STATE ESTIMATION USING OBSERVERS FOR A CONTINUOUS STIRRED TANK REACTOR (CSTR)

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Abstract: *The design of various feedback controllers, optimal controllers require the information about all the states present in the system. Not all the states in the system will be available for direct measurement. In order to estimate all the states of the system the observers are designed. In this paper the state estimation problem of the CSTR is considered, the observers used include Luenberger Observer, Kalman Observer, and Sliding Mode Observer. The states that are estimated using the observers are utilized by the state feedback controllers and the optimal controllers, to ensure the convergence of the states to the equilibrium point. The designed observers had the residuals converging to zero in finite time and the comparison in terms of estimation errors resulted in better performance of the sliding mode observer.*

Keywords: Luenberger Observer, Sliding Mode Observers (SMO), Kalman Observers (KO), State feedback, optimal control.

1. Introduction

The CSTR is important process equipment and the reactor considered here is exothermic. The distinguished property of a CSTR is that it has non linearitires such as bifurcations [1], multiple steady states [2], Chaos [3], limit cycle [4] and potential safety issues [5]. In some cases state variables of the reactor are not completely measurable for economic or technical reasons so a T-S based observer was used to estimate the states and the H infinity controller was used to ensure robust tracking performance [6], [7].The process variables (states) may not available for direct measurement, but they can be inferred from readily accessible states by means of the competent design of observers. The observers are used in places where the sensors are costly or where the sensors are not available for direct measurement of the state variables. The most common type of observer used is Luenberger observer it is known for its simple structure [8].In case of presence of disturbances the Kalman observer can be used [9]. The observers can also be used in fault detection and also as disturbance estimator. The sliding mode observer method incorporates a switching function into the observer design to make the error dynamics to converge to zero asymptotically [10].

The organization of the paper is as follows. In Section 2 the modeling of the CSTR is given in detail. The various models of state observers are briefed in section 3. The controller design is given in Section 4. The simulation results of observer based controller of CSTR are reported in section 5. Finally the comparison among the observers is given in the conclusion.

2. Modeling of CSTR

Modeling of the CSTR involves using the first principles to obtain the model of a system. Here the species balance and the energy balance of the CSTR is carried out to derive the state space model and the transfer function model of the system. During the modeling of the CSTR the following assumptions are made
1. Perfect mixing of the reactants &
2. Constant volume of the reactor.

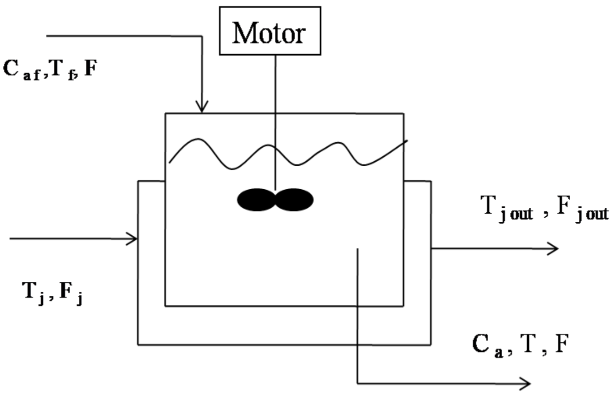

Fig.1 Typical CSTR

Table.1: Parameters of the CSTR

States	Measured Variable	Estimated Variable
Concentration in the rector (mol/m^3)	Concentration in the rector (mol/m^3)	Temperature in the reactor(K)
Temperature in the reactor(K)		

The mathematical model equations are obtained by a component mass balance and energy balance principle in the reactor.

(Accumulation of component Mass) = (Component Mass) $_{in}$ - (component Mass) $_{out}$ + (generation of component Mass)

(Accumulation U + PE + KE) = (H + PE + KE) $_{in}$ - (H+PE+KE) $_{out}$ + Q-Ws

The species balance is given as

$$V\frac{dC_a}{dt} = F\left(C_{a,f} - C_a\right) - K_0 \exp\left[\frac{-E}{RT}\right] C_a V \qquad (1)$$

The Energy balance is given as

$$V\rho C_p \frac{dT}{dt} =$$

$$\rho F C_p\left(T_f - T\right) - \Delta H\left[K_0 \exp\left[\frac{-E}{RT}\right] C_a\right] V - UA\left(T_j - T\right) \qquad (2)$$

The state space representation of the CSTR is given as

$$\begin{bmatrix} \dot{C}_a \\ \dot{T} \end{bmatrix} = \begin{bmatrix} -K_0 \exp\left[\frac{-E}{RT}\right] & 0 \\ -\frac{\Delta H}{\rho c_p} \exp\left[\frac{-E}{RT}\right] & \frac{UA}{\rho c_p V} \end{bmatrix} \begin{bmatrix} C_a \\ T \end{bmatrix} + \begin{bmatrix} 0 \\ -\frac{UA}{\rho c_p V} \end{bmatrix} \left[T_j\right] \qquad (3)$$

$$y = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} C_a \\ T \end{bmatrix} \qquad (4)$$

Where the states of the process are Concentration of the Reactor (C_a), Temperature of the Reactor (T). Manipulated input is the Temperature of the Cooling Jacket (T_j). Controlled outputs are Concentration of the Reactor (C_a) and Temperature of the Reactor (T).

Table.2: Parameter values of the model

T_j	Temperature of cooling jacket (K)	270
F	Volumetric Flow rate(m^3/sec)	100
V	Volume of CSTR(m^3)	100
ρ	Density of A-B Mixture(kg/m^3)	1000
C_p	Heat capacity of A-B mixture(J/kg-K)	0.239
ΔH	Heat of reaction for A → B (J/mol)	5×10^4
E/R	EoverR	8750
K_0	Pre exponential factor(1/sec)	7.2×10^{10}
UA	Overall heat transfer coefficient (U=W/m^2-K)	5×10^4
$C_{a,f}$	Feed concentration	1
T	Temperature in CSTR (K)	350
C_a	Concentration of A in CSTR	0.989

The CSTR is linearized around the operating points C_a = 0.989 mol/m^3 and T = 296.6 K and the state space representation of the nominal plant model is obtained.

$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t) + Du(t)$$

Where,

A is $n \times n$ the system matrix, a constant

B is $n \times r$ the input matrix, a constant

C is $m \times n$ the output matrix, a constant

D is $m \times r$ the direct feed through, a constant

x is $n \times 1$ the state vector, a function of time

u $r \times 1$ is the input, a function of time

y $m \times 1$ the output, a function of time

3. Models of observers

3.1 Luenberger Observer

For the continuous system of the form

$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t) + Du(t) \qquad (5)$$

The pair [A, C] should be observable for the application of observer to the system. The observer equation is given as

$$\dot{\hat{x}} = A\hat{x} + Bu + L(y - \hat{y})$$
$$\hat{y} = C\hat{x} \qquad (6)$$

L is the observer gain

The Estimation error is given as $e = x - \hat{x}$; Residual of the observer is given as $(y - \hat{y})$.

The observer gain L must be chosen in such a way that the error dynamics converges to zero when time tends to infinity. The closed loop poles of the observer have to be 3 to 4 times greater than the poles of the system [11].

3.2 Continuous Time Kalman Observer

Kalman observer is a recursive predictive filter that is based on the use of state space techniques and recursive algorithms, i.e. only the estimated state from the previous time step and the current measurement are needed to compute the estimate of the current state. The Kalman filter operates by propagating the mean and covariance of the state through time [12].

For the continuous system of the form

$$\dot{x} = Ax + Bu + Gw$$

$$y = Cx + Du + Hw + v \qquad (7)$$

With inputs *u*, white process noise *w*, and white measurement noise *v* satisfying

$E(w)=E(v)=0$, $E(ww^T)=Qn$, $E(vv^T)=Rn$, $E(wv^T)=Nn$

The observer equation is given as

$$\dot{\hat{x}} = A\hat{x} + Bu + L(y - \hat{y} - Du)$$

$$\hat{y} = C\hat{x} \qquad (8)$$

L is the observer gain.

The steady-state error covariance is given by

$$P = \lim_{t\to\infty} E(\{x - \hat{x}\} - \{x - \hat{x}\}^T \qquad (9)$$

The filter gain L is determined by solving an algebraic Riccati equation to be

$$L = (PC^T+N)\, R^{-1} \qquad (10)$$

3.3 Sliding Mode Observer

For the continuous system of the form

$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t) + Du(t) \qquad (11)$$

Where $A \in R^{n \times n}$, $B \in R^{n \times m}$, $C \in R^{p \times n}$ and $p \geq m$. The pair [A, C] should be observable for the application of observer to the system

Consider the change of coordinates $x \rightarrow T_c\, x$ whereby

$$T_c = \begin{bmatrix} N_c{}^T \\ C \end{bmatrix} \qquad (12)$$

Where the columns of $N_C \in R^{n \times (n-p)}$ span the null space of C. This transformation is nonsingular.

The canonical form for the nominal system is given as

$$\dot{x}_1 = A_{11}x_1 + A_{12}y + B_1u$$
$$\dot{y} = A_{21}x_1 + A_{22}y + B_2u \qquad (13)$$

Where $T_c\, X = \begin{bmatrix} x_1 \\ y \end{bmatrix}$

The observer is given as

$$\dot{\hat{x}}_1 = A_{11}\hat{x}_1 + A_{12}\hat{y} + B_1u + L\upsilon$$
$$\dot{\hat{y}} = A_{21}\hat{x}_1 + A_{22}\hat{y} + B_2u - \upsilon \qquad (14)$$

Where $(\hat{x}_1, \hat{y}_1)$ represent the state estimates, $L \in R^{(n-p) \times p}$ is a gain matrix and $\upsilon = M\, \mathrm{sign}\, (\hat{y} - y)$ where $M \in R_+$. L is the observer gain and it can be chosen to make the spectrum of $A_{11} + LA_{21}$ lie in the left of the complex plane [13].

4. Controller Design

4.1 State feedback control

For a system of the form

$$\dot{x}(t) = Ax(t) + Bu(t)$$

$$y(t) = Cx(t) + Du(t) \quad (15)$$

A state feedback control places the closed loop poles at the desired location. The poles of the system is given by the Eigen values of the A matrix. This can be done using methods namely Pole placement, Ackermann's formula. For the application of the State feedback controls the necessary and the sufficient condition is that the system is controllable. For the above mentioned system the control vector u is given by

$$u = -Kx(t) \quad (16)$$

The closed loop system is given as

$$\dot{x}(t) = (A - BK)x(t) = A_{cl}x(t)$$

$$A_{cl} = (A - BK) \quad (17)$$

The gain matrix is designed in such a way that Determinant of (sI - (A - BK)) = (s-μ_1) (s-μ_2) (s-μ_3)….. Where μ_1, μ_2, μ_3 are the desired pole locations [14].

4.2 Optimal Control

For a system of the form

$$\dot{x}(t) = Ax(t) + Bu(t)$$

$$y(t) = Cx(t) + Du(t)$$

The optimal controllers are designed in such a way that it minimizes the Quadratic cost function (J). $J = \int_0^\infty (x^T Qx + u^T Ru)\,dt$. Here x is the state variable, u is the control variable, Q and R are the penalty on the state variables and control variables. In order to optimize the gain value (K) in the state feedback control u=-K$\times$x (t) the optimal control is used. The value of K is obtained by solving $K = R^{-1} \times B^T \times P$. The value of P is found by solving the Algebraic Ricatti Equation $PA^T + PA - PR^{-1}B^T P + Q = 0$ [15].

5. Simulation Results

The state space representation of the CSTR is obtained by linearizing the non linear model around the steady state operating points.

$$A = \begin{bmatrix} -1.0111 & -0.0110 \\ 2.3216 & -3.0922 \end{bmatrix} \quad C = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

$$B = \begin{bmatrix} 0 & -0.0110 \\ 2.0920 & 53.400 \end{bmatrix} \quad D = 0$$

5.1 Luenberger Observer

For the design of the Luenberger Observer location of the desired poles of the plant are μ_1=-0.0281, μ_2=-0.1480.The observer poles are chosen to be -0.0842, -0.4441which is 3 times greater than the poles of the plant. The calculated value of the observer gain is $L = \begin{bmatrix} 0.3522 \\ 13.3910 \end{bmatrix}$.Using the poles and the observer gain the observer is constructed. The Fig.2 shows that the residuals of the observer tend to zero in a finite time.

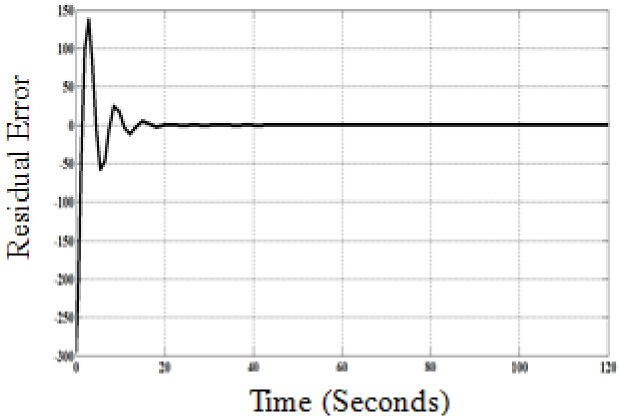

Fig.2. Residual of Luenberger Observer

The measured state which is the concentration (mol/m^3) is also estimated as we are invloved in designing if full order observers. The Fig.3, 4 shows the convergence of the estimated states (x_1, x_2) to the plant's real states. Table 3 shows the values of estimation error at different time.

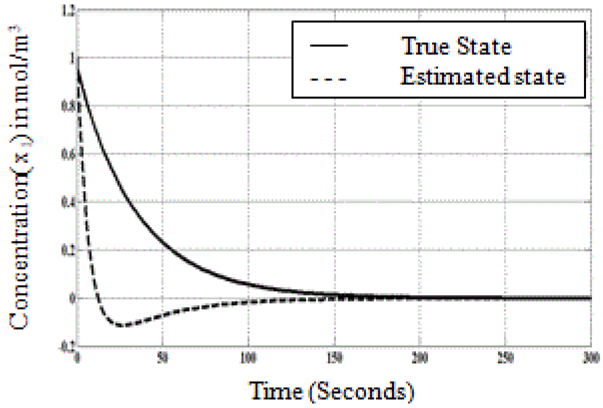

Fig.3. Convergence of Concentration (x_1) in mol/m^3 of Luenberger Observer

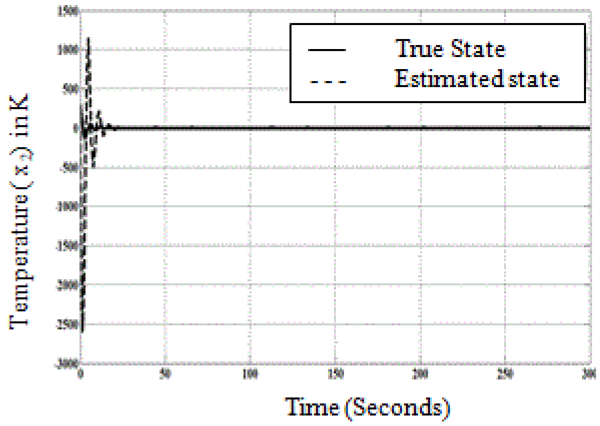

Fig.4. Convergence of Temperature (x_2) in Kelvin (K) of Luenberger Observer

Table 3: Estimation Error calculation for Luenberger Observer

Time (Seconds)	Estimation Error in states	
	$x_1 - \hat{x}_1$ Concentration(mol/m^3)	$x_2 - \hat{x}_2$ Temperature (K)
10	3.9563	1.7212
20	2.2881	0.3273
30	1.2923	0.0124
40	0.4999	0.0062

5.2. Continuous time Kalman Observer

The greater advantage of the Kalman Observer is the consideration of the process noise and the measurement noise. The weighing matrices Q_n and Rn which satisfies E(w)=E(v)=0, E(ww^T)=Qn, E(vv^T)=Rn, E(wv^T)=Nn; R depends on the sensor sensitivity. If this is a real world problem this can be obtained from the manufacturer. If not an identity matrix multiplied by a scalar that is less than 1is used. Q is the covariance of the process noise. Again if this is a real world problem this can be obtained in the noise level in the states of the system at steady state. A non-zero Q helps achieve good convergency characteristics

$$R_n = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad Q_n = [1].$$

The steady state Covariance matrix for the design of Kalman observer is given as $P = \begin{bmatrix} 0.1639 & -0.0948 \\ -0.0948 & 0.0613 \end{bmatrix}$.

The observer gain L is a column vector with values $L = \begin{bmatrix} 0.0617 \\ -0.0384 \end{bmatrix}$.

5.2.1 Kalman Observer Based Optimal Controller

The Optimal controller design requires information about the solution to the Algebraic Ricatti-Equation, (ARE) $PA^T + PA - PR^{-1}B^T P + Q = 0$. The value of $Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ $R = [1]$ and the solution to the ARE is $P = \begin{bmatrix} 8.5120 & 0.2139 \\ 0.2139 & 3.1937 \end{bmatrix}$.The obtained value of the controller gain (K) is shown in the tabulation. The residuals of the observer which is the difference between the output y (t) of the plant and the output $\hat{y}(t)$ of the observer tend to zero in finite time. The Fig.5 shows that the residuals of the observer tend to zero in a finite time. The measured state which is the concentration (mol/m^3) is also estimated as we are invloved in designing if full order observers. The Fig.6, 7 shows the convergence of the estimated states (x_1, x_2) to the plant's real states. Table 4 shows the values of estimation error at different time.

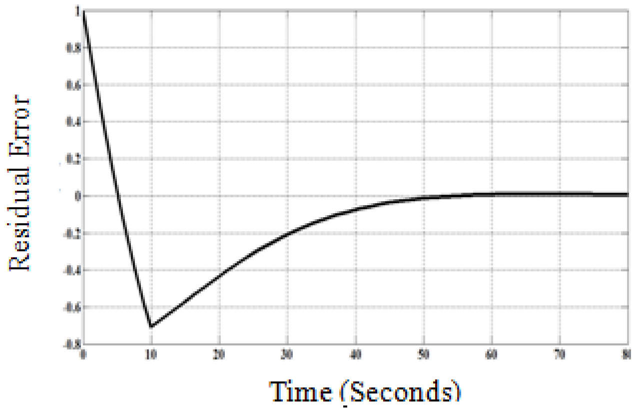

Fig.4. Residual of LQR based Kalman Observer

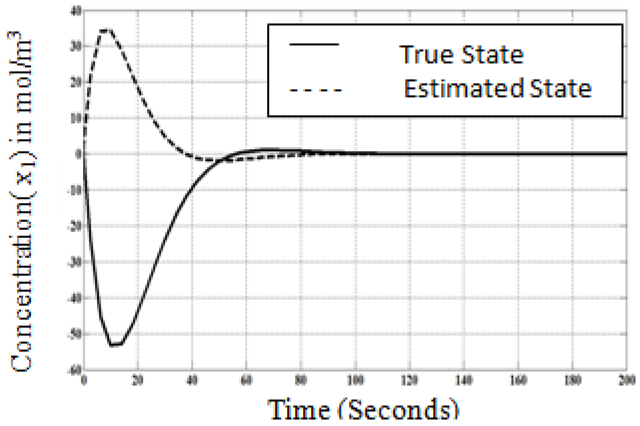

Fig.5. Convergence of Concentration (x_1) in mol/m^3 of LQR based Kalman Observer

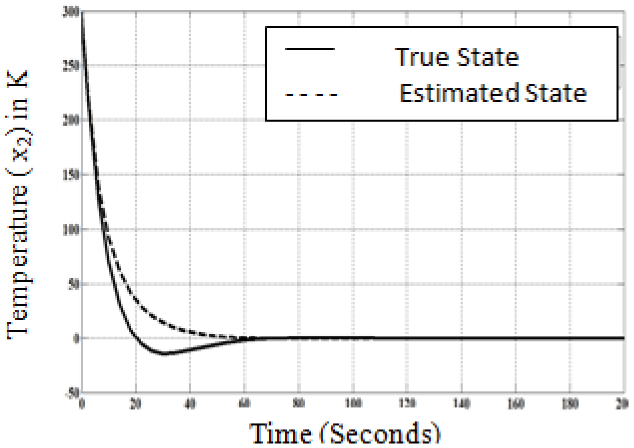

Fig.6. Convergence of Temperature (x_2) in Kelvin (K) of LQR based Kalman Observer

Table 4: Estimation Error and Gain calculation for LQR based Kalman Observer

Time (Seconds)	Estimation Error in states		Controller Gain $[K_1\ K_2]$
	x_1-$\hat{x}_1$ Concentration (mol/m^3)	x_2-$\hat{x}_2$ Temperature (K)	
10	0.6773	0.8931	[0.3251 -0.3008]
20	0.1741	0.2483	
30	0.0802	0.0017	
40	0.0172	0.0027	

5.2.2 Kalman Observer based State Feedback Controller

For the design of the State feedback control law the location of the desired poles is required. Here μ_1=-0.0903, μ_2=-0.1476. Once the locations of the desired poles are known the controller gain can be calculated. The Fig.8 shows that the residuals of the observer tend to zero in a finite time. The measured state which is the concentration (mol/m^3) is also estimated as we are invloved in designing if full order observers. The Fig.9, 10 shows the convergence of the estimated states (x_1, x_2) to the plant's real states. Table 5 shows the values of estimation error at different time.

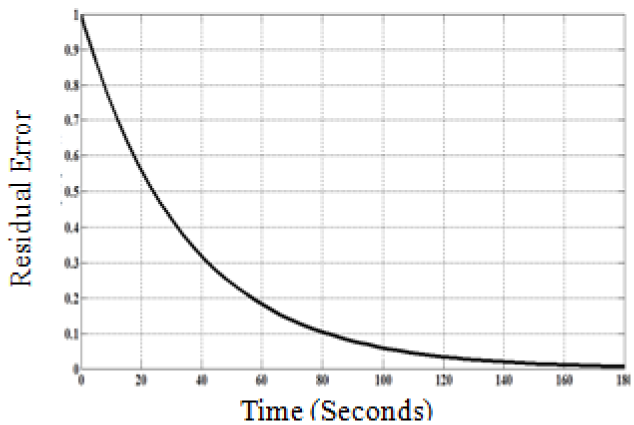

Fig.8. Residual of state feedback based Kalman Observer

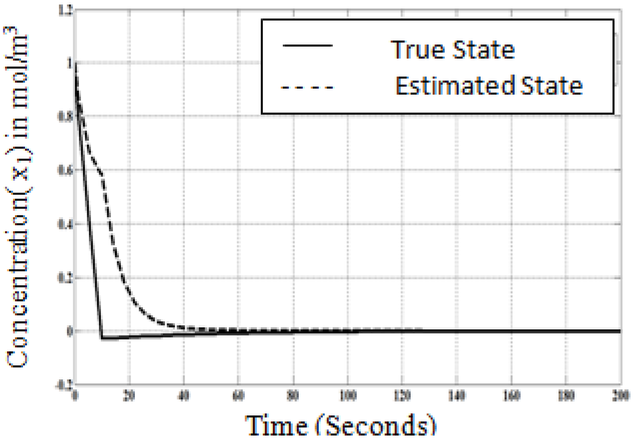

Fig.9. Convergence of Concentration (x_1) in mol/m^3 of State feedback based Kalman Observer

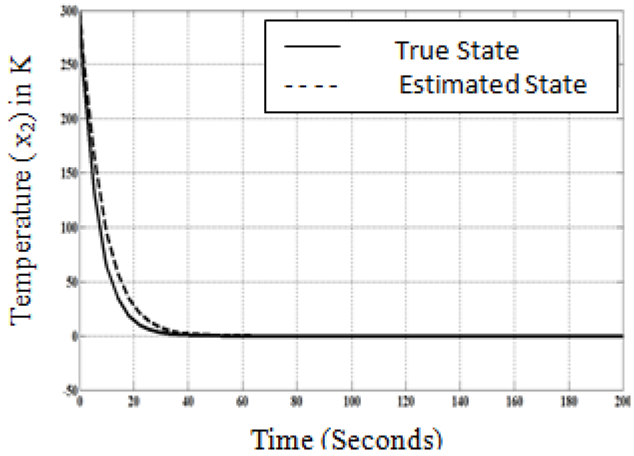

Fig.10. Convergence of Temperature (x_2) in Kelvin (K) of State feedback based Kalman Observer

Table 5: Estimation Error calculation for state feedback based Kalman Observer

Time (Seconds)	Estimation Error in states		Controller Gain [K_1 K_2]
	x_1 - $\hat{x}_1$ Concentration(mol/m^3)	x_2 - $\hat{x}_2$ Temperature (K)	
10	0.3820	0.9704	[0.4212 0.1936]
20	0.3452	0.3963	
30	0.0215	0.2610	
40	0.0020	0.3434	

5.3. Sliding Mode Observer

To design a SMO the change of coordinates x →T_c x has to be calculated $T_c = \begin{bmatrix} N_c^T \\ C \end{bmatrix}$ $N_c = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $T_c = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. The change of coordinates leads to $X = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} C_a \\ T \end{bmatrix}$. As υ = M sign ($\hat{y} - y$), the value of M is 0.1.

The canonical form of the nominal system is

$$\dot{\hat{x}}_1 = -0.0285\,\hat{x}_1 - 0.0014\,\hat{y} - 0.0850\,u - 0.069 \times 0.1 \times \text{sign}(\hat{y} - y)$$

$$\dot{\hat{y}} = -0.0371\,\hat{x}_1 - 0.1472\,\hat{y} + 0.0802\,u - 0.1 \times \text{sign}(\hat{y} - y)$$

The observer gain L= -0.069.

5.3.1. Sliding Mode Observer based Optimal Controller

The Optimal controller design requires information about the solution to the Algebraic Ricatti Equation (ARE) $PA^T + PA - PR^{-1}B^T P + Q = 0$. The value of $Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ $R = [1]$ and the solution to the ARE is $P = \begin{bmatrix} 8.5122 & 0.2149 \\ 0.2149 & 3.2015 \end{bmatrix}$.The obtained value of the controller gain (K) is shown in the tabulation. The residuals of the observer which is the difference between the output y (t) of the plant and the output $\hat{y}(t)$ of the observer tend to zero in finite time. The Fig.11 shows that the residuals of the observer tend to zero in a finite time. The measured state which is the concentration (mol/m^3) is also estimated as we are invloved in designing if full order observers. The Fig.12, 13 shows the convergence of the estimated states (x_1, x_2) to the plant's real states. Table 6 shows the values of estimation error at different time.

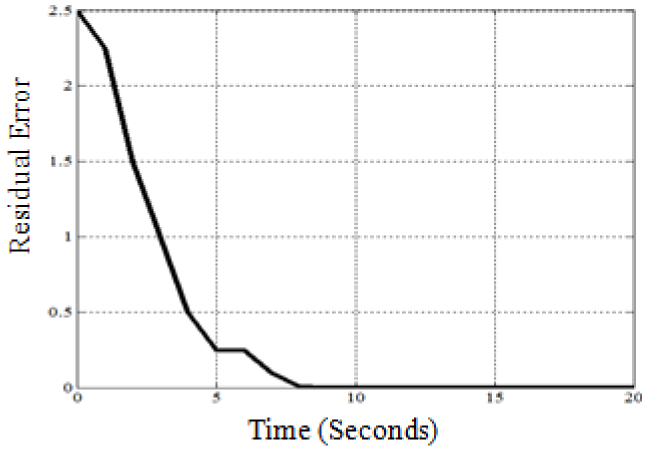

Fig.11. Residual of LQR based Sliding Mode Observer

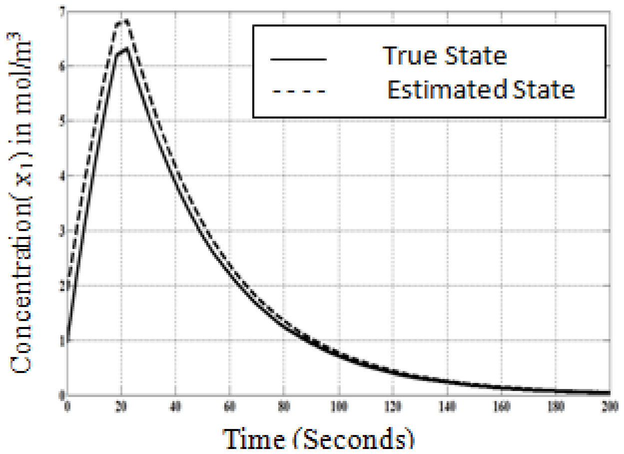

Fig.12.Convergence of Concentration (x_1) in mol/m^{3}of LQR based sliding mode observer

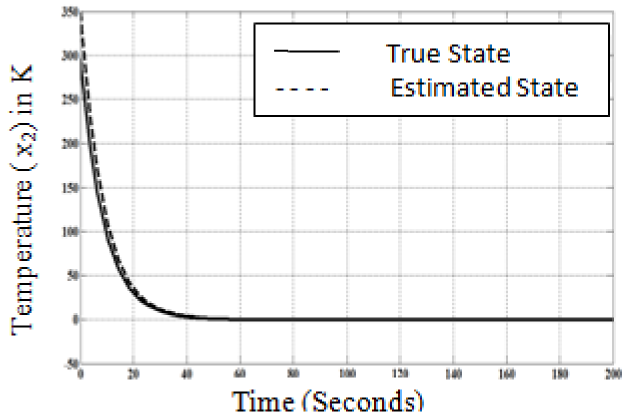

Fig.13. Convergence of Temperature (x_2) in Kelvin (K) of LQR based sliding mode observer

Table.6. Estimation Error calculation using LQR based sliding mode observer

Time (Seconds)	Estimation Error in states		Controller Gain $[K_1\ K_2]$
	x_1-$\hat{x}_1$ Concentration(mol/m^3)	x_2-$\hat{x}_2$ Temperature (K)	
10	0.0455	0.412	[-0.7064 0.2379]
20	0.0124	0.3065	
30	0.0034	0.2283	
40	0.0009	0.1704	

5.3.2 Sliding Mode Observer based State Feedback Controller

For the design of the State feedback control law the location of the desired poles is required. Here μ_1=-0.0281, μ_2=-0.1476. Once the locations of the desired poles are known the controller gain can be calculated. The Fig.14 shows that the residuals of the observer tend to zero in a finite time. The measured state which is the concentration (mol/m^3) is also estimated as we are invloved in designing if full order observers. The Fig.15, 16 shows the convergence of the estimated states (x_1, x_2) to the plant's real states. Table 7 shows the values of estimation error at different time.

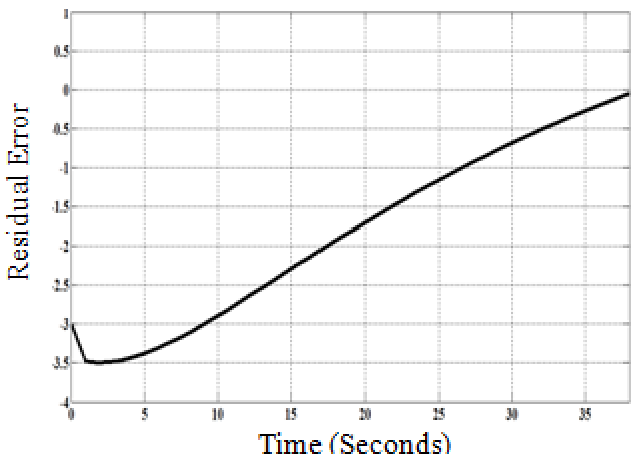

Fig.14. Residual of State feedback based Sliding Mode Observer

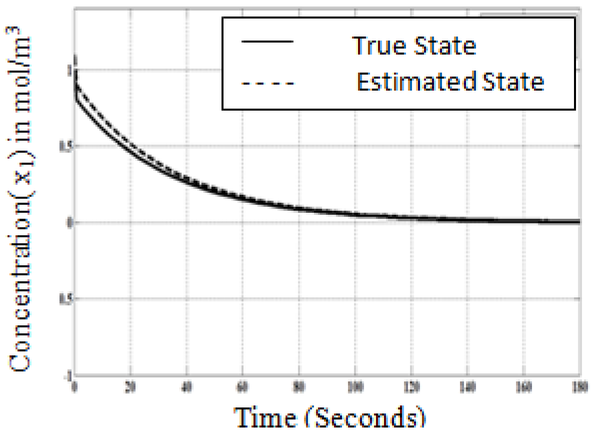

Fig.15. Convergence of Concentration (x_1) in mol/m^{3}of state feedback based sliding mode observer

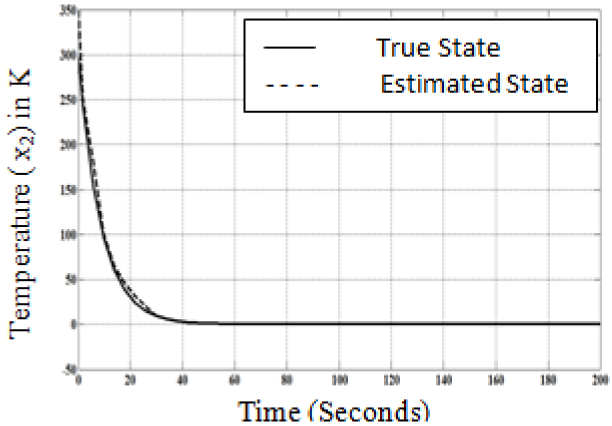

Fig.16. Convergence of Temperature (x_2) in Kelvin (K) of state feedback based sliding mode observer

Table.7. Estimation Error calculation for state feedback based sliding mode observer

Time (Seconds)	Estimation Error in states		Controller Gain $[K_1\ K_2]$
	$x_1 - \hat{x}_1$ Concentration(mol/m^3)	$x_2 - \hat{x}_2$ Temperature (K)	
10	0.0676	0.4548	[0.3251 -0.3008]
20	0.0182	0.3351	
30	0.0050	0.2493	
40	0.0014	0.1860	

In order to ensure the robustness of the Sliding Mode Observers the disturbance rejection and the tracking performance of the observers were calculated in terms of the steady state error and tabulated.

Table.8. Comparison of the Disturbance rejection and Tracking performance of the Observer Based Controllers in terms of Steady State Error

Observer/ Controller	Luenberger Observer		Kalman Observer		SMO	
	Tracking	Disturbance Rejection	Tracking	Disturbance Rejection	Tracking	Disturbance Rejection
State feedback	0.1779	0.1107	-0.85903	-0.85549	0.0046	0.0230
Optimal	0.0175	0.0585	0.0081	0.0082	0.2193×10^{-5}	2.8696×10^{-6}

6. Conclusion

The estimation error calculations from the simulations confirm that the Sliding Mode Observers had minimum deviation between the true state and the estimated states. The sliding observer tracked the true states when both the state feedback and optimal control laws were used. The Luenberger Observer had the advantage of its simple structure and design and the Kalman Observer had the advantage of including the process noise and measurement noise into the system. The observer gains and the controller gains which are important for the design for observers are tabulated. The observers are also being compared in terms of its disturbance rejection and tracking performances which ensure the robustness of the sliding mode observers due to the reduced values of the steady state error comparing to Luenberger and Kalman Observers which is shown in Table 8.

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