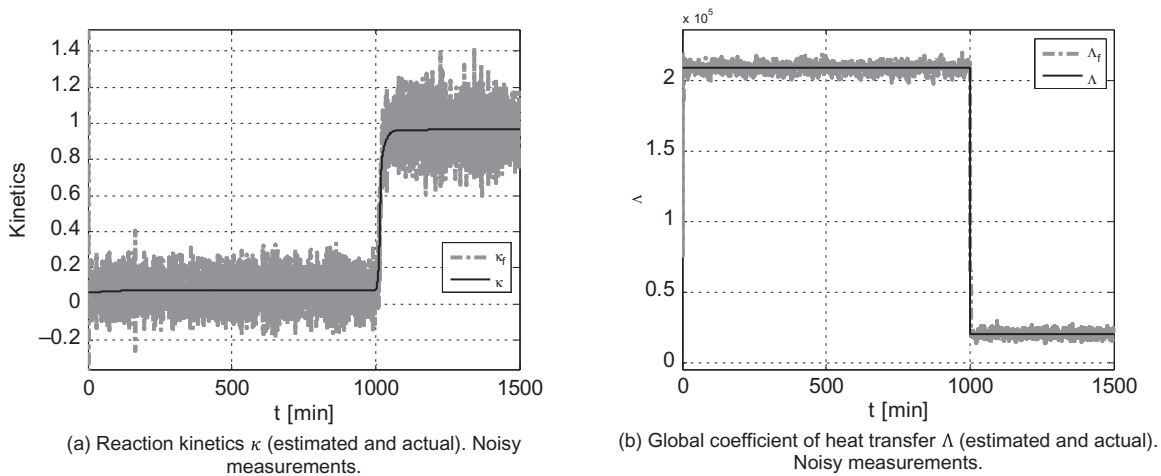

(a) Reaction kinetics κ (estimated and actual). Noisy measurements.

(b) Global coefficient of heat transfer Λ (estimated and actual). Noisy measurements.

Figure 6: Reaction kinetics κ and global coefficient of heat transfer Λ (estimated and actual). Noisy measurements.

instead, there is included a normally distributed random signal as measurement noise in the temperature.

4.1 Noiseless measurements

In this subsection, it is assumed no noise in the measurements. The following results were obtained:

Figures 1–3 show the comparison between the actual and estimated variables corresponding to the concentration of reactive inside the reactor C_A, the temperature inside the reactor T and the temperature inside the jacket T_j, the reaction kinetics κ and the global coefficient of heat transfer Λ, respectively, for noiseless measurements. It is observed the fast convergence of the variables T, T_j and Λ, while the variables C_A and κ converge exponentially with a time constant of $\frac{F}{V}$.

4.2 Noisy measurements

In this subsection, it is assumed that the temperature measurements were corrupted by a normally distributed random signal with zero mean and unitary variance; this assumed variance corresponds to temperature sensors with an accuracy of $\pm 3[K]$. The following results were obtained:

Figures 4–6 show the comparison between the actual and estimated variables corresponding to the concentration of reactive inside the C_A, the temperature inside the reactor T and the temperature inside the jacket T_j, the reaction kinetics κ and the global coefficient of heat transfer Λ, respectively, for noisy measurements.

Based on the presented simulations results, it can be observed a good performance of the proposed observer

scheme, also under noisy measurement conditions. The observer for C_A presents a correct estimation of this variable due to its independence of the unknown terms Λ and κ (Figures 1 and 4). In addition, a correct simultaneous estimation of T, T_j, κ and Λ using the high order sliding mode observer is achieved (Figures 2, 3, 5 and 6), making the proposed system suitable for observer-based control applications. Furthermore, under noisy conditions, the estimated temperatures are much closer to their actual values than their measurements (Figure 5).

5 Conclusions

An estimation scheme based on an asymptotic observer working jointly with a second order sliding mode estimator, was proposed for a CSTR. Measuring the temperature inside the reactor and the temperature inside the jacket, this scheme achieves the asymptotic estimation of the concentration, despite of changes in the global coefficient of heat transfer Λ, the Arrhenius constant k_0 and the activation energy E. Additionally, the proposed scheme allows to estimate the terms Λ and $k_0 e^{-\frac{E}{RT}}$ which are well-known as very difficult to measure, especially for real-time applications. These terms were considered as unknowns but with known bounds of their time derivatives. Hence, this configuration ensures an estimation of the concentration, which is robust with respect to variations of the mentioned above terms. With a suitable selection of the observer gains, the proposed scheme presents a fast observer error convergence with high accuracy.

The performance of the proposed approach was verified via numerical simulations, showing characteristics as good estimation of the state variable and both terms, and robustness with respect to plant parameter variations under noisy measurements.

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