2012-10

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Giraldo, B.; Sánchez-Torres, J.D. and Botero-Castro, H. (2012). State and Parameter Estimation of a CSTR. 15th Latinamerican Control Conference.

State and Parameter Estimation of a CSTR

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Abstract: In the continuation of authors' studies on estimation and control for Continuous Stirred-Tank Reactors (CSTR), a new structure to estimate the concentration of reactive state, the global heat transfer coefficient, and the heat of reaction parameters is proposed here. This scheme consist of an Observer Based Estimator (OBE) connected in cascade with a High Order Sliding Mode Observer (HOSMO). The OBE estimates the global heat transfer coefficient, and the HOSMO estimates the heat of reaction, and the concentration of reactive. Numerical simulations show that the whole structure presents a good performance in presence of parametric variations, which often are presented in chemical processes.

Keywords: Continuous Stirred-Tank Reactor (CSTR), Observer Based Estimator (OBE), High Order Sliding Mode (HOSM) Algorithms, State and Parameter Estimation

1. INTRODUCTION

The aim of this paper is to present a nonlinear estimation structure for a CSTR, it is composed by a linear OBE coupled with a HOSMO. It is well known that nonlinear state observers have becoming of great interest for the design of observer-based controllers, and the synthesis of fault detection and isolation methods (Walcott and Zak, 1987; Drakunov, 1992; Spurgeon, 2008), among other applications. A class of nonlinear observers are the Sliding Mode Observers (SMO) which have features of the sliding mode algorithms.

The Sliding Mode (SM) 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). These algorithms exhibit very interesting features such as to work with reduced observation error dynamics, the possibility of obtaining a step by step design, robustness 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 et al., 2010) and to *Fixed Time Stability* (Polyakov, 2012), allowing the design of controllers and estimators with convergence time independent to the initial conditions.

On the other hand, the sliding mode algorithms present two main disadvantages: (i) they are usually assumed to be more sensitive to noise than the most of smooth controllers and estimators (Boukhobza and Barbot, 1998), and (ii) the so-called *chattering* which is an oscillation due to the high frequency and discontinuity of the functions, as the sign, used to implement the sliding manifolds (Utkin, 1992). However, for the case (i), using the steady state error as performance index, it is shown that, under the bounded disturbance hypothesis, linear and discontinuous algorithms are equally sensitive to noise. Therefore, discontinuous are the optimal selection under both noise and perturbation (Angulo et al., 2012). Besides, for case (ii), several approaches have been proposed to reduce or avoid chattering. A first example is the use of continuous and smooth approximations of the sign function as linear saturation or sigmoid functions (Wang et al., 1997; Barbot et al., 2002); with this solution only a quasi-sliding motion can be forced in a vicinity of the desired manifold, reducing the performance and the robustness of the algorithm (Utkin et al., 2009). A different approach to implement the manifold with chattering reduction is the use of continuous functions with discontinuous derivatives, instead of a discontinuous function; these methods are the so-called HOSM algorithms, which extend the idea of the SM actuating on the time derivatives of the sliding manifold, and preserving the main features of the original SM approach. In addition, for a SMO design case, the chattering reduces to a numerical problem (Slotine et al., 1986). Hence, some SMO have attractive properties similar to those of the Kalman filter but with simpler implementation (Drakunov, 1983).

The idea of applying a HOSMO for state and parameter estimation in a CSTR, assuming the parameter to be estimated as an unknown input, was introduced by Giraldo Osorio et al. (2011). Here, employing measurements of the temperature inside the reactor, the observer estimates the heat of reaction, and the concentration of reactive. In addition, in order to facilitate the estimation procedure, the global heat transfer coefficient was assumed to be a known constant. No dynamics of the temperature inside the jacket was considered in the mentioned approach.

This paper proposes an extension of the last approach, considering the global heat transfer coefficient as an unknown variable, to be estimated. This assumption conduces to a better approximation of the CSTR real operation conditions. As first step, an OBE for the global heat transfer coefficient estimation is used. With this estimation, a HOSMO for state and input estimation (Fridman et al., 2008) is used to estimate the heat of reaction, and the concentration of reactive. The heat of reaction is a parameter which is considered as an unknown input for the observer design. The HOSM is based on real time differentiation (Levant, 1998) with a *Super-Twisting* algorithm (Levant, 1993).

In the following: 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, here the proposed structure is compared with a first order SMO. Finally, the conclusions of this paper are included in Section 5.

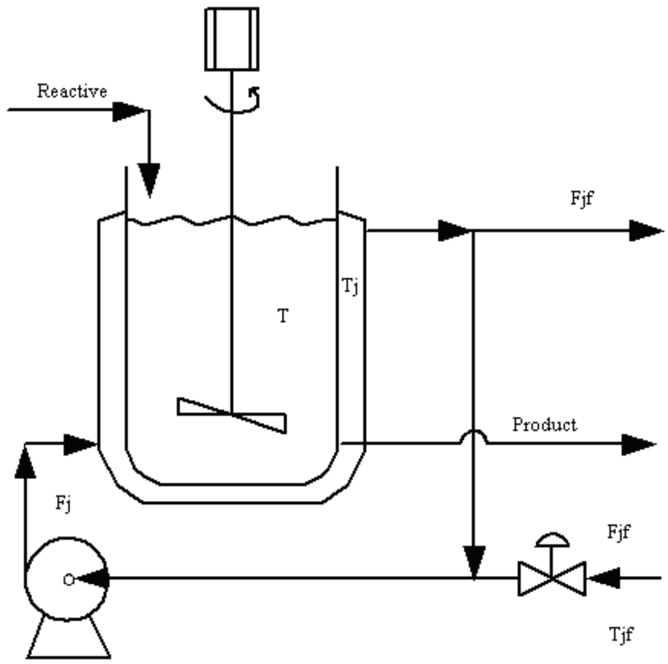

Fig. 1. Scheme of CSTR

2. MATHEMATICAL MODEL FOR THE CSTR

The CSTR is one of the most studied operation units due its wide application in several processes. The diagram of a CSTR is shown in the Fig. 1. This plant performs an exothermic chemical reaction from reactant A to product B ($A \rightarrow B$). The CSTR from Fig. 1 has a recirculation flow in the jacket, allowing to improve its controller design (Bequette, 2002).

The state equations of CSTR are presented in two subsystems as follows:

$$\left\{ \frac{dT_j}{dt} = \frac{F_{jf}}{V_j}\left(T_{jf} - T_j\right) - \frac{UA}{\rho_j C_{pj} V_j}\left(T_j - T\right) \right. \tag{1}$$

$$\left\{ \begin{array}{l} \dfrac{dT}{dt} = \dfrac{F}{V}\left(T_{in} - T\right) - \dfrac{\Delta H}{\rho C_p} k_0 C_A e^{-\frac{E}{RT}} + \dfrac{UA}{\rho C_p V}\left(T_j - T\right) \\ \dfrac{dC_A}{dt} = \dfrac{F}{V}\left(C_{in} - C_A\right) - k_0 C_A e^{-\frac{E}{RT}} \end{array} \right. \tag{2}$$

with outputs T and T_j.

Here, F is the flow into the reactor, V is the volume of the reaction mass, C_{in} is the reactive input concentration, C_A is the concentration of reactive inside the reactor, k_0 is the Arrhenius kinetic constant, E is the activation energy, R is the universal gas constant, T is the temperature inside the reactor, T_{in} is the inlet temperature of the reactant, ΔH is the heat of reaction, and in this article is considered an unknown input because of it is a uncertainty parameter, ρ is the density of the mixture in the reactor, C_p is the heat capacity of food, U is the overall coefficient of heat transfer, A is the heat transfer area, and T_j is the temperature inside the jacket, 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 (Bequette, 2002).

3. ESTIMATION SYSTEM DESIGN

In this section the estimation system for the CSTR in proposed, it estimates the following variables:

- The concentration of reactive inside the reactor, C_A (state variable), due to expensive sensors.
- The global coefficient of heat transfer, UA (parameter), which depends on tank level, the stirring speed inside the reactor, the cleaning degree of the surface inside the reactor, and speed of the cooling flow inside the jacket; making its estimation a hard task (Poling et al., 2001).
- The heat of reaction, ΔH (parameter), which is uncertain due to experimental measurement complexity of thermal and kinetic phenomena that involve it (Martínez-Guerra et al., 2004).

Considering Subsystem(1), it can be noted that the global coefficient of heat transfer, UA, is the only unknown variable. Taking advantage of this characteristic, an estimation system based on cascade connection of an OBE with a HOSMO is proposed as follows:

- Using measurements of T, T_j and, an OBE based on Subsystem (1), an estimation of the parameter UA ($\widehat{UA}$), is obtained.
- Using measurements of T, T_j, the estimated parameter $\widehat{UA}$ and, a HOSMO based on Subsystem (2), estimations of the state variable C_A ($\hat{C}_A$), and the parameter ΔH ($\widehat{\Delta H}$) are obtained.

For this case, the HOSMO structure allows to consider the parameter ΔH as an unknown input. With this assumption, the estimation system is robust against variations of ΔH.

For the OBE design, it is assumed that the global coefficient of heat transfer, UA, is piecewise constant or slowly varying with respect to system state variables. This means $\dot{UA} = 0$.

The whole structure for state and parameter estimation of CSTR is shown in Fig. 2.

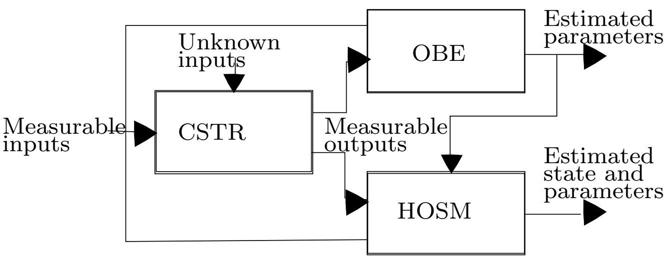

Fig. 2. Structure for state and parameter estimation of CSTR

A detailed explanation for each of the observers is presented in the following.

3.1 OBE Design

Regarding the cascade structure of the estimation system, it will be started with the parameter UA estimation. At first, it must be noted that the HOSMO allows the joint estimation of state an parameters, considering the last ones as unknown inputs. However, it is no possible to achieve the form required by the HOSM in order to estimate simultaneously the parameters UA and ΔH. Therefore, the use of an OBE to estimate UA is proposed here.

Taking into account the Subsystem (1), the OBE design considers a model in the form presented by Oliveira et al. (2002). Hence, in this way, using the jacket temperature equation T_j as coupling equation to calculate UA; the resulting estimator is:

$$\begin{aligned} \frac{d\hat{T}_j}{dt} &= \frac{F_{jf}}{V_j}\left(T_{jf} - \hat{T}_j\right) - \frac{\widehat{UA}}{\rho_j C_{pj} V_j}\left(T_j - T\right) + \omega\left(T_j - \hat{T}_j\right) \\ \frac{d\widehat{UA}}{dt} &= \gamma\left(T_j - \hat{T}_j\right) \end{aligned} \tag{3}$$

where, ω and, γ are the OBE gains.

In order to analyze the OBE convergence, notice that the estimation error dynamics is given by:

$$\begin{bmatrix} \dot{\widetilde{T}}_j \\ \dot{\widetilde{UA}} \end{bmatrix} = \begin{bmatrix} \frac{F_{jf}}{V_j} - \omega & \frac{-\left(T_j - T\right)}{\rho_j C_{pj} V_j} \\ -\gamma & 0 \end{bmatrix} \begin{bmatrix} \widetilde{T}_j \\ \widetilde{UA} \end{bmatrix} + \begin{bmatrix} 0 \\ \dot{UA} \end{bmatrix} \tag{4}$$

where $\widetilde{T}_j = T_j - \hat{T}_j$ and, $\widetilde{UA} = UA - \widehat{UA}$.

Given $\dot{UA} = 0$, the estimation error dynamics is globally exponentially stable for suitable values of ω and γ. Thus, the OBE convergence analysis is based on the following characteristic equation:

$$s^2 + \left(\omega - \frac{F_{jf}}{V_j}\right) s - \gamma\left(\frac{T_j - T}{\rho_j C_{pj} V_j}\right) = 0 \tag{5}$$

Hence, for ensure exponential stability of system (4), its eigenvalues given by the roots of the characteristic equation (5) must have negative real part. For this case, this is achieved equaling the characteristic polynomial to a desired Hurwitz polynomial and calculating the values for ω and γ. For this case, the desired polynomial is an ITAE polynomial of the form $s^2 + 1.4\omega_n s + \omega_n^2$.

3.2 HOSMO Design

Once a time the estimation of $\widehat{UA}$ is obtained, a HOSMO is designed based on Subsystem (2) to provide the estimation of the state variable C_A, $\hat{C}_A$, and the parameter ΔH, $\widehat{\Delta H}$.

In the general case, a nonlinear locally stable MIMO system is considered (Fridman et al., 2008):

$$\begin{aligned} \dot{x} &= f(x) + G(x)\varphi(t) \\ y &= h(x) \end{aligned} \tag{6}$$

where $x \in \mathbb{R}^n$, $y, \varphi \in \mathbb{R}^m$, $f(x) = [f_1(x), \ldots, f_n(x)]^T \in \mathbb{R}^n$, $h(x) = [h_1(x), \ldots, h_m(x)]^T \in \mathbb{R}^m$, $G(x) = [g_1(x), \ldots, g_m(x)] \in \mathbb{R}^{n\times m}$, and $g_i(x) \in \mathbb{R}^n$, $i = 1, \ldots, m$; are smooth vector and matrix functions defined over an open set $\Omega \subset \mathbb{R}^n$. Local weak observability is a basic assumption for system (6).

Therefore, a HOSMO to estimate the state $x(t)$ and, the unknown inputs $\varphi(t)$, using the measurements $y = h(x)$ is designed. This observer is asymptotically stable, that means:

$$\lim_{t\to\infty} \|\hat{x}(t) - x(t)\| = 0 \tag{7}$$

$$\lim_{t\to\infty} \|\hat{\varphi}(t) - \varphi(t)\| = 0. \tag{8}$$

The HOSMO is designed, transforming (6) to the Brunovsky canonical form and calculating the derivatives by means of a robust exact sliding mode differentiator (Levant, 1998).

For the case of CSTR, the parameter ΔH is considered as an unknown input and is defined as $\varphi(t) = \Delta H$.

In addition, it is observed that the output T has a relative degree equal to one with respect with the unknown input $\varphi(t)$. Hence, employing the usual notation, the variables $\xi = T$ and, $C_A = \eta$ are defined.

Therefore, the HOSM structure is:

$$\begin{aligned} \frac{d\hat{\eta}}{dt} &= \frac{F}{V}\left(C_{in} - \hat{\eta}\right) - k_0 \hat{\eta} e^{\frac{-E}{R z_0}} \\ \frac{d\hat{\varphi}(t)}{dt} &= \left(\frac{-k_0\hat{\eta}}{\rho C_p} e^{\frac{-E}{R z_0}}\right)^{-1} \Bigg(z_1 - \frac{F}{V}\left(T_{in} - z_0\right) - \\ &\qquad \frac{\widehat{UA}}{\rho C_p V}\left(T_j - z_0\right)\Bigg) \end{aligned} \tag{9}$$

where z_0 is the estimation of ξ and, z_1 is the estimation of ξ time derivative $\dot{\xi}$.

The estimated variables z_0 and, z_1 are calculated by means of a *Super-Twisting* differentiator of the form:

$$\begin{aligned} \frac{dz_0}{dt} &= -\lambda_0 |z_0 - \xi|^{1/2} \operatorname{sign}\left(z_0 - \xi\right) + z_1 \\ \frac{dz_1}{dt} &= -\lambda_1 \operatorname{sign}\left(z_0 - \xi\right) \end{aligned} \tag{10}$$

with $\lambda_0, \lambda_1 > 0$.

Due the existence of the Brunovsky canonical form for the system (2) the convergence proof of HOSMO can be reduced to prove the differentiator (10) stability.

Let $e_0 = z_0 - \xi$ and, $e_1 = z_1 - \dot{\xi}$. Therefore, the differentiator error dynamics is given by:

$$\begin{aligned}\frac{de_0}{dt} &= -\lambda_0 |e_0|^{1/2} \operatorname{sign}(e_0) + e_1 \\ \frac{de_1}{dt} &= -\lambda_1 \operatorname{sign}(e_0) + \ddot{\xi}\end{aligned} \tag{11}$$

thus, assuming $|\ddot{\xi}| < \xi^+$, with $\xi^+ > 0$ a known constant and, choosing $\lambda_0 > 0$, $\lambda_1 > 3\xi^+ + 4\left(\frac{\xi^+}{\lambda_0}\right)^2$, then $(e_0, e_1) = (0, 0)$ in finite time (Moreno and Osorio, 2008). Establishing a finite time sliding mode for the constraint $e_1 = 0$, that is $z_1 = \dot{\xi}$, despite of the perturbation $\ddot{\xi}$.

Finally, with the convergence the OBE, the convergence of the HOSMO, and the cascade connection; it can be ensured the convergence of the whole estimation system (Sundarapandian, 2004).

4. NUMERICAL SIMULATION RESULTS

The numerical simulations results of the proposed estimation structure applied to a CSTR are presented in this section. The method is compared with a first order SMO as is presented by Wang et al. (1997). The CSTR parameters are shown in Table 1.

Table 1. Nominal Parameters of CSTR

Parameter	**Value**	**Unit**
F	0.1605	$m^3 \cdot min^{-1}$
V	2.4069	m^3
C_{in}	2114.5	$gmol \cdot m^{-3}$
k_0	$2.8267 \cdot 10^{11}$	min^{-1}
E	75361.14	$J \cdot gmol^{-1}$
R	8.3174	$J \cdot gmol^{-1} K^{-1}$
T_{in}	295.22	K
ΔH	$-9.0712 \cdot 10^4$	$J \cdot gmol^{-1}$
ρ	1000	$kg \cdot m^{-3}$
C_p	3571.3	$J \cdot kg^{-1}$
U	$2.5552 \cdot 10^4$	$J \cdot (s \cdot m^2 \cdot K)^{-1}$
A	8,1755	m^{-2}
T_j	279	K^o

In order to verify the observers performance in presence of parametric variations, the changes shown in Table 2 have been introduced in the simulation. Is worth to notice that this changes are unknown for the proposed estimation system.

Table 2. CSTR Parametric Variations

Parameter	**Variation Time**	**Variation Magnitude**
ΔH	45 s	10% Negative step
UA	100 s	50% Negative exponential

For OBE the selected parameter was $\omega_n = 1.429$, leading to $\omega = 1.5096$ and, $\gamma = 93.37$. For HOSMO, the parameters $\lambda_0 = 10$ and, $\lambda_1 = 15$ was used.

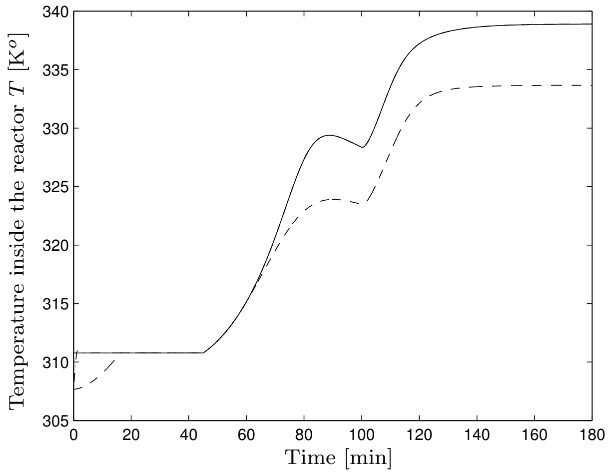

Fig. 3. Temperature T. Real *(solid)*, First Order SMO *(dashed)*, OBE-HOSMO *(dot-dashed)*.

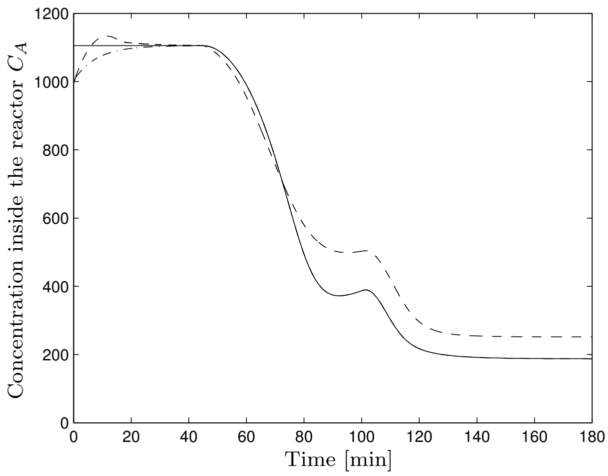

Fig. 4. Concentration C_A. Real *(solid)*, First Order SMO *(dashed)*, OBE-HOSMO *(dot-Dashed)*.

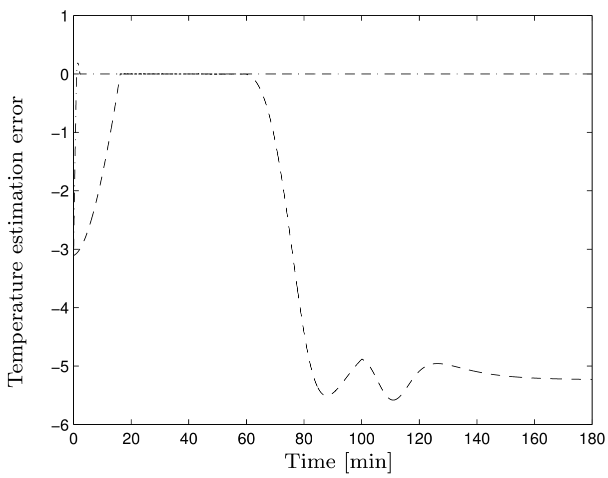

Fig. 5. Temperature estimation error. First Order SMO *(dashed)*, OBE-HOSMO *(dot-dashed)*.

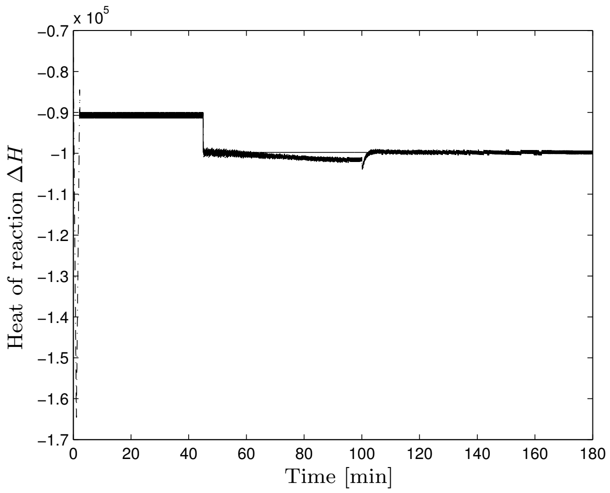

Fig. 6. Heat of reaction ΔH. Real *(solid)*, OBE-HOSMO *(dot-dashed)*.

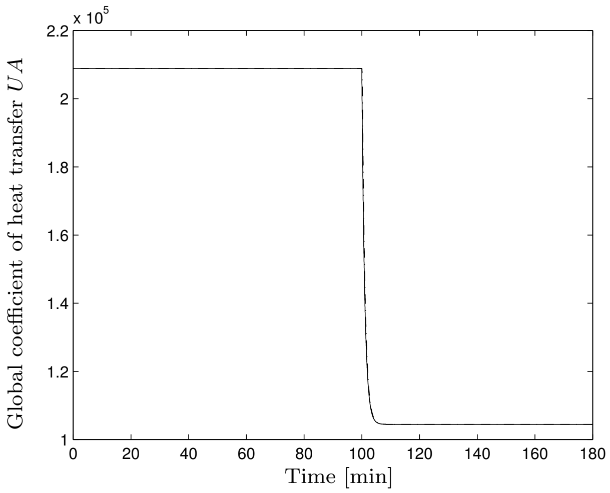

Fig. 7. Global coefficient of heat transfer UA. Real *(solid)*, OBE-HOSMO *(dot-dashed)*.

Figures 3 to 7 show the temperature inside the reactor T, the concentration of reactive inside the reactor C_A, temperature estimation error e_0, the heat of reaction ΔH and, the global coefficient of heat transfer UA, respectively.

Based on the presented figures, it can be observed the good performance of the proposed scheme. The introduced parametric change for ΔH at 45 min induces a steady state error for the first order SMO estimation. In contrast, the HOSMO presents a correct estimation due to its capacity to calculate the ΔH parameter (Figs. 3, 4 and 5). In addition, the simultaneous estimation of UA using the OBE makes the proposed system robuster against this parameter variations (Figs. 6 and 7).

Besides, it can be noted that the HOSMO presents a little chattering due to its discontinuous stabilizing terms (Fig. 6). On the other hand, as is expected, the continuous OBE does not presents similar oscillations phenomena (Fig. 7).

Also, the $|\sigma|$ measure was applied in order to quantify the chattering for the first order SMO and for the HOSMO. This measuring was taken in the interval from 20 min to 44 min, which is the time where both observers present sliding mode motion, before the introduction of the ΔH variation (Fig. 5). The results are the following: for the first order SMO $|\sigma| \leq 0.00311$ and, for the HOSMO $|\sigma| \leq 0.00008$. This means that the chattering generated by the first order SMO is approximately 38.87 times higher than the presented by the HOSMO.

5. CONCLUSIONS

An estimation structure for a CSTR based on an OBE with series connection to a HOSMO observed was proposed. This scheme allows to consider the estimation of two parameters of the process which are well-known as very difficult to measure, specially for real-time applications. One of this parameters was considered as an unknown parameter in the HOSMO, and the second one is estimated by a OBE. Hence, this configuration ensures, a state estimation that is robust against variations of the mentioned parameters. With a suitable selection of the observer parameters, the structure presents a fast convergence with high accuracy.

The simulations present a comparison with a first order SMO. It can be observed the performance of the proposed approach, showing characteristics as good estimation of both parameters and state, robustness, and a short time convergence of the whole system.

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