I J C T A, 7(2) December 2014, pp. 155-164

State Estimation Using Kalman Filtering Approach Case Study: Nonlinear Process Control Reactor – CSTR

M. Shyamalagowri[*] and R. Rajeswari[**]

ABSTRACT

This paper presents the State Estimation problem using Kalman filtering approach for Nonlinear Process Control Reactor (Continuous Stirred Tank Reactor) to simulate the circumstances of real case studies. The well-known conventional Kalman filters give the optimal solution but require synchronous measurements, an accurate system model and exact stochastical noise characteristics. The conventional estimation algorithm with incomplete information may be degraded or even diverged. In order to reduce the effect of noise variance uncertainty, adaptive fading Kalman filter is proposed to overcome this drawback. On the other hand, received data to estimation nodes from multi-sensors have different communication delays and various sampling rates. In this paper, conventional Kalman filter has been implemented in a way to be workable for state estimation in plants with different communication delays in their sensors. The estimation, prediction and error correction algorithm has been used to estimate states in presence nonlinearities and process variances. The feasibility and effectiveness of the presented methods are demonstrated through simulation studies on a continuous stirred tank reactor (CSTR) benchmark problem.

Keywords: State Estimation, Kalman Filter, Nonlinearity, Continuous Stirred Tank Reactor, Prediction.

INTRODUCTION

For a particular industrial process application, there might be plenty of associated process variance and nonlinear measurements located at different operational levels and having various accuracy and reliability specifications[1]. One of the key issues in developing a nonlinear system is the question of how can design the fused or combined to overcome uncertainty associated with individual data sources and obtain an accurate joint estimate of the system state vector. There exist various approaches to resolve this nonlinear problem, of which the KF or its information form is one of the most significant and applicable candidate solutions [2]. In nonlinear systems, the Kalman filtering approach use the first order Taylor series to transform nonlinear system to linear system, and it is a used widely in nonlinear system. The KF approximates the probability density resulting from the non-linear transformation of a random variable instead of approximating the nonlinear functions with a Taylor series expansion[3]. The classical Kalman filter is a centralized fusion filter that assumes all observation coming synchronously to a control computing facility. This approach is usually related to solving a partial differential equation and boundary condition equations which do not have an explicit solution in general[4]. For the case of discrete-time systems, the problem has been investigated via system augmentation and standard Kalman filtering [5]. The main idea of this methodology is to recalculate Kalman filter in the delay time period [6]. Simulation results depict the efficiency of the Kalman filter approach for state estimation purpose. Basically, the conventional Kalman filter methodology hinge on prior knowledge about statistical characteristics of measurement and process noises. But when these are unknown, using adaptive Kalman filter strategy is imperative for state estimation purpose. In order to reduce the effect of prior measurement, fading memory algorithm has been applied in this work.

[*] Associate Professor / EEE, Erode Sengunthar Engineering College, Thudupathi, Erode, *E-mail: mshyamalagowri2011@gmail.com*

[**] Professor / EEE, Government College of Technology, Coimbatore, *E-mail: rree@gct.ac.in*

This paper is organized as follows: Section1 explains the CSTR description, Section 2 derives state estimation procedure on the basis of KF, Section 3 shows how the KF algorithm can be used to estimate the various states of the nonlinear process control reactor CSTR, Section 4, CSTR industrial plant will be simulated. Simulation results are presented in section 5. Finally, section 6 summarizes the main conclusions.

CSTR SYSTEM DESCRIPTION

The Continuous stirred Tank Reactor (CSTR) having a wide application in process control industries. The detailed diagram of CSTR is presented in the Fig. 1.

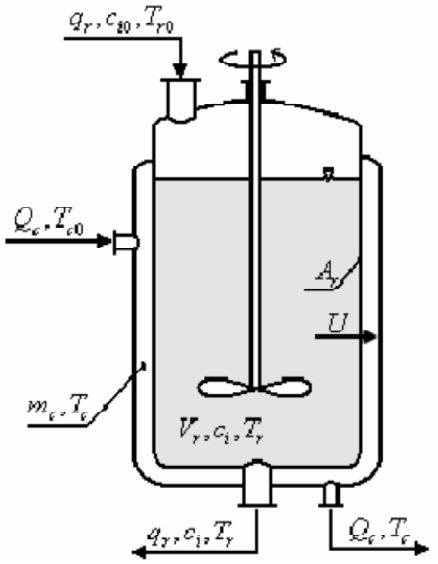

Figure 1: Schematic Diagram of the CSTR

In order to reduce the heat created in the CSTR, a cooling jacket has been used which will be carrying out the Vander Vusse reaction scheme described by the following reactions:

$$A \xrightarrow{K_1} B \xrightarrow{k_2} C \tag{1}$$

$$2A \xrightarrow{K_3} D \tag{2}$$

Here B is the required product,

C and D are the undesired byproducts

k_1, k_2 and k_3 are considered as the reaction rate constants.

In this reactor, a product A is to be transformed to the desired product B by an exothermic reaction in CSTR, but the product B is again degraded to product C. In addition to this successive reaction, a high order parallel reaction occurs and A is converted to by product D. The mathematical modeling of this non linear process control reactor is explained as the four set of Ordinary Differential Equations (ODE) is derived from material and heat balances inside the reactor.

$$\frac{dC_A}{dt} = \frac{q_r}{V_r}(C_{A0} - C_A) - k_1 C_A - k_3 C_A^2 \tag{3}$$

$$\frac{dC_B}{dt} = -\frac{q_r}{V_r} C_B + k_1 C_A - k_2 C_B \tag{4}$$

$$\frac{dT_r}{dt} = \frac{q_r}{V_r}(T_{r0} - T_r) - \frac{h_r}{\rho_r c_{pr}} + \frac{A_r U}{V_r \rho_r c_{pr}}(T_c - T_r) \tag{5}$$

$$\frac{dT_r}{dt} = \frac{1}{m_c c_{pc}}(Q_c + A_r U(T_r - T_c)) \tag{6}$$

Where $C_A \geq 0$, $C_B \geq 0$

In the differential equations, t denotes time, c denotes concentrations, T denotes temperatures, c_p represents the specific heat capacities, q represents the volumetric flow rate, Q_c represents the heat removal, V represents the volumes, ρ represents the densities, A_r is the heat exchange surface and U represents the heat transfer coefficient. Indexes $(.)_A$ and $(.)_B$ represents the compounds A and B, $(.)_r$ given for the reactant mixture, $(.)_c$ denotes the cooling liquid and $(.)_0$ denotes the feed (inlet) values. The mathematical modeling of the nonlinear process control reactor has been derives by considering the four states namely concentrations of the product A (C_A) and the concentration of the product B (C_B), temperature of the reactor T and the temperature of the coolant T_c.

The model of the reactor describes the nonlinear process control reactor. Nonlinearity calculated in reaction rates (k_j) which are described via Arrhenius law:

$$k_j(T_r) = k_{0j}.\exp\left(\frac{-E_i}{kT_r}\right), \; for \;\; j = 1,2,3 \tag{7}$$

Where k_0 denotes the pre-exponential factors and E denotes the activation energies.

The reaction heat (h_r) in the equation (2) is expressed as:

$$h_r = h_1 k_1 c_A + h_2 k_2 C_B + h_3 k_3 c_A^2 \tag{8}$$

Where h_j means reaction enthalpies.

Table 1
Parameters of the Reactor

$k_{01} = 2.145 \cdot 10^{10}$ min^{-1}	$k_{02} = 2.145 \cdot 10^{10}$ min^{-1}	$k_{03} = 1.5072 \cdot 10^{8}$ min^{-1}mol^{-1}
$E_1/R = 9758.3$ K	$E_2/R = 9758.3$ K	$E_3/R = 8560$ K
$h_1 = -4200$ kJ.kmol^{-1}	$h_2 = 11000$ kJ.kmol^{-1}	$h_3 = 41850$ kJ.kmol^{-1}
$V_r = 0.01$ m^3	$\rho_r = 934.2$ kg.m^{-3}	$c_{pr} = 3.01$ kJ.kg^{-1}.K^{-1}
$U = 67.2$ kJ.min^{-1}m^{-2}K^{-1}	$c_{pc} = 2.0$ kJ.kg^{-1}.K^{-1}	$A_r = 0.215$ m^2
$c_{A0} = 5.1$ kmol.m^{-3}	$T_{r0} = 387.05$ K	$U = 67.2$ kJ.min^{-1}m^{-2}K^{-1}
$m_c = 5$ kg	$c_{B0} = 0$ kmol.m^{-3}	

This reaction describes the nonlinear chemical reaction, under ultimate environment, of an inflow of substance A to a product B. a heat exchanger with coolant flow has been used for controlling the heat created inside the reactor due to chemical reaction. The various parameters of the reactor are given in the table 1. In order to make easier the problem, some of the assumptions have been considered:

- The mixing of the liquid has been carried out ideally.
- The density and the physical properties are assumed to be constant.
- The tank liquid level h is assumed as constant and water flows in the input and output are considered as equal: $Q1 = Q2$.

- The first order reaction with a temperature relation was carried out based on the Arrhenius law.
- The work in the shaft was neglected.
- The temperature increase in the coolant on the coil was neglected.

In the CSTR, it is considered that the reaction has been carried out in the two chemicals to produce a product compound A with the concentration $C_A(t)$, with the reactor temperature T(t). The heat created by the exothermic reaction slows down the reaction. A coolant is used with coolant flow-rate $Q_c(t)$, the temperature is to be reduced which will control the concentration of the product. C_A denotes the concentration of the inlet feed, Q denotes the process flow-rate, T represented the temperature of the inlet feed and T_C denotes the temperature of the coolant, all of which are understood as constant at nominal values.

KALMAN FILTER

The Kalman filter, also known as linear quadratic estimation (LQE), is an algorithm that uses a series of measurements observed over time, containing noise (random variations) and other inaccuracies, and produces estimates of unknown variables that tend to be more precise than those based on a single measurement alone. More formally, the Kalman filter operates recursively on streams of noisy input data to produce a statistically optimal estimate of the underlying system state. The filter is named for Rudolf (Rudy) E. Kalman, one of the primary developers of its theory.

The Kalman filter has numerous applications in technology. A common application is for guidance, navigation and control of vehicles, particularly aircraft and spacecraft. Furthermore, the Kalman filter is a widely applied concept in time series analysis used in fields such as signal processing and econometrics.

The algorithm works in a two-step process. In the prediction step, the Kalman filter produces estimates of the current state variables, along with their uncertainties. Once the outcome of the next measurement (necessarily corrupted with some amount of error, including random noise) is observed, these estimates are updated using a weighted average, with more weight being given to estimates with higher certainty. Because of the algorithm's recursive nature, it can run in real time using only the present input measurements and the previously calculated state and its uncertainty matrix; no additional past information is required.

It is a common misconception that the Kalman filter assumes that all error terms and measurements are Gaussian distributed. Kalman's original paper derived the filter using orthogonal projection theory to show that the covariance is minimized, and this result does not require any assumption, e.g., that the errors are Gaussian.

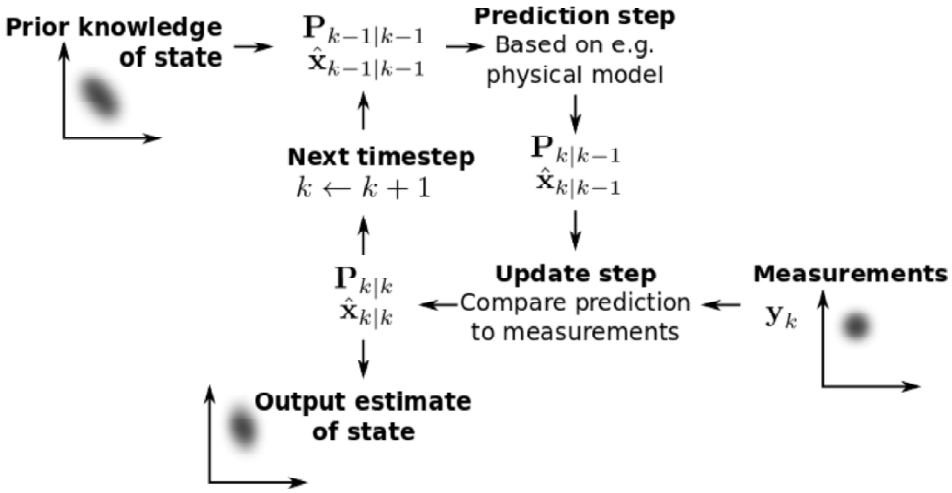

Figure 2: Kalman Filtering Approach

The Kalman filter is a recursive estimator. The step by step procedure of the Kalman filtering approach is given in the figure 2. This means that only the estimated state from the previous time step and the current measurement are needed to compute the estimate for the current state. In contrast to batch estimation techniques, no history of observations and/or estimates is required. In what follows, the notation $\hat{\mathbf{X}}_{n|m}$ represents the estimate of **X**at time *n* given observations up to, and including at time *m*. The Kalman filtering steps for state estimation is illustrated in the figure 3.

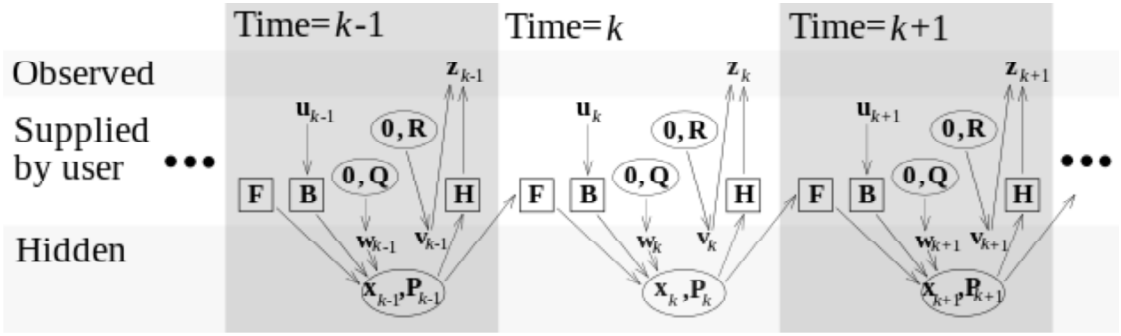

Figure 3: Kalman Filtering Steps for State Estimation

The state of the filter is represented by two variables:

- $\hat{\mathbf{X}}_{k|k}$, the *a posteriori* state estimate at time *k* given observations up to and including at time *k*;
- $\mathbf{P}_{k|k}$, the *a posteriori* error covariance matrix (a measure of the estimated accuracy of the state estimate).

The Kalman filter can be written as a single equation; however it is most often conceptualized as two distinct phases: “Predict” and “Update”. The predict phase uses the state estimate from the previous time step to produce an estimate of the state at the current time step. This predicted state estimate is also known as the a priori state estimate because, although it is an estimate of the state at the current time step, it does not include observation information from the current time step. In the update phase, the current a priori prediction is combined with current observation information to refine the state estimate. This improved estimate is termed the a posteriori state estimate.

Typically, the two phases alternate, with the prediction advancing the state until the next scheduled observation, and the update incorporating the observation. However, this is not necessary; if an observation is unavailable for some reason, the update may be skipped and multiple prediction steps performed. Likewise, if multiple independent observations are available at the same time, multiple update steps may be performed (typically with different observation matrices $\mathbf{H}_k$).

Predict

Predicted (*a priori*) state estimate

$$\hat{\mathbf{X}}_{k|k-1} = \mathbf{F}_k \hat{\mathbf{X}}_{k-1|k-1} + \mathbf{B}_k \mathbf{u}_k$$

Predicted (*a priori*) estimate covariance

$$\mathbf{P}_{k|k-1} = \mathbf{F}_k \mathbf{P}_{k-1|k-1} \mathbf{F}_k^T + \mathbf{Q}_k$$

Update

Innovation or measurement residual

$$\tilde{\mathbf{y}}_k = \mathbf{z}_k - \mathbf{H}_k \hat{\mathbf{X}}_{k|k-1}$$

Innovation (or residual) covariance

$$\mathbf{S}_k = \mathbf{H}_k \mathbf{P}_{k|k-1} \mathbf{H}_k^T + \mathbf{R}_k$$

Optimal Kalman gain

$$\mathbf{K}_k = \mathbf{P}_{k|k-1} \mathbf{H}_k^T \mathbf{S}_k^{-1}$$

Updated (*a posteriori*) state estimate

$$\hat{\mathbf{X}}_{k|k} = \hat{\mathbf{X}}_{k|k-1} + \mathbf{K}_h \tilde{\mathbf{y}}_k$$

Updated (*a posteriori*) estimate covariance

$$\mathbf{P}_{k|k} = (I - \mathbf{K}_k \mathbf{H}_k) \mathbf{P}_{k|k-1}$$

The formula for the updated estimate and covariance above is only valid for the optimal Kalman gain. Usage of other gain values requires a more complex formula found in the *derivations* section.

Invariants

If the model is accurate, and the values for $\hat{\mathbf{X}}_{0|0}$ and $\mathbf{P}_{0|0}$ accurately reflect the distribution of the initial state values, then the following invariants are preserved: (all estimates have a mean error of zero)

- $\mathbf{E}[\mathbf{x}_k - \hat{\mathbf{x}}_{k|k}] = \mathbf{E}[\mathbf{x}_k - \hat{\mathbf{x}}_{k|k-1}] = 0$
- $\mathbf{E}[\tilde{\mathbf{y}}_k] = 0$

where $\mathbf{E}[\xi]$ is the expected value of ξ, and covariance matrices accurately reflect the covariance of estimates

- $\mathbf{P}_{k|k} = \mathrm{cov}(\mathbf{x}_k - \hat{\mathbf{x}}_{k|k})$
- $\mathbf{P}_{k|k-1} = \mathrm{cov}(\mathbf{x}_k - \hat{\mathbf{x}}_{k|k-1})$
- $\mathbf{S}_k = \mathrm{cov}(\tilde{\mathbf{y}}_k)$

Estimation of the Noise Covariance's $\mathbf{Q}_k$ and $\mathbf{R}_k$

Practical implementation of the Kalman Filter is often difficult due to the inability in getting a good estimate of the noise covariance matrices Q_k and R_k. Extensive research has been done in this field to estimate these covariance's from data. One of the more promising approaches to do this is the Auto covariance Least-Squares (ALS) technique that uses auto covariances of routine operating data to estimate the covariances. The GNU Octave code used to calculate the noise covariance matrices using the ALS technique is available online under the GNU General Public License license.

KALMAN FILTER DESIGN

In this paper the ability of the Kalman filtering is explained as both a steady state filter and a time varying filter.

Let us assume

$x(n + 1) = Ax(n) + Bu(n)$

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

design a Kalman filter to estimate the output y based on the noisy measurements $yv[n] = C\,x[n] + v[n]$

Steady-State Kalman Filter Design

The function KALMAN to design a steady-state Kalman filter. This function determines the optimal steady-state filter gain M based on the process noise covariance Q and the sensor noise covariance R.

First specify the plant + noise model. Set the sample time to –1 to mark the plant as discrete.

Design the steady-state Kalman filter with the equations

Time update:

$x[n + 1|n] = Ax[n|n–1] + Bu[n]$

Measurement update:

$x[n|n] = x[n|n–1] + M\,(yv[n] – Cx[n|n–1])$

where M = optimal innovation gain

The working of the Kalman filter is as follows and the block diagram of Kalman filtering is given in the figure 4, which generate some data and compare the filtered response with the true plant response:

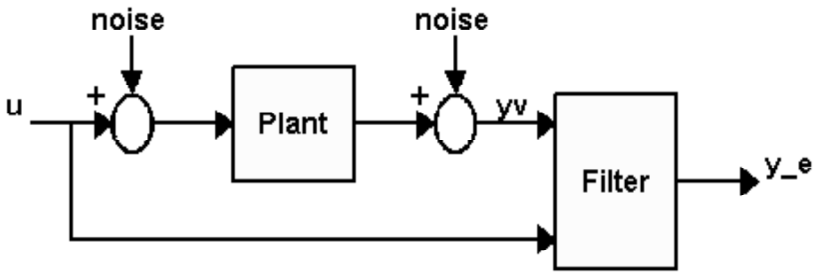

Figure 4: Block Diagram of Kalman Filtering

Next, connect the plant model and the Kalman filter in parallel by specifying u as a shared input:

Finally, connect the plant output *yv* to the filter input *yv*. The resulting simulation model has *w*, *v*, *u* as inputs and *y*, *y_e* as outputs. The Kalman filter reduces the error *y–yv* due to measurement noise. To confirm this, compare the error covariances, Covariance of error before filtering (measurement error), Covariance of error after filtering (estimation error).

Time-Varying Kalman Filter Design

A time-varying Kalman filter can perform well even when the noise covariance is not stationary. The time varying Kalman filter has the following update equations.

Time update:

$x[n+1|n] = Ax[n|n] + Bu[n]$

$P[n+1|n] = AP[n|n]A' + B*Q*B'$

Measurement update:

$x[n|n] = x[n|n–1] + M[n](yv[n]–Cx[n|n–1]) –1$

$M[n] = P[n|n–1]\ C'\ (CP[n|n–1]C'+ R)$

$P[n|n] = (I – M[n]C)\ P[n|n–1]$

The time varying filter also estimates the output covariance during the estimation. Plot the output covariance to see if the filter has reached steady state

SIMULATION RESULTS

The estimation of all two process variables of nonlinear process control reactor Continuous Stirred Tank Reactor was given in the Figure 5 and 6. In Figure 5, gives the estimation of Concentration in steady state analysis and the estimation of Concentration in time varying Kalman filter. The actual and estimated state simulation of process variables was compared which will shows the efficient tracking capability of the Kalman filter.

CONCLUSION

The ability to incorporate data from a large, possibly changing variety of sources and to accommodate sensing delays without derogating estimation is extremely valuable in systems. The inaccurate estimation of states in Kalman filter approach is due to a lack of solid consideration of existing model uncertainty and also a nonrealistic pre-assumption on noise distribution matrices has been alleviated by incorporation of an adaptive fading method into KF strategies. Moreover, the simulation results denote the improvement of nonlinear state estimation using KF that approximates the probability density from the non-linear

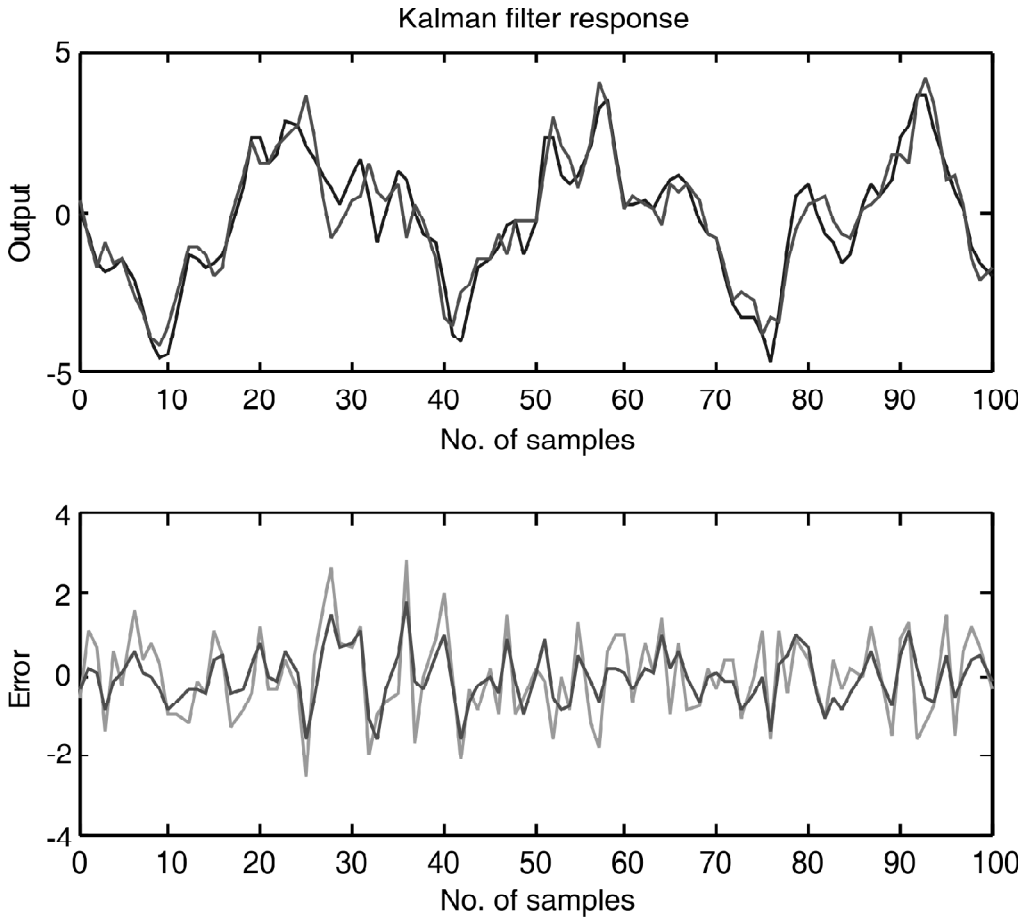

Figure 5: Steady state Kalman Filtering Approach for State Estimation of CSTR

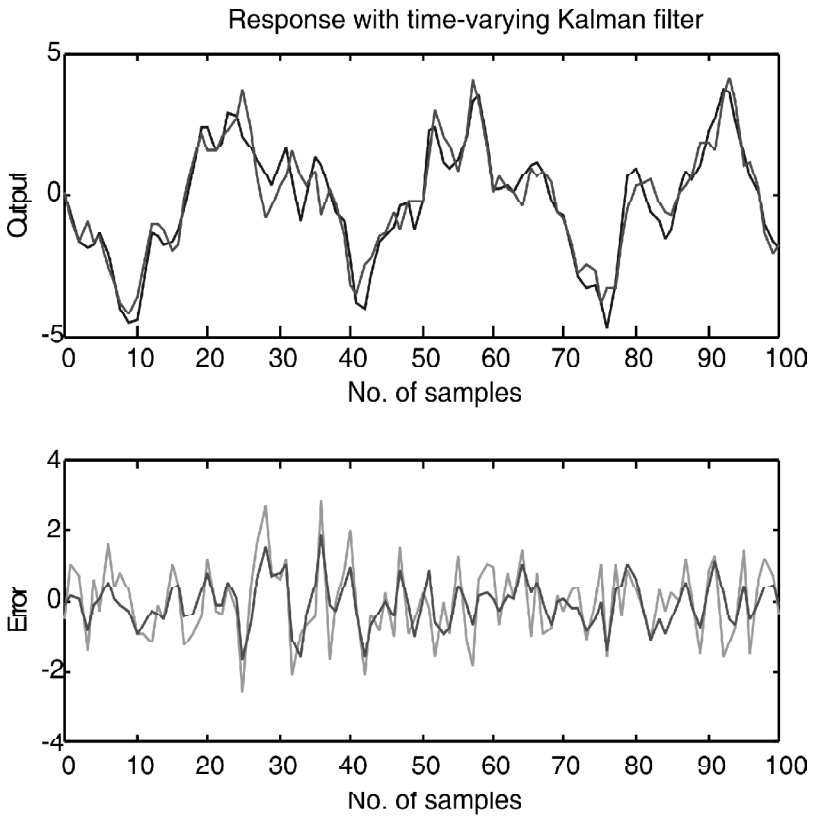

Figure 6: Time Varying Kalman Filtering Approach for State Estimation of CSTR

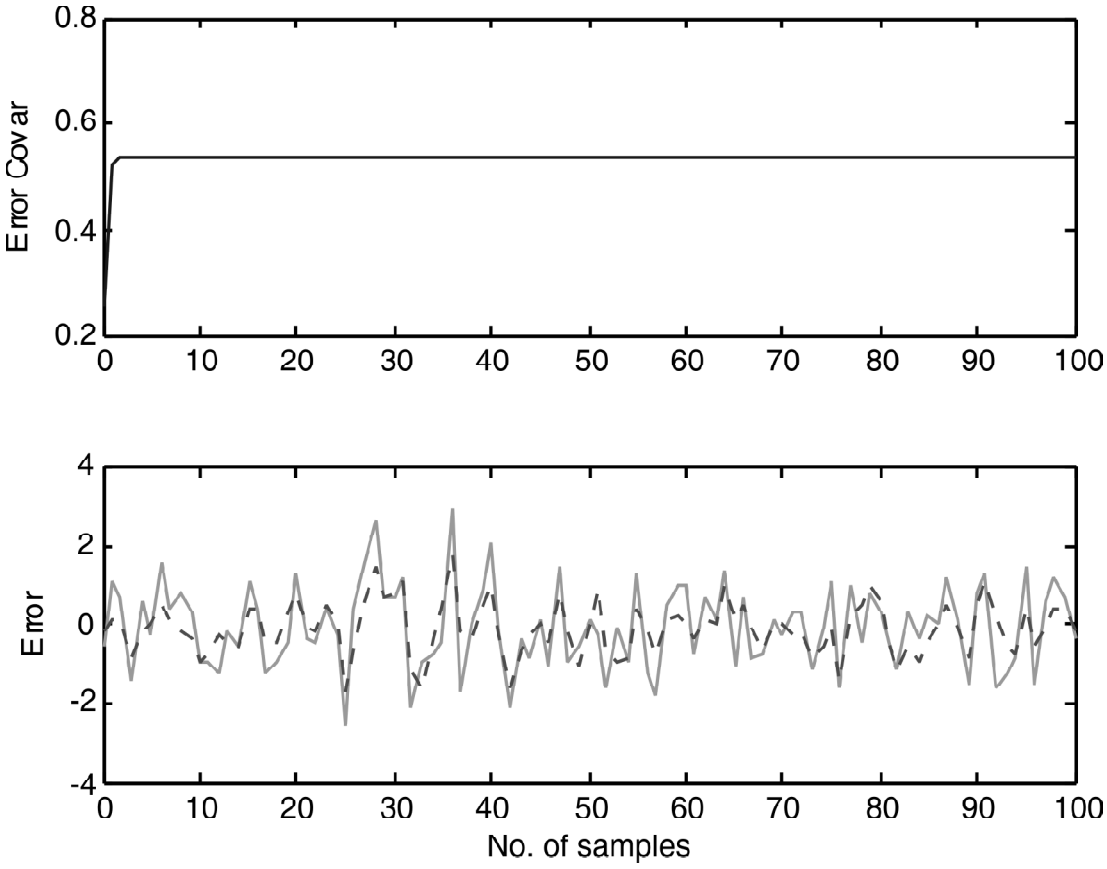

Figure 7: Simulation Result of Error Covariance and Error

transformation of a random variable, compared to other estimation method in which approximation is done employing Taylor series expansion. This paper presents the real-time implementation of a Kalman ûlter based estimator in order to overcome the simultaneous estimation problem of the variations in heat removal rate Q and volumetric flow rate q and all states required for the state and parameter estimation of the Continuous Stirred Tank Reactor. As it is well known, nonlinear behavior of the process control reactor, processing errors of data acquisition devices, modeling errors, parameter uncertainties, and noise adversely affects the performance of any estimation algorithm in real-time experiments. In this paper, the KF based estimation technique introduced to solve the simultaneous estimation problem of the uncertainties associated with the system and all states required for the nonlinearities in continuous Stirred Tank Reactor via measuring Concentration of A and B and to overcome the limited number of state and parameter estimations that would be possible with a single KF algorithm.

REFRENCES

[1] Balaji. V, Dr. N.Vasudevan, E. Maheswari, "MATLAB Simulation for continuous Stirred Tank Reactor", *The Pacific Journal of Science and Technology*, Vol. 9, No. 1, p. 127 – 136, May-June 2008.

[2] Julier. S. J and J. K. Uhlmann, "A New Extension of the Kalman Filter to Nonlinear Systems," in Proc. of AeroSense: The 11th Int. Symp. On Aerospace Defence Sensing, Simulation and Controls, 1997.

[3] Juraj Voros, Jan Mikles, Lubos Cirka, "Parameter Estimation of Nonlinear Systems", *Journal of Acta Chimica Slovaca*, Vol. 1, No. 1, p. 309 – 320, 2008.

[4] Mansouri, M, Nounou, H, Nounou, M., "State estimation of a chemical reactor process model - A comparative study", IEEE Transaction on Systems, Signals & Devices (SSD), E-ISBN : 978-1-4673-6458-4, p. 1 – 6, DOI : 10.1109/ SSD.2013.6563998, 2013.

[5] S. Popova, M. Ignatova, V. Lyubenova, "State and Parameter Estimation by Extended Kalman Filter for studying Inhomogeneous Dynamics in Industrial Bioreactor, *Journal of Recent Advances in Mechanical Engineering and Automatic Control*, ISBN: 978-1-61804-142-5, p.43-47, 2012.

[6] Speyer, J. L., "Computation and transmission requirements for a decentralized linear-quadratic-Gaussian problem," *IEEE 7Ians. Automatic Control*, Vol. AC-24, 1979.