

Design of a Kalman Filter and Three Observers in a CSTR for the Estimation of Concentration and Temperature in Jacket.

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Abstract— The control implementation loops for the chemical process require measurements and variable estimations that are hard, difficult, and expensive; this is due to the lack of reliable devices, delays, wrong measurements, and expensive devices. The state estimation and non-linear systems parameters let restores state variables that the process requires to identify using the input and output known variables. This paper presents four-state estimators, Luenberger observer, Unknown Inputs, Sliding modes, and Kalman Filter, applied to a chemical process in a Continuous Stirred-Tank Reactor (CSTR) at three dynamics: concentration (C_A), temperature (T), and temperature of the jacket (T_j). The estimation of the dynamics is carried out from the measurement of the values of the inputs and outputs of the process. Each estimator was tuned to have values close to the real ones. The three dynamics of the CSTR were assessed with perturbations and parametric changes based on the chemical process's phenomenological model. The estimators' results were close to those of the real process, with estimated deviations of the state variables between 5% and 10% of the real value. The SMO algorithm accepts a greater range of variation at nominal flow input F until 30%, while KF, UIO, and OL reach 5% maximum; this makes possible better estimation of chemical process variables in a CSTR using SMO.

Keywords— Observer; sliding surface; Kalman filter; continuous stirred-tank reactor; Luenberger.

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I. INTRODUCTION

At an industrial level, knowing dynamics with veracity, such as angular velocity, temperatures, torque, and concentration, allows identifying variables that directly affect a process in order to make the necessary corrections and maneuvers as a response to failures. With this consideration in mind, several state estimators have been proposed to tackle certain requirements, such as convergence time, type of process (chemical, electromechanical, pneumatic, among others), dynamics, parameters to estimate, as well as other guidelines present at the time of performing mathematical development in a state observer. Based on a review of the reconstruction of variables from data acquisitions, in the 1960s, the search for solutions to the estimation of states began with the Kalman filter [11],[14] and the Luenberger observer [13], becoming the major references in the field. It has also been proven that the estimation from unknown inputs is of significant importance due to the scarce knowledge or the difficult reconstruction of a physical input (manipulated

or not) of the process [4]. In addition to those mentioned, there are estimators that use different tools or mathematical concepts, such as the observer-based estimator [15] and the high-order sliding-mode observer [8-9, 21], which provide a wide range for the study of specific cases.

A CSTR (Continuous Stirred-Tank Reactor) chemical processes have dynamics and parameters, generally unknown in mathematical modeling, obtained from mass and energy balances equations, such as concentration and temperature. The mass and energy balances allow identifying both the number of state variables and the minimum number of parameters for their correct operation. Additionally, the convergence, stability, and observability criteria allow defining the best estimation strategy to use. At an industrial level, the excessive cost and availability of final control elements [10], such as sensors, have increased software used to estimate non-measurable parameters.

In industrial processes, it is usually difficult to know the variables and parameters of the model in real-time due to instrumentation, excessive costs, coupling with other control systems, noise levels, among other factors [16]. In addition to

the estimation of states, using the same algorithms used in the estimators, it is possible to reconstruct the model's unknown parameters from the input and output readings of the real process.

Chemical processes have been highly studied in the industrial sector. Process Engineering currently supports the use of estimators in heat exchangers, continuous reactors, distillation towers, among others [17]. This work proposes the construction and performance evaluation of four estimators, the Kalman filter, the Luenberger observer, the Unknown Input observer, and the sliding-mode observer [12]. The estimators' design was carried out in a linearized plant from a non-linear one, showing the process of linear approximation and choosing the operation points that allow building the theory of the estimators on linear and smooth models. Fig. 1 shows a flow chart so that the estimation research stages are seen properly and systematically.

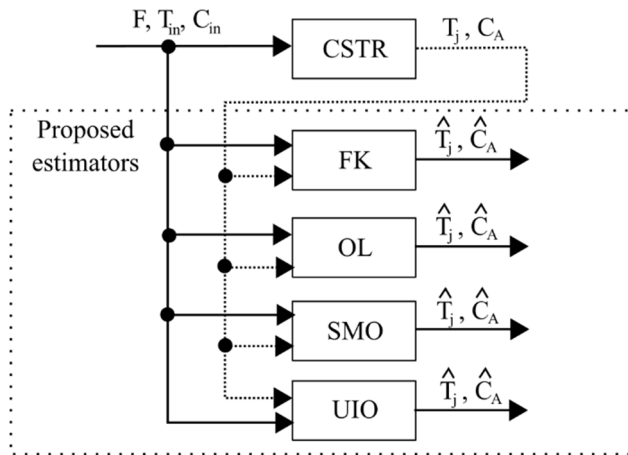


Fig. 1 Flow chart of research stages

II. MATERIAL AND METHOD

A. Continuous Stirred-Tank Reactor (CSTR)

In this work, a chemical reactor, operated in continuous mode, is approached with the dynamics of concentration and temperature to estimate the four aforementioned estimators' efficiency. Internally, the CSTR produces a chemical reaction inside the tank that transfers energy from the reactive mass within the cooling fluid that recirculates through the jacket, covering the reactive mass on the outside [6].

An exothermic reaction, $A \rightarrow B$, occurs inside the tank. Fig. 2 shows the CSTR reactor structure, the dynamics process, the manipulated inputs, and the control elements. The constructed model is based on mass and energy balances, where the concentration dynamic, C_A , is the first balance per component followed by the energy balance of temperature for the reactive mass, T , and by the temperature of the cooling fluid the jacket, T_j . Given the existence of external dynamics that affect the behavior of the CSTR, assumptions were made to the model to limit the problem and reduce the number of dynamics to work with [1],[3].

B. Model Equations and Assumptions

In this case, study, since we assume that the level is controlled, the volume is constant; therefore, the model is composed of three state variables: C_A , T , and T_j . In addition, the following assumptions were made [1]:

- The concentration of the reagent is uniform inside the reactor.
- The reactor operates at a constant volume.
- The temperature of the jacket and the reactive mass are uniform.
- The heat retained by the metal walls inside the reactor is insignificant.
- The densities of the fluids remain constant.

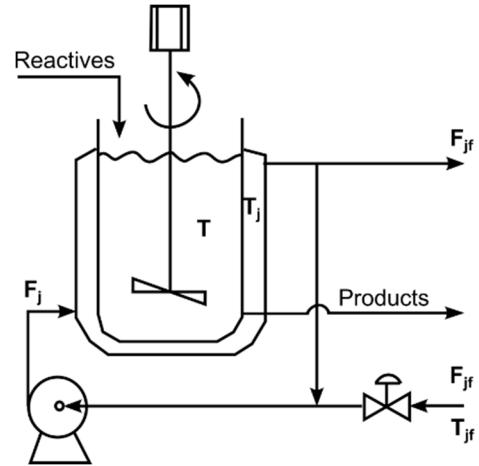


Fig. 2 Diagram of the CSTR process with recirculation in jacket.

Equations 1-3 are commonly referenced in CSTR chemical process studies and are derived from the results of materials and energy balances [1], [3]. Equation 1 corresponds to the balance of the components of reagent A, Equation 2 corresponds to the energy balance of the reactor's internal temperature, and Equation 3 corresponds to the energy balance of the jacket's temperature.

$$\dot{C}_A = \frac{F}{V} (C_{in} - C_A) - k_0 C_A e^{\frac{-E}{RT}} \quad (1)$$

$$\dot{T} = \frac{F}{V} (T_{in} - T) - \frac{\Delta H}{\rho c_p} k_0 C_A e^{\frac{-E}{RT}} + \frac{UA}{\rho c_p V} (T_j - T) \quad (2)$$

$$\dot{T}_j = \frac{F_{jf}}{V_j} (T_{jf} - T_j) - \frac{UA}{\rho_j c_{pj} V_j} (T_j - T) \quad (3)$$

The actual parameters that feed the modeling equations were chosen for the simulation prior to constructing the estimators in MATLAB® Simulink. Table 1 details the nominal values and units [1].

Where F is the inflow to the reactor, V is the volume of the reactive mass, C_{in} is the concentration of the reagent at the entrance to the reactor, C_A is the concentration of the reagent inside the reactor, k_0 is the Arrhenius constant of the reaction, E is the activation energy, R is the gas constant, T is the temperature inside the reactor, T_{in} is the input temperature of the reagent, ΔH is the heat of reaction, ρ is the density of the mixture in the reactor, c_p is the specific calorific capacity, U is the heat transfer coefficient, A is the heat transfer area, T_j is the temperature inside the jacket, F_{jf} is the jacket flow, V_j is the jacket volume, T_{jf} is the input temperature of the jacket, ρ_j is the density of the fluid in the jacket, and c_{pj} is the calorific capacity of the fluid in the jacket [3].

TABLE I
NOMINAL PARAMETERS OF THE CSTR

Variable	Value	Variable	Value
F	0.1605	ρ	1000
V	2.4069	c_p	3571.3
C_{in}	2114.5	U	2.6×10^4
k_0	2.83×10^{11}	A	8.1755
E	75361.1	F_{jf}	0.3776
R	8.3174	V_j	0.2407
T_{in}	295.22	T_{jf}	282.96
ΔH	-9×10^{14}	ρ_j	1000

C. Linearization

As a previous step to the construction of the estimators based on linear models, we propose a linearization under an operating point (as seen in Table. 2) with the model Equations 1-3.

TABLE II
STATES AND STEADY-STATE INPUTS

Variables	Operative points	
	Value	Unit
	663.862501612603	gmol m^{-3}
T	320.236393435742	K
T_j	287.775973873343	K
F	0.1605	$\text{m}^3 \text{min}^{-1}$
F_{jf}	0.3776	$\text{m}^3 \text{min}^{-1}$

Once the partial derivatives with respect to the states and inputs were found, the linearization process is performed under a dynamic operating point by taking a non-linear system to a linearizing one [20]. Equations 4-5 explain the model in state-space with incremental variables.

$$\begin{bmatrix} \Delta \dot{C}_A \\ \Delta \dot{T} \\ \Delta \dot{T}_j \end{bmatrix} = \begin{bmatrix} -0.212 & -8.545 & 0 \\ 0.004 & 0.126 & 0.024 \\ 0 & 0.233 & -1.802 \end{bmatrix} \begin{bmatrix} \Delta C_A \\ \Delta T \\ \Delta T_j \end{bmatrix} + \begin{bmatrix} 602.7 \\ -10.4 \\ 0 \end{bmatrix} \Delta F \quad (4)$$

$$\begin{bmatrix} \Delta C_A \\ \Delta T \\ \Delta T_j \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \Delta C_A \\ \Delta T \\ \Delta T_j \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \Delta F \quad (5)$$

With the linearized system in deviation variables, the concept of stability by location of poles in the real-imaginary plane is identified within matrix A of the CSTR reactor dynamics. There is the possibility to analyze the stability of the system using the Lyapunov functions. For the system described in Equation 4, based on system A's matrix, we used the direct method to identify the poles through A's eigenvalues. The location of the poles of A was obtained using Equation 6.

$$\lambda_1 = -0.0417 + 0.0494i; \lambda_2 = -0.0417 - 0.0494i \\ \lambda_3 = -1.8045 \quad (6)$$

From Equation 6, it can be concluded that the poles of our system have negative real and imaginary parts, guaranteeing

the stability condition of the three dynamics by being located in the left half-plane of poles and zeros.

D. Comparison of Linear vs Non-linear Model

The Kalman filter and the state observer models work correctly once the corresponding plant is in its deviation variables, based on a linearized model under a neighborhood around the operating point. The Kalman state and filter observer models work correctly once the corresponding plant is in its deviation variables in a linearized manner under one operating point boundary. The comparison between the linear and the non-linear model of the CSTR was carried out under a 5% change in parameters at the entrance of F, validating its maximum tracking of the states of the system in the vicinity-

E. Observability

After reviewing the stability and linearization of the chemical process, it is necessary to know the observability test, where, for linear systems, it is sufficient to obtain the range of the observability matrix that involves the previously linearized matrix. The output matrix C directly involves the states to be measured and known. In this paper, we propose to measure the internal temperature of the reactor T (reactive mass) and to estimate the dynamics of the concentration of A (C_A) and of the temperature of the jacket T_j [9]. In Equation 7, the matrix of order 3x1 and its range are identified.

$$\text{Range}(M_{OBS}) = \begin{bmatrix} C \\ CA \\ CA^2 \end{bmatrix} = 3 \quad (7)$$

Equation 7 shows a complete column equal to three, concluding that the three mentioned states could be observed. It is thus guaranteed that the system is observable and that the Luenberger observer will have no restrictions. For the Unknown Input Observer (UIO), the proposed observability matrix was analyzed in detail to use two inputs: feed flow F and flow entering the reactor's jacket F_{jf} .

III. RESULTS AND DISCUSSION

A. Luenberger Linear Observer

For the Luenberger Linear Observer, the linearized plant was considered as described in Equation 8.

$$\Delta \dot{x}(t) = A \Delta x(t) + B \Delta u(t) \\ \Delta y(t) = C \Delta x(t) \quad (8)$$

Where Equation 8 represents the plant in deviation variables, with states and inputs $x(t)$ and $u(t)$, respectively. For the design of the Luenberger observer, a structure was proposed in Equation 9 [13].

$$\Delta \hat{x}(t) = A \Delta \hat{x}(t) + B \Delta u(t) + K_e (y - \hat{y}) \quad (9)$$

The correction in the estimation of the proposed model is directly reflected in the choice of the correction matrix K_e , showing that it can be forced to have an adjustable dynamic, with the direct design under the location of poles in the desired polynomial that meets the conditions of convergence, stability, and speed [13].

$$Pd = s^2 + 10.8s + 29.3 \quad (10)$$

The fastest pole from Equation 6 was chosen for the desired polynomial. The desired polynomial is exposed in Equation 10, and the Luenberger matrix K_e is chosen in Equation 11.

$$K_e = \begin{bmatrix} -0.6718 \\ -0.0004 \\ 0.28500 \end{bmatrix} \quad (11)$$

From the Luenberger observer of the linear and non-linear models, the estimates were analyzed by assuming the temperature T and estimating the concentration of A and the jacket's temperature. By measuring the temperature in the reactive mass of the CSTR, both C_A and T_j were estimated using a linear Luenberger observer (see Fig. 3 and 4).

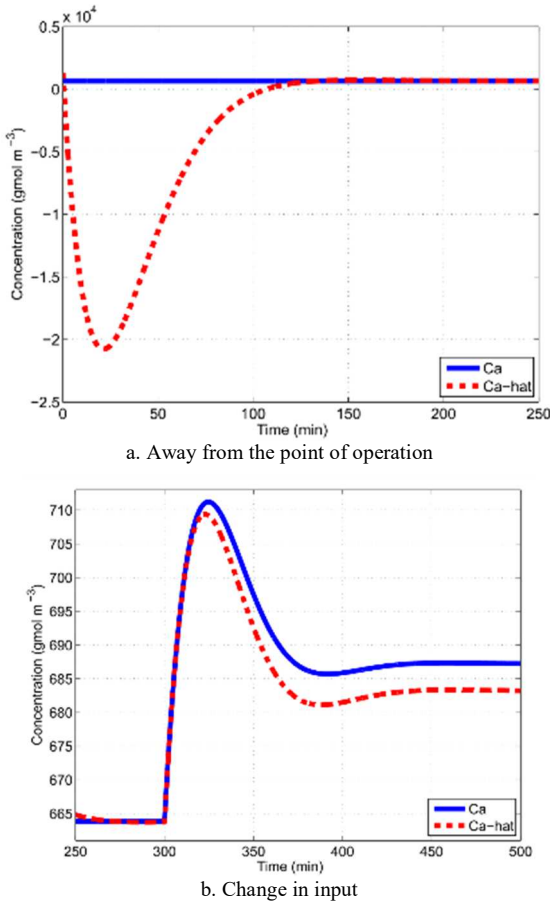
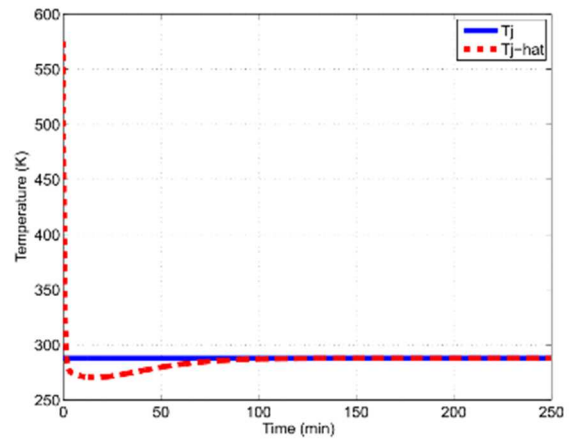


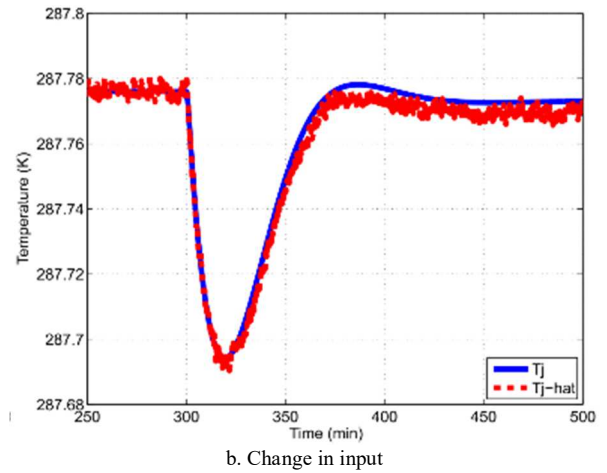
Fig. 3 Estimation of C_A by the Luenberger Observer.

Fig. 3(a) and Fig. 4(a) show changes in the input of 5%, which suggests that the concentration estimate is more difficult to correct than the error it generates, with changes in the input in the minute 300.

The temperature in the jacket, estimated in Fig. 4(a), begins from a point far from the operating point and, in the face of changes in the inputs and the noise in the measurement, it is identified in Fig. 4(b) that the dynamics T_j and \hat{T}_j do not undergo changes before the flow F due to the disturbance at 300 minutes.



a. Away from the point of operation



b. Change in input

Fig. 4 Estimation of T_j by the Luenberger Observer.

B. Unknown Input Observer (UIO)

A linearized plant is proposed under an operating point, described by Equation 12. The model is described in deviation variables, and the adjustment matrix for the UIO is identified by the letter D , multiplied by the vector of unknown inputs.

$$\begin{aligned} \Delta \dot{x}(t) &= A \Delta x(t) + B \Delta u(t) + D v(t) \\ \Delta y(t) &= C \Delta x(t) \end{aligned} \quad (12)$$

Where $x \in \mathbb{R}^k$, $u \in \mathbb{R}^n$, $v \in \mathbb{R}^p$ and $y \in \mathbb{R}^p$, are the state vector, the known inputs vector, the unknown inputs vector, and the output system, respectively [5]. The inputs are defined to perform the observer with unknown inputs as follows: the first input is the flow to the reactive mass F (unknown), and the second input, the known, is the flow that feeds the jacket F (known). Once the inputs were chosen, the value of matrix B in Equation 12 changes. Finally, matrices B and D are shown in Equation 13.

$$B = \begin{bmatrix} 0 \\ 0 \\ -20.09 \end{bmatrix}; \quad D = \begin{bmatrix} 602.6995 \\ -10.3936 \\ 0 \end{bmatrix} \quad (13)$$

To obtain matrices B and D , we follow the steps proposed in [15], in which an estimator of unknown inputs is proposed, shown in Equation 14, where \hat{z} is the new estimated vector that feeds back from the original estimated state of Equation 12, and the matrices N , L and G are known. Following the steps proposed in [15], the range of observability of (PA, C)

gave a value. It can be concluded that the temperature of the jacket T_j is estimated from the measured state T .

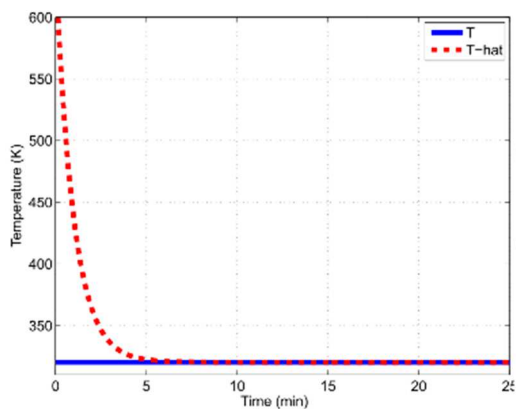
$$\begin{aligned}\dot{\hat{z}} &= Nz + Ly + Gu \\ \hat{x}(t) &= z - Ey\end{aligned}\quad (14)$$

From the identification of the location of the eigenvalues of N , it is observed that the first is in the right half-plane and represents instability and is not observable (see Fig. 7). The non-estimated state is concentration. The poles of the matrix N are shown in Equation 15.

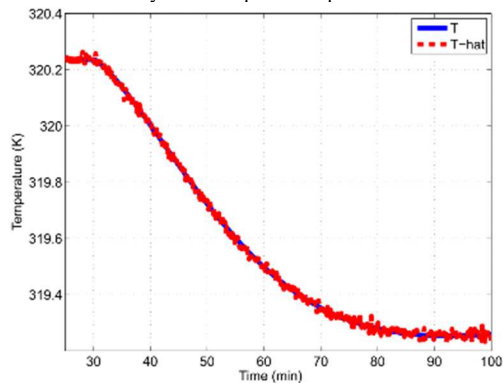
$$\begin{aligned}\lambda N_1 &= 0.0022 \\ \lambda N_2 &= -1.802 \\ \lambda N_3 &= -1.000\end{aligned}\quad (15)$$

Following the steps of [15], from the UIO design, it was obtained that the gain of the observer K_{UIO} has two static dynamics, one of them being variable. The dynamics were modified to guarantee convergence in the estimation of the states T and T_j , related to the temperature of the reactive mass in the CSTR.

Estimates of T and T_j were obtained from the Unknown Input Observer, as shown in Fig. 5 and Fig. 6. From Fig. 5(b) and Fig. 6(b) it can be seen that, before the noise in the measurement of T , the same variable can be estimated correctly and, in addition, the temperature of the jacket in the reactor can be estimated, having as an aggravating factor that, for this system, the feed flow to the reactor is unknown. Fig. 5(a) and Fig. 6(a), with a different operating point, correctly observe the state.

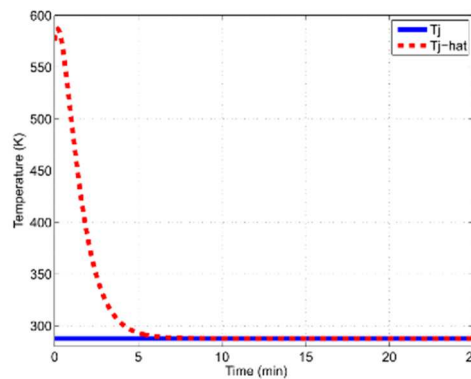


a. Away from the point of operation

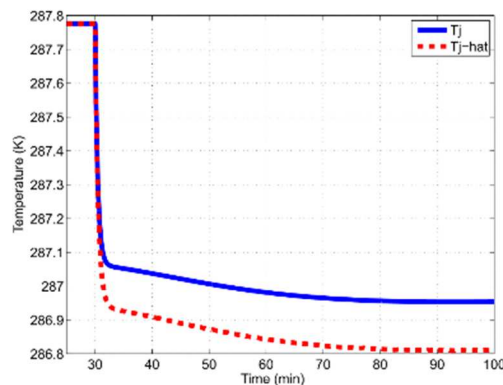


b. Change in input

Fig. 5 Estimation of T by the UIO.



a. Away from the point of operation



b. Change in input

Fig. 6 Estimation of T_j by the UIO

In Fig. 7 it is observed that the estimate of C_A never really converges due to the reason explained above that the poles are located in the right half-plane.

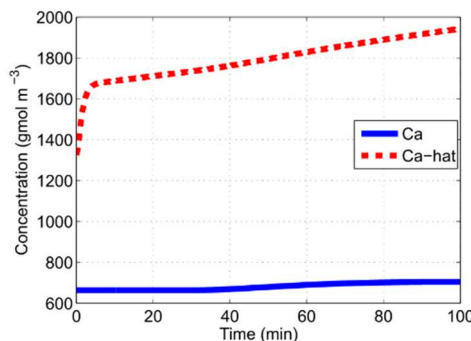


Fig. 7 Estimation of C_A by the UIO.

C. Kalman Filter

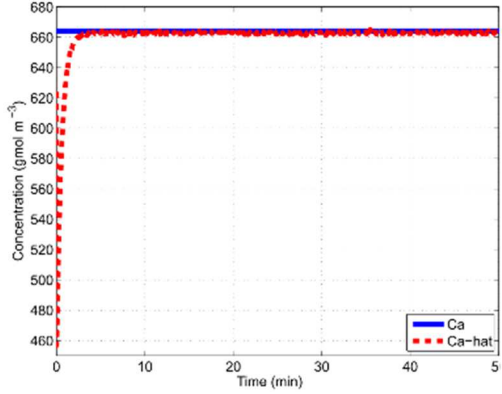
The Kalman filter is a state estimator that calculates the state of a linear dynamic system, disturbed by noisy signals, from measurements that are linearly related to the state, without any filter, similar to noisy signals found in real life [3]. From the proposed deduction of the Kalman filter, the improvements proposed [3], and the equations that govern this filter [11], the design of the Kalman filter is proposed using the algorithm developed in the MATLAB® subroutines, where it is only necessary to have the system in the linearized state space and choose the tuning matrices Q and R .

As presented in previous observers, the Kalman filter has a correction factor that helps filter the corresponding signal in the estimation. The tuning matrices and Kalman gain matrices

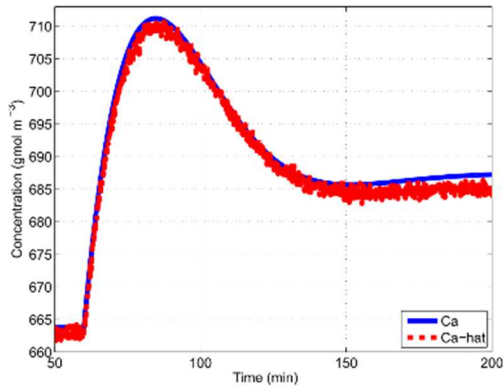
(KKalman) were chosen for the filter operation as shown in Equation 16, respectively.

$$Q = 100; \quad R = 1; \quad K_{Kalman} = \begin{bmatrix} -5898.56 \\ 103.85 \\ 0.2286 \end{bmatrix} \quad (16)$$

As in the two previous estimators, the variable measured in the CSTR was the reactive mass temperature. The estimation of C_A and T_j was performed, as shown in Fig. 8 and Fig. 9. In Fig. 8(a) and Fig. 9(a) the estimator reaches the desired value out of its operating point.



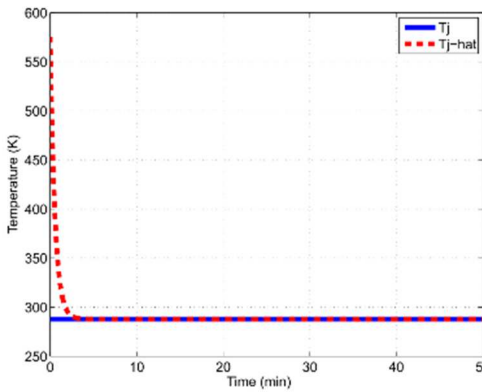
a. Away from the point of operation



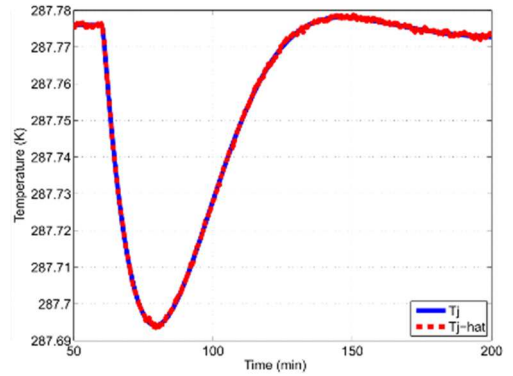
b. Change in input

Fig. 8 Estimation of C_A using the Kalman Filter.

From the tuning of the Q and R matrices, a good response to the estimation of C_A and T_j was obtained by considering that the observer was launched from an arbitrary point and that the input had a change in the step of 5% at 60 minutes (see Fig. 8(b) and Fig. 9(b)).



a. Away from the point of operation



b. Change in input

Fig. 9 Estimation of T_j using the Kalman Filter.

D. Sliding Mode Observer (SMO)

Consider the plant described in Equation 17, where $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$, $u \in \mathbb{R}^p$ are defined as states, outputs, and inputs, respectively.

$$\Delta \dot{x}(t) = A \Delta x(t) + B \Delta u(t)$$

$$\Delta y(t) = C \Delta x(t) \quad (17)$$

To apply this method, the system of Equations 17 must be transformed into two dynamics: one of the measured states and the other of unmeasured states [9]. The discriminated model is shown in Equation 18.

$$\dot{y} = A_{11}y + A_{12}x_1 + B_1u$$

$$\dot{x}_1 = A_{21}y + A_{22}x_1 + B_2u \quad (18)$$

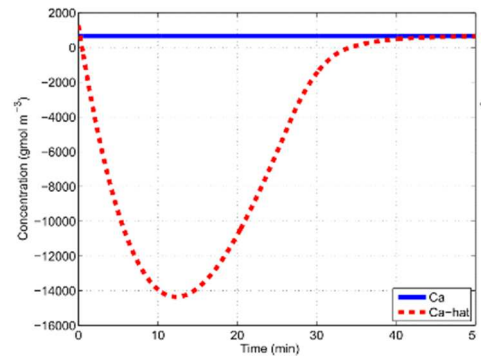
In Equation 18, \dot{y} is measurable and \dot{x}_1 is not measurable, considering that the values of A_{11} , A_{12} , A_{21} , A_{22} , B_1 and B_2 are known. Once the model has been transformed into measurable and non-measurable dynamics [7],[18], the extended Equation 19 describes the Sliding Mode Observer (SMO) [19].

$$\hat{y} = A_{11}\hat{y} + A_{12}\hat{x}_1 + B_1u + L_1 \text{sign}(y - \hat{y})$$

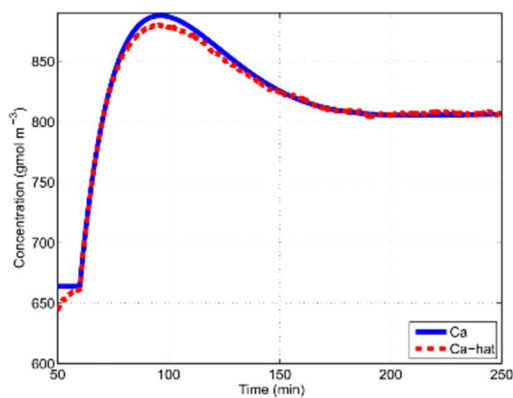
$$\hat{x}_1 = A_{21}\hat{y} + A_{22}\hat{x}_1 + B_2u + L_2 L_1 \text{sign}(y - \hat{y}) \quad (19)$$

The estimator's correction factor is chosen between L_1 and L_2 , multiplied by the function $\text{sign}(x)$. To find these values, the dynamics of the error is developed in the measurable part $e(y) = \bar{y} = y - \hat{y}$. From the linearized plant under a neighborhood and the procedure proposed in [7],[18], the estimator was performed with the gain values determined as follows:

$$L_1 = 10; \quad L_2 = 1 \quad (20)$$



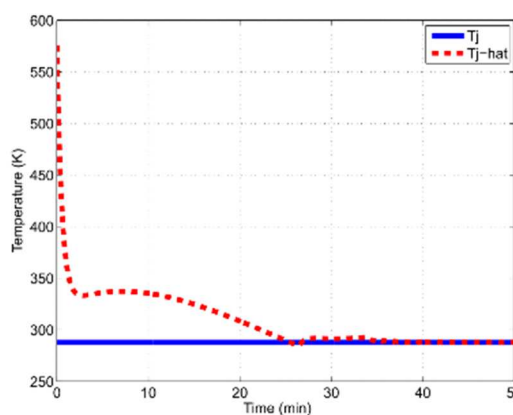
a. Away from the point of operation



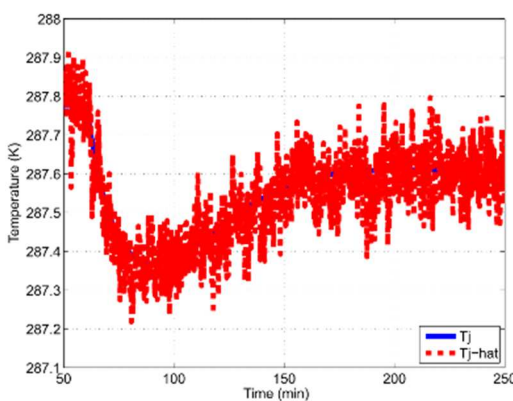
b. Change in input

Fig. 10 Estimation of C_A by the SMO.

C_A and T_j were estimated using a sliding-mode observer by employing, as a measured variable, the reactor's internal temperature. Fig. 10 and Fig. 11 show such behavior. According to the sliding-mode observer, the gains L_1 and L_2 vary, the chattering directly affects the estimation [2].



a. Away from the point of operation



b. Change in input

Fig. 11 Estimation of T_j by the SMO.

As L_1 increases, the robustness improves considerably, as seen in Fig. 10 (b) and Fig. 11 (b). The C_A and T_j estimate under a first-order SMO show good monitoring since 20% changes were introduced in the input at 60 minutes of the simulation, and they presented greater robustness concerning other observers and estimators made with parametric changes at the input.

IV. CONCLUSION

In industry, the implementation of an estimator is determined according to the accuracy of the model and the relevance of using an approximation of a variable of interest. Therefore, the proposed estimators performed correctly in simulation. In the CSTR study case, the KF, UIO, and OL algorithms accept a range of variations at nominal flow input F until 5%. At the same time, SMO achieves a higher one, up to 30%, using SMO provides a higher range of operation in the tuning of control algorithms, after these disturbance values at the input, the C_A and T_j dynamics estimations have high steady-state errors, hence applying SMO makes possible better estimation of chemical process variables in a CSTR. Despite chattering in SMO (unwanted phenomenon), it can be reduced by applying robust differentiators through the Super-twisting algorithm (STA), which reduces the estimation error and gets a faster response.

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