State and unknown input estimation in a CSTR using higher-order sliding mode observer

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Abstract— **The aim of this paper is to design and analyze an observer based on high-order sliding mode to estimate states and unknown inputs in a continuous stirred tank reactor (CSTR). Additionally, the designed HOSM allows to reduce the chattering. The performance of HOSM observer is compared with a 1-order sliding mode observer.**

Keywords: Sliding mode observer, higher-order sliding mode observer, observability, sliding surface.

I. Introduction

State estimation using 1-order sliding mode observer or simply sliding mode observer (SMO) has attractive features as: to work with reduced observation error dynamics, the possibility of obtaining a step by step design, finite time convergence for all observable states, and robustness under parameter variations [1], [2], [3]. However, the main disadvantage of the sliding mode observer is the chattering ([1], [4]) which consists of oscillations in the estimated variables. Chattering arises due to high, theoretically infinite, frequency action of the sign function, applied in order to reach the constraint manifold $\sigma=0$. In the observer σ is the difference between estimated and measured variables.

In order to alleviate the chattering the constraint manifold is changed by continuous functions around $\sigma=0$, like lineal saturation or sigmoid [1], [4]. Nevertheless in some cases, the use of saturation or sigmoid functions decreases the advantage of robustness of the sliding observer. Also in such cases, main features of sliding mode approach, like finite time convergence to sliding surface and insensitivity to a particular class of disturbances and uncertainty in the system are lost.

Another method which reduces chattering is high-order sliding mode (HOSM). It preserves advantages of sliding mode, but it is restricted at the observation case because is necessary to know derivatives of σ [3], [5].

HOSM has many applications in the field of control, but not much in the estimation. Some considerations are made in order to use HOSM in the design of observers [6], [7]. In this sense, several applications of HOSM have been reported for hypothetical systems [3]. However, these systems do not necessarily have physical meaning. In contrast few applications of HOSM in chemical process models have been reported.

The aim of this paper is to design and analyze an observer based on HOSM to estimate states and unknown inputs in a continuous stirred tank reactor (CSTR). Additionally, the designed HOSM allows to reduce the chattering. The CSTR model is a recognized benchmark, since results can be extended to others process.

This paper is organized as follows: in Section II a CSTR model is presented, and its observability conditions are analyzed. Also, for comparison aims, the design of a classic SMO is revised. Section III presents the design of HOSM observer based on robust sliding mode differentiators. In section IV the comparison between SMO and HOSM observer are analyzed by means of simulation results and comparing the $|\sigma|$ between observers as a measure of chattering [8]. Finally, in section V some conclusions are given.

II. Sliding mode observer in a CSTR

A. CSTR model

The diagram of a CSTR is shown in the Fig 1. This plant performs an exothermal chemical reaction from reactant A to product B (A→B).

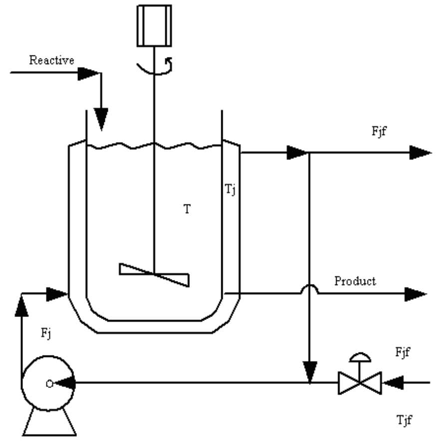

Figure 1. Diagram of a CSTR.

The CSTR model is taken from [9]. It consists of two state equations: temperature and concentration. This model considers that the dynamic of the jacket temperature is fast compared with the mentioned dynamics and that this temperature is kept in a constant value by a control loop. Other modeling assumptions are: perfect mixing in reactor and jacket, constant volume reactor and jacket (level is perfectly controlled), constant parameter values, the heat retained by the walls is negligible. The state equations of CSTR are:

$$\frac{dT}{dt} = \frac{F}{V}(T_{in} - T) + \frac{(-\Delta H)}{\rho C_p} k_0 C_A exp\left(\frac{-E}{RT}\right) - \frac{UA}{\rho C_p V}(T - T_j) \quad (1)$$

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{in} - C_A) - k_0 exp\left(\frac{-E}{RT}\right) C_A \quad (2)$$

where 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, k_0 is the Arrhenius's 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 reaction heat 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. The Table 1 shows the values of the parameters.

B. *Observability of the CSTR*

The Process observability can be proved using (1) and (2). In this study, nonlinear observability was based on differential geometric observability and the results are shown in Table 2 [10].

As is shown in Table 2 the conditions required for the full range of the observability distribution were achieved in a common operation region for the CSTR. The CSTR are often operated in this region because the temperature is always positive and the concentration is greater than zero. Therefore, state observers with arbitrary dynamics for either of the two cases can be designed in a wide region of state space.

Table 1. Parameters of CSTR [11]

Parameter	Value	Unit
F	0.1605	$m^3.min^{-1}$
V	2.4069	m^3
C_{in}	2114.5	$gmol.m^{-3}$
k_0	$2.8267x10^{11}$	min^{-1}
E	75361.14	$Jgmol^{-1}$
R	8.3174	$Jgmol^{-1}K^{-1}$
T_{in}	295.22	K
ΔH	$-9.0712x10^4$	$Jgmol^{-1}$
ρ	1000	$kg.m^{-3}$
C_p	3571.3	Jkg^{-1}
U	$2.5552x10^4$	$J.(s.m^2.K)^{-1}$
A	8.1755	m^2

Table 2. Observability conditions of the CSTR.

Measure variable y=h(x)	Estimate variable $\hat{x}$	Observability distribution ΔS_0	Conditions for full range
C_A	T	A1	T>0 T≠∞
T	C_A	A2	C_A>0 T≠∞

Where A1 and A2 are respectively:

$$span\begin{bmatrix} 1 & 0 \\ \frac{F}{V}(C_{in} - C_A) - k_0 C_A exp\left(\frac{-E}{RT}\right) & \frac{-E k_0 C_A}{RT^2} exp\left(\frac{-E}{RT}\right) \end{bmatrix} \quad (3)$$

$$span\begin{bmatrix} 1 & 0 \\ \frac{F}{V}(C_{in} - C_A) k_0 C_A exp\left(\frac{-E}{RT}\right) & \frac{-E k_0 C_A}{RT^2} exp\left(\frac{-E}{RT}\right) \end{bmatrix} \quad (4)$$

C. *Sliding Mode Observer*

In order to compare the HOSM performance, a classic SMO is designed. The following design is based on the methodology by [1] and applied by [11] to CSTR, but here is only considered the single input single out (SISO) case. Consider the CSTR nonlinear system model in the form:

$$\dot{x} = f(x, u) \quad (5)$$

$$y = x_1 = T \quad (6)$$

Where $x=[T, C_A]^T$ is in $\mathbf{R}^2$, y and u are in $\mathbf{R}$, u is the external input, x_i are smooth functions and the output measured is $y = x_1 = T$, the reactor temperature.

The SMO can be represented as:

$$\dot{\hat{x}} = f(\hat{x}, u) + K(t)sign(x_1 - \hat{x}_1) \quad (7)$$

$$\hat{y} = \hat{x}_1 = \hat{T} \quad (8)$$

Were K(t) is the observer matrix gain. The objective of the sliding observer is to ensure the constraints $\sigma = x_1 - \hat{x}_1 = 0$, by a right selection of K(t). The constraint σ is also named the sliding surface.

The steps for calculating the sliding observer are:

- Organize the model equation so that the output measured is $y = x_1$ = reactor temperature.
- Define the estimation error as $\sigma = x_1 - \hat{x}_1$
- Get a sliding condition for σ by $d\sigma/dt=-\eta sign(\sigma)$, with $\eta>0$ such that dσ/dt has sign opposite to σ.
- Obtain the $K(t)$ matrix gain of the observer according to the procedure by [1].
- Check by simulating the observer performance.

III. HOSM OBSERVER

In HOSM observers the r-order of the sliding mode is defined by a smooth function which meets the constraint $\sigma=\sigma^{(1)}=\ldots=\sigma^{(r-1)}=0$ [7]. The term $\sigma^{(r)}$ is discontinuous or nonexist. So, the first order mode (r=1), only satisfies σ=0, and is the most sliding mode known. For r≥2, the sliding mode is named HOSM.

A. System representation

In order to estimate states and unknown inputs, the model of the system are to be in the Brunovsky canonical form. Reference [2] proposes a methodology to estimate the state and unknown inputs in nonlinear systems based on [7], [12]. The model equations are to be expressed in the form:

$$\dot{x} = f(x) + G(x)\varphi(t) \quad (9)$$

$$y = h(x) \quad (10)$$

For the CSTR equation (9) written in expanded form is:

$$\begin{bmatrix} \dot{T} \\ \dot{C}_A \end{bmatrix} = \begin{bmatrix} \frac{F}{V}(T_{in} - T) + \frac{UA}{\rho C_p V}(T_j - T) \\ \frac{F}{V}(C_{in} - C_A) - k_0 C_A exp\left(\frac{-E}{RT}\right) \end{bmatrix} + \begin{bmatrix} \frac{-k_0}{\rho C_p} C_A exp\left(\frac{-E}{RT}\right) \\ 0 \end{bmatrix} \varphi(t) \quad (11)$$

Where x, f(x), G(x)=g_1, are in $\mathbf{R}^2$, y is in $\mathbf{R}$, φ(t) (the unknown input) is in $\mathbf{R}$. Here, the unknown input represents the uncertain parameter ΔH and y=T. The heat of reaction is an uncertain term because of the fact that thermal and kinetic phenomena related are complex and difficult to measure experimentally [13].

B. Design of HOSM observer for a CSTR

The steps for designing the HOSM observer are:

- The system represented by (11), are to be transformed to the Brunovsky canonical form.
- To apply HOSM differentiators in order to estimate temperature.
- Based on estimated temperature to estimate x_2 and φ(t).

Because of the system model consists of two state variables, the state equations of the transformed system are equal to (11), then with $\xi=T=x_1$, $\eta=C_A=x_2$, these equations are:

$$\begin{bmatrix} \dot{\xi} \\ \dot{\eta} \end{bmatrix} = \begin{bmatrix} \frac{F}{V}(T_{in} - \xi) + \frac{UA}{\rho C_p V}(T_j - \xi) \\ \frac{F}{V}(C_{in} - \eta) - k_0 \eta exp\left(\frac{-E}{R\xi}\right) \end{bmatrix} + \begin{bmatrix} \frac{-k_0}{\rho C_p} \eta exp\left(\frac{-E}{R\xi}\right) \\ 0 \end{bmatrix} \varphi(t) \quad (12)$$

For the transformed system (12) the temperature ξ is estimated using a robust 2-order sliding mode differentiator and hereafter is named second-order sliding mode observer (SOSMO) with the form of the equations (13) to (15). These equations are the typical in the design of HOSM [7].

$$\frac{dz_0}{dt} = v_0 \quad (13)$$

$$v_0 = -\lambda_0 \sqrt{|z_0 - T|} sign(z_0 - T) + z_1 \quad (14)$$

$$\frac{dz_1}{dt} = -\lambda_1 sign(z_0 - T) \quad (15)$$

Where z_0 is the the estimation of ξ and z_1 its velocity. The constants λ_i are positive, $\lambda_0>\lambda_1$ and must be adjusted by simulation. The main features of this observer are that preserves advantages of sliding modes like the possibility of obtaining a step by step design, finite time convergence for all the observables states, and robustness under parameter variations.

The estimated equations for the concentration and the parameter unknown are taken from (12):

$$\frac{d\hat{\eta}}{dt} = \frac{F}{V}(C_{in} - \hat{\eta}) - k_0 \hat{\eta} exp\left(\frac{-E}{R\hat{T}}\right) \quad (16)$$

$$\hat{\varphi}(t) = \left(\frac{-k_0}{\rho C_p} \hat{\eta} exp\left(\frac{-E}{R\hat{\xi}}\right)\right)^{-1} \left[z_1 - \frac{F}{V}(T_{in} - \hat{\xi}) - \frac{UA}{\rho C_p V}(T_j - \hat{\xi})\right] \quad (17)$$

IV. SIMULATIONS RESULTS

The two designed observers (SMO and SOSMO) were simulated. Euler integration method with step size 0.01min was used. The values of the constants λ_0=2 and λ_1=1.3 were adjusted by simulation looking at the temperature graph and calculating the value maximums of |σ| for SMO and SOSMO.

Initial conditions are as a follows (units are omitted): T(0)=310.77, $T_{SO}(0)$=307.66, $T_{SOSO}(0)$=307.66, $C_A(0)$=1105.21, $C_{ASMO}(0)$=994.70, $C_{ASOSMO}(0)$=994.70. The value of ΔH is -9.0712×10^4 and at 45 min is multiplied by a factor of 1.1. The Fig. 2 shows the real temperature, the estimated temperatures with SMO and SOSMO, Fig. 3 shows the concentration, Fig. 4 shows the reaction heat ΔH and its estimation, Fig. 5 show σ functions related with SMO and SOSMO and Fig. 6 shows the estimation error for the concentration variable.

In Fig. 2 note that the settling time is lower in SOSMO than in SMO, but after the change in ΔH, SMO temperature does not track the others ones. A Similar behavior is found in the concentration variable, which shows greater robustness of the SOSMO observer compared with the SMO one.

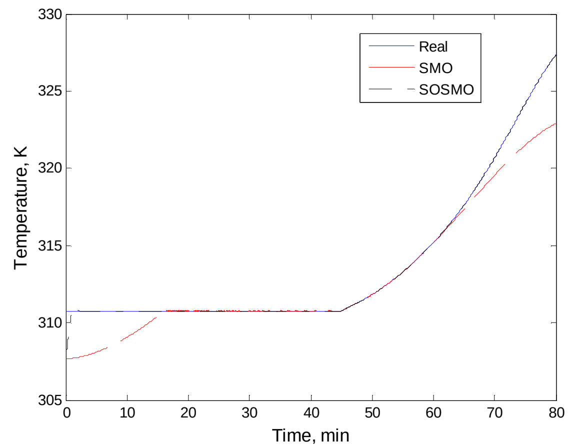

Figure 2. Reactor temperature.

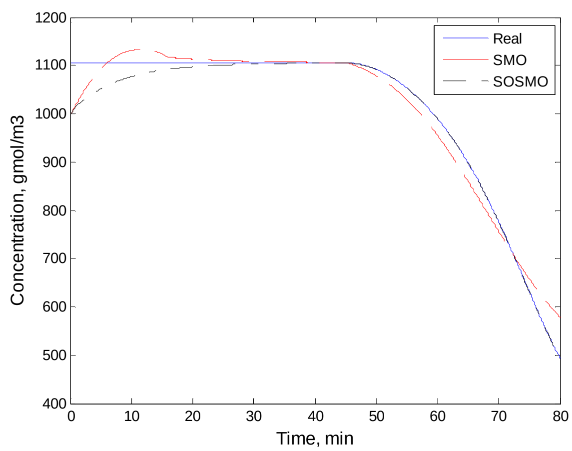

Figure 3. Concentration C_A.

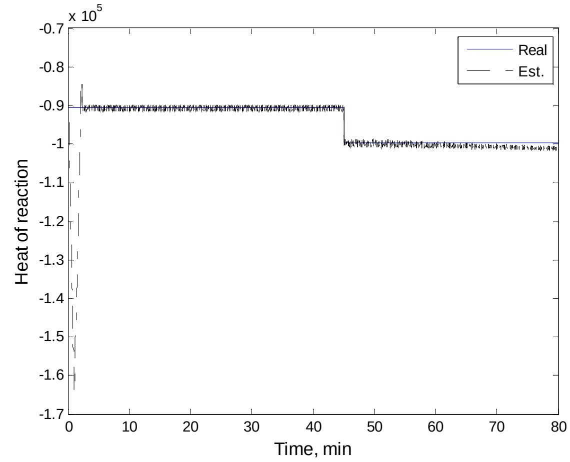

Figure 4. Real and estimated heat of reaction.

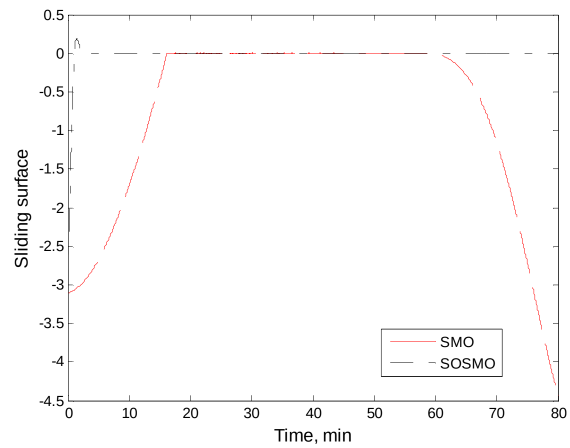

Figure 5. Sliding surface.

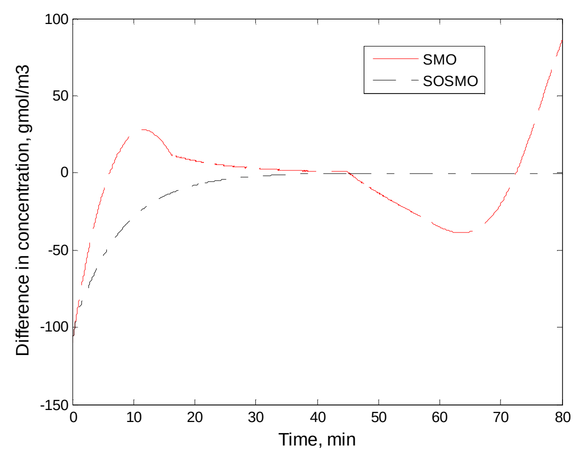

Figure 6. Difference estimation C_A

New steady state values are caused by the change in ΔH for temperature and concentration, but those achieved by SMO are incorrect, which are shown in Fig. 7 and Fig. 8.

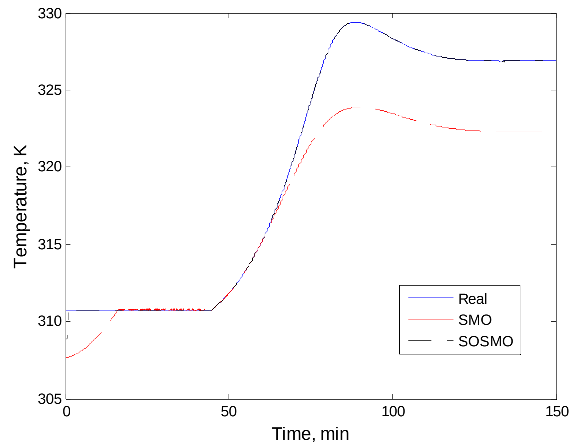

Figure 7. Reactor temperature.

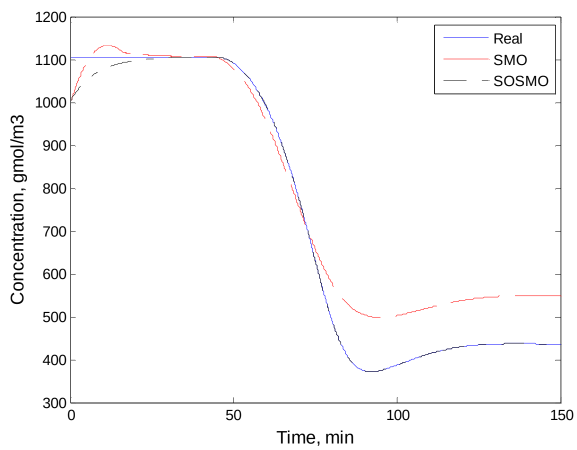

Figure 8. Concentration C_A.

The Fig. 4 shows the quick estimation of heat reaction, at the beginning and after the change in ΔH.

Additionally the criterion of small value of $|\sigma|$ is considered to prove the reduction of chattering [8]. Therefore, the $|\sigma|$ are calculated for SMO and SOSMO and compared between them in order to feature the lowest chattering. These results were obtained between 20 and 44 min. Then, for SMO $|\sigma|\leq 0.00311$ and for SOSMO $|\sigma|\leq 0.00008$, the ratio between them is 38.87 which feature a lower chattering in the SOSMO. By other hand, Fig 5 shows the convergence to zero of the SOSMO sliding surface, which is also observed in Fig. 2.

V. CONCLUSIONS

An observer based on HOSM (SOSMO) to estimate states and unknown inputs in a continuous stirred tank reactor was designed. This observer allows to reduce the chattering compared with SMO. Also, the settling time of the sliding surface is lower in SOSMO than in SMO. The observer using HOSM estimated the state and the heat reaction in a CSTR. Only SOSMO is robust to changes in heat reaction.

The model of CSTR is a recognized benchmark, and represent several chemical process, therefore the results can be extended to others process.

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