HOSM State Estimation and Robust PID Control of a Chemical Process

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Abstract: This paper presents some results of the authors' studies on robust estimation and control for chemical processes. Here, an observer-based controller is designed for a chemical process. A High Order Sliding Mode Observer (HOSMO) for state and parameter estimation is synthesized and, a Multi-Variable PID (MV-PID) controller is calculated using the estimated variables. The HOSMO presents insensitivity and robustness against a class of uncertainties in the system, and the MV-PID allows the tracking of slow-varying and piecewise constant references, which are often proposed to drive chemical processes. Numerical simulations show that the observer-based controller presents a good performance in presence of parametric variations, which often are presented in chemical processes; the proposed structure is compared with a First Order Sliding Mode Observer (FOSMO) coupled with a MV-PID.

Keywords: Continuous Stirred-Tank Reactor (CSTR), High Order Sliding Mode (HOSM) Algorithms, Multi-Variable PID Controller.

1. INTRODUCTION

This paper tackles with the design of an observer-based controller for a chemical process. One of the main characteristics of the proposed approach is the use of a HOSMO. In addition, a MV-PID controller uses the estimated variables to track the process to desired references.

Due to its wide application in several processes and the possibility to represent many processes typically employed in industry, the CSTR is one of the most studied operation units and is a recognized benchmark frequently used for controller proofs (Bequette, 2002). Therefore, the proposed scheme will be applied to a CSTR unit.

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 designing, at first place, a HOSMO to estimate the process variables. After that, with the robust estimation provided for the HOSM, a MV-PID controller tracks the CSTR temperature and reactive concentration to desired references.

The Sliding Mode Observers (SMO) are based on the idea of the sliding mode algorithms. As a class of nonlinear state observers, SMO are used 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.

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). 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).

In the following: Section 2 presents the mathematical model of the CSTR. The observer-based controller is presented in Section 3. The Section 4 presents results of numerical simulation, here the proposed controller is compared with one based on a first order SMO. Finally, the conclusions of this paper are included in Section 5.

2. MATHEMATICAL MODEL FOR THE PROCESS

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).

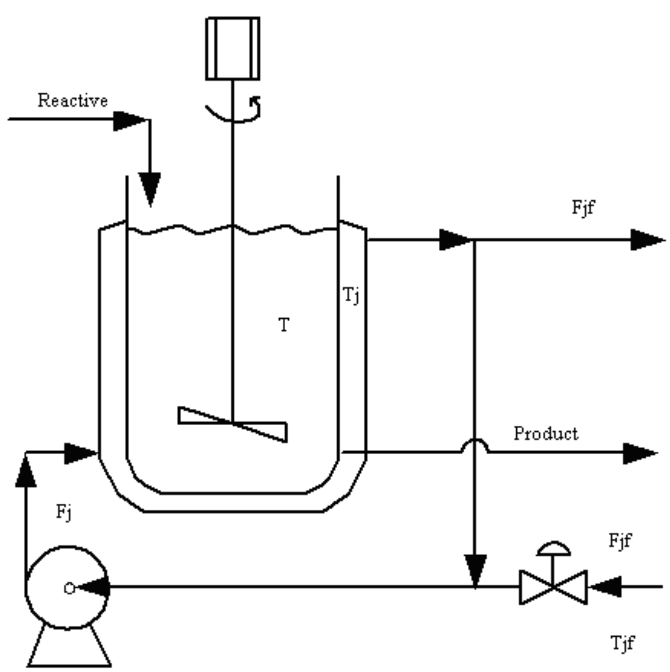

Fig. 1. Scheme of CSTR

The state equations of CSTR are presented as follows:

$$\begin{aligned}
\frac{dT}{dt} &= \frac{F}{V}\left(T_{in} - T\right) - \frac{\Delta H}{\rho C_p} k_0 C_A e^{-\frac{E}{RT}} + \frac{UA}{\rho C_p V}\left(T_j - T\right) \\
\frac{dC_A}{dt} &= \frac{F}{V}\left(C_{in} - C_A\right) - k_0 C_A e^{-\frac{E}{RT}} \\
\frac{dT_j}{dt} &= \frac{F_{jf}}{V_j}\left(T_{jf} - T_j\right) - \frac{UA}{\rho_j C_{pj} V_j}\left(T_j - T\right)
\end{aligned} \tag{1}$$

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 cooling 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.

3. OBSERVER BASED CONTROLLER FOR A CSTR

In this section the observer-based controller is designed. At first, the HOSMO is presented. Then, with the estimated variables, a MV-PID controller is calculated to track the temperature inside the reactor T and, is the concentration of reactive inside the reactor C_A.

3.1 Observer Design

For the CSTR, it is considered the estimation of the concentration of reactive inside the reactor, C_A (state variable), due to expensive sensors. Also, the heat of reaction, ΔH (parameter), is uncertain due to experimental measurement complexity of thermal and kinetic phenomena that involve it (Martínez-Guerra et al., 2004). Therefore, using measurements of T, T_j, the estimated parameter $\widehat{UA}$ and, a HOSMO based on the system (1), estimations of C_A ($\hat{C}_A$), and 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.

In order to apply the design procedure proposed by Fridman et al. (2008), the system (1) must be written in the following general form:

$$\begin{aligned}
\dot{x} &= f(x) + G(x)\varphi(t) \\
y &= h(x)
\end{aligned} \tag{2}$$

where $x \in \mathbb{R}^n$, $y, \varphi \in \mathbb{R}^m$, $f(x) = \left[f_1(x), \ldots, f_n(x)\right]^T \in \mathbb{R}^n$, $h(x) = \left[h_1(x), \ldots, h_m(x)\right]^T \in \mathbb{R}^m$, $G(x) = \left[g_1(x), \ldots, g_m(x)\right] \in \mathbb{R}^{n \times m}$, 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 and, locally stability are basic assumptions for system (2).

The HOSMO is designed, transforming (2) 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:

$$\begin{aligned}\frac{d\hat{\eta}}{dt} =& \frac{F}{V}\left(C_{in} - \hat{\eta}\right) - k_0 \hat{\eta} e^{\frac{-E}{Rz_0}} \\ \frac{d\hat{\varphi}(t)}{dt} =& \left(\frac{-k_0\hat{\eta}}{\rho C_p} e^{\frac{-E}{Rz_0}}\right)^{-1}\left(z_1 - \frac{F}{V}\left(T_{in} - z_0\right) - \right. \\ & \left. \frac{\widehat{UA}}{\rho C_p V}\left(T_j - z_0\right)\right)\end{aligned} \tag{3}$$

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* (Levant, 1993) differentiator of the form:

$$\begin{aligned}\frac{dz_0}{dt} =& - \lambda_0 |z_0 - \xi|^{1/2} \text{sign}\left(z_0 - \xi\right) + z_1 \\ \frac{dz_1}{dt} =& - \lambda_1 \text{sign}\left(z_0 - \xi\right)\end{aligned} \tag{4}$$

with $\lambda_0, \lambda_1 > 0$.

Due the existence of the Brunovsky canonical form for the system (1) the convergence proof of HOSMO can be reduced to prove the differentiator (4) stability.

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

$$\begin{aligned}\frac{de_0}{dt} =& - \lambda_0 |e_0|^{1/2} \text{sign}\left(e_0\right) + e_1 \\ \frac{de_1}{dt} =& - \lambda_1 \text{sign}\left(e_0\right) + \ddot{\xi}\end{aligned} \tag{5}$$

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 $\ddot{\xi}$.

3.2 Controller Design

With the estimated variables provided by the HOSMO, a MV-PID is designed. The controlled variables are the temperature inside the reactor T and, is the concentration of reactive inside the reactor C_A. and, the control input variables are the flow into the reactor F and, the feeding cooling flow F_{jf}.

The MV-PID has the well-known structure given by:

$$u = -\mathbf{K}_p\left(y - y_r\right) - \mathbf{K}_i \int_0^t \left(y - y_r\right) d\tau - \mathbf{K}_d \frac{d}{dt}\left(y - y_r\right) \tag{6}$$

where $u = [F \; F_{jf}]^T$ is the control input, $y = \left[T \; \hat{C}_A\right]^T$ is the controlled output, $y_r = [T_r \; C_{A_r}]^T$ is the controller reference, $\mathbf{K}_p$ is the proportional gain matrix, $\mathbf{K}_i$ is the integral gain matrix, and $\mathbf{K}_d$ is the derivative gain matrix; with $\mathbf{K}_p, \mathbf{K}_i, \mathbf{K}_d \in \mathbb{R}^{2\times 2}$.

The PID tunning is based on minimize the maximal relation complex/real of the characteristic matrix eigenvalues for the closed-loop system linearized on a stable operation point. This criteria provides robustness of the closed-loop system, but does not guarantees a good performance for the controller. Therefore, in order to improve the controller, a tunning method which minimizes a Lyapunov quadratic index is coupled to the first tunning approach (Ruiz-López et al., 2006). The quadratic index depends on the system output.

4. NUMERICAL SIMULATION RESULTS

The numerical simulations results of the proposed observer-based controller applied to a CSTR is presented in this section. The method is compared with one based on 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 observer-based controller performance in presence of ΔH parametric uncertainty, and variations in the references, the changes shown in Table 2 have been introduced in the simulation. Is worth to notice that the parametric uncertainty is unknown for the proposed controller.

Table 2. CSTR Parametric Variations

Variable	**Variation Time [min]**	**Variation Magnitude**
C_A reference	4	5% Negative step
T reference	4	2% Negative step
ΔH parameter	10	2% Positive step

For HOSMO, the parameters $\lambda_0 = 10$ and, $\lambda_1 = 15$ was used. And, for the MV-PID presented in Eq. (6), the following gains are tunned:

$$\mathbf{K}_p = \begin{bmatrix} 7732.5 & -13770.9 \\ -673.64 & 0 \end{bmatrix},$$

$$\mathbf{K}_i = \begin{bmatrix} 93938.6 & -97506.6 \\ -6634.2 & 142.36 \end{bmatrix}.$$

For this case the derivative gain matrix is equal to zero. Besides, the initial condition for the temperature T, and the concentration C_A are 438.54 [K^o], and 0.1 [Mol/l], respectively.

4.1 FOSMO Results

For the FOSMO-based controller, Fig. 2 to Fig. 4 show the temperature inside the reactor T, the concentration of reactive inside the reactor C_A, the tank feeding flow F and, the cooling flow F_{jf}, respectively.

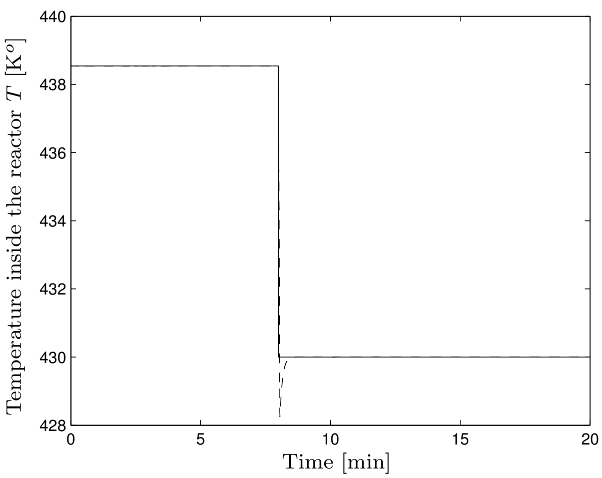

Fig. 2. Temperature T. Reference *(solid)*, Real *(dashed)*.

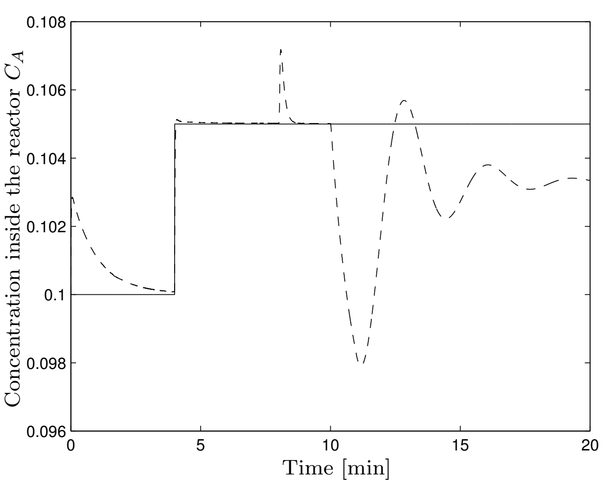

Fig. 3. Concentration C_A. Reference *(solid)*, Real *(dashed)*.

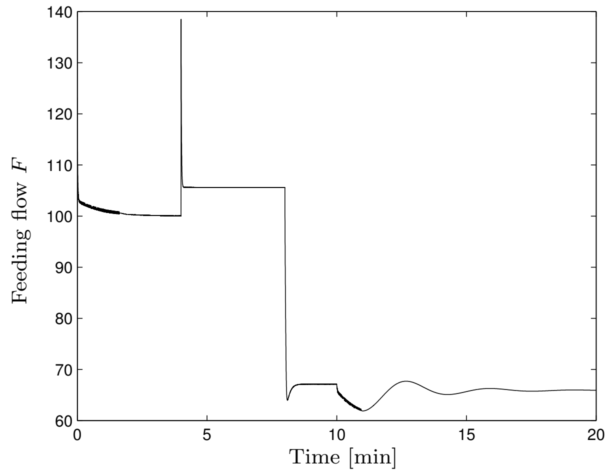

Fig. 4. Feeding flow F.

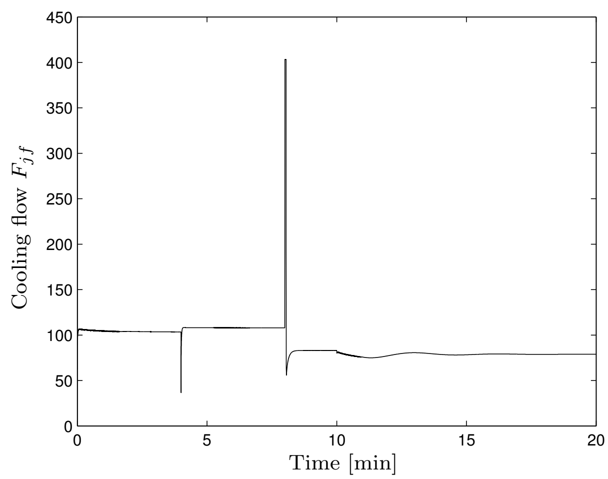

Fig. 5. Cooling flow F_{jf}.

4.2 HOSMO Results

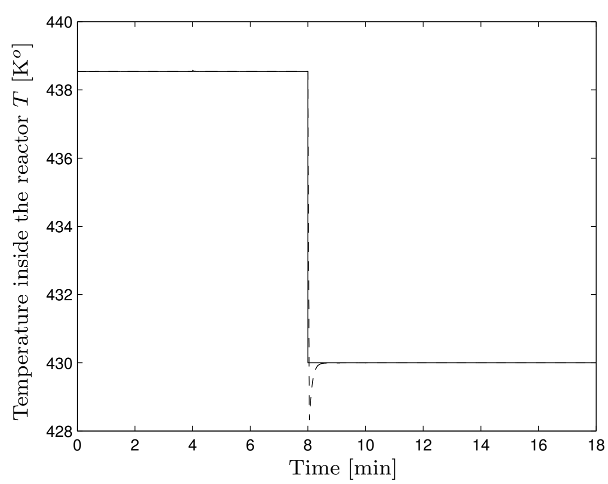

Fig. 6. Temperature T. Reference *(solid)*, Real *(dashed)*.

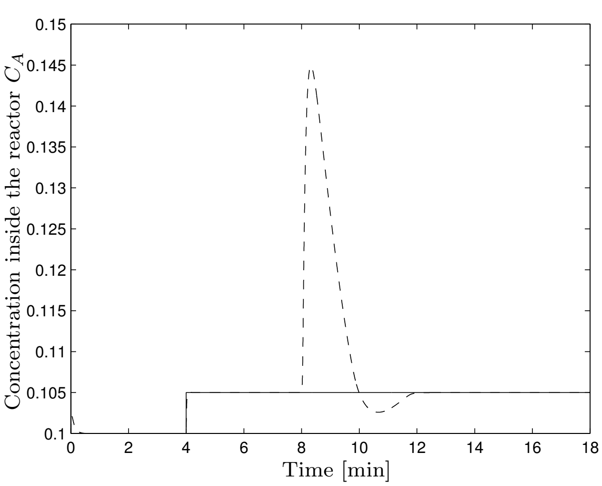

Fig. 7. Concentration C_A. Reference *(solid)*, Real *(dashed)*.

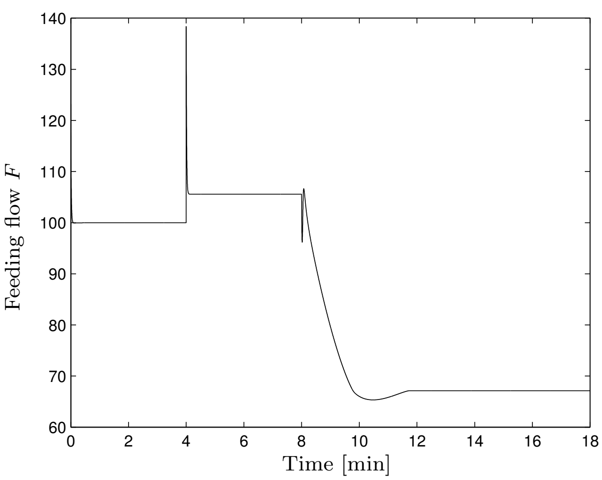

Fig. 8. Feeding flow F.

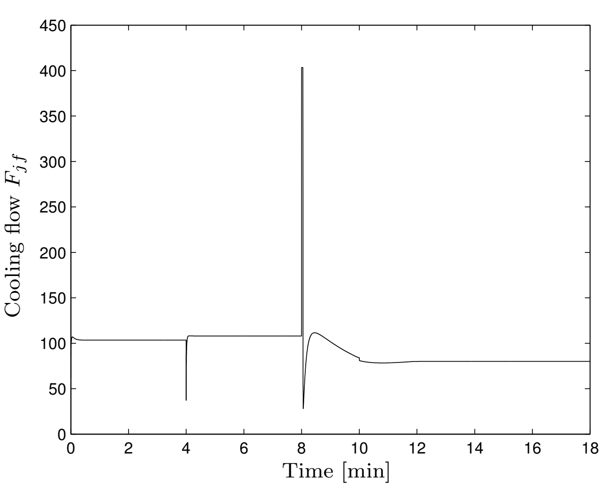

Fig. 9. Cooling flow F_{jf}.

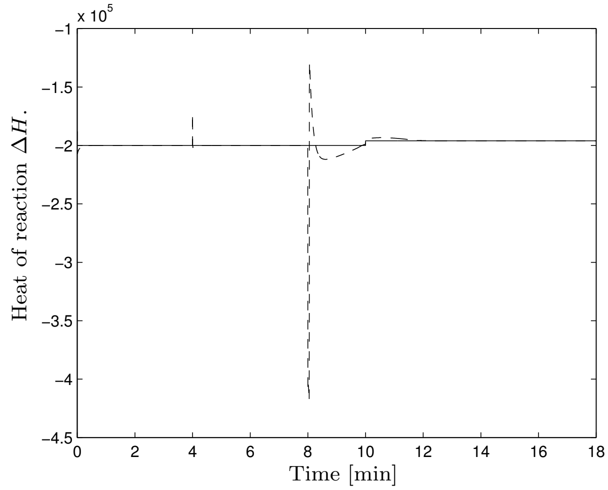

Fig. 10. Heat of reaction ΔH. Real *(solid)*, Estimated *(dashed)*.

In a similar way to FOSMO, for the HOSMO-based controller, Fig. 6 to Fig. 10 show the temperature inside the reactor T, the concentration of reactive inside the reactor C_A, the tank feeding flow F, the cooling flow F_{jf} and, the heat of reaction ΔH estimation, respectively.

4.3 Analysis

With the use of both observer-based controllers, and only considering variations for the references; the tracking presents a good performance as is shown in Figs. 2, 3, 6, and 7. However, the introduced parametric change for ΔH induces a steady state error for the first order SMO estimation, which produces and steady state error in the tracking of the concentration C_A (Fig. 3).

On the other hand, the HOSMO presents a correct estimation due to its capacity to calculate the ΔH parameter (Figs. 7, and 10), providing a good performance and robustness of the closed- loop system. However, due the MV-PID effort to provide an accurate tracking, high values are obtained in the concentration C_A when the temperature T reference is changed. These high values are attenuated in approximately 4 min (Fig. 7) and, are produced by the reduction of the input flow F velocity response (Fig. 8).

With both schemes, the temperature T tracking is accurate and, its dynamics is robust against variations of the ΔH parameter.

5. CONCLUSIONS

An state and parameter estimation structure based on a HOSMO observed was proposed for a CSTR controlled by a MV-PID. The controller uses the estimation of the HOSMO to reference tracking purposes. This configuration ensures, closed-loop robustness against variations of the temperature and heat of reaction parameter. With a suitable selection of the observer and controller parameters, the structure presents a fast convergence with high accuracy.

The simulations present a comparison of the proposed observer-based controller with one based on a FOSMO. It can be observed the performance of the proposed approach, showing characteristics as good estimation of parameter and state, robustness, and a short time convergence of the closed-loop system. In addition, due to the estimation of heat of reaction, the closed-loop system does not exhibits steady state error. In contrast, this error is unavoidable in the FOSMO-based approach.

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