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Nonlinear State Estimation Using Extended Kalman Filter Approach Case Study – Nonlinear Process Control Reactor (Continuous Stirred Tank Reactor)

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ABSTRACT

In the process industries one of the main goals is to make the end product at the lowest possible cost while satisfying product quality constraints. State estimation often plays an important role in accomplishing this goal in process control and performance monitoring applications. There are many uncertainties to deal with in process control; model uncertainties, measurement uncertainties and uncertainties in terms of different noise sources acting on the system. State estimation is a means to propagate the pdf of the system states over time in some optimal way. The Extended Kalman Filter (EKF) has become a standard technique used in a number of nonlinear estimation and machine learning applications. These include estimating the state of a nonlinear dynamic system, estimating parameters for nonlinear system identification (e.g., learning the weights of a neural network), and dual estimation (e.g., the Expectation Maximization (EM) algorithm) where both states and parameters are estimated simultaneously. In this kind of environment, representing the model state by an (approximated) probability distribution function (pdf) has distinct advantages. It is most common to use the Gaussian pdf to represent the model state, process and measurement noises. The Gaussian pdf can be characterized by its mean and covariance. The Extended Kalman Filter propagates the mean and covariance of the pdf of the model state in an optimal (minimum mean square error) way in case of linear dynamic systems. The efficiency of the proposed state estimation schemes using the Extended Kalman Filter is validated on benchmark problem a nonlinear process control reactor (Continuous Stirred Tank Reactor) involving constraints on estimated state variables.

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INTRODUCTION

Many various problems in science and especially many various control algorithms require determination of the states for studied or controlled system. In more realistic cases only the outputs of the plant (rather than the state vector) can be measured. In this case the state estimation process often plays an important role in the process control implementation and in the monitoring applications. In case of the industrial processes there are many disturbing factors which influence the process control such as model and measurement uncertainties. All practical systems possess some degree of nonlinearity. Depending on the type of process and the operating region of the process, some processes can be approximated with a linear model and the EKF can be used for state estimation. In some cases the linear approximation may not be accurate enough, and state estimator designs using nonlinear process models are necessary. The most

common way of applying the KF to a nonlinear system is in the form of the extended Kalman filter (EKF).

The Extended Kalman Filter (EKF) algorithm is the widely used method for solving nonlinear state estimation applications. In this paper the Gaussian probability distribution function is used to represent these uncertainties. The Extended Kalman filter (EKF) can be used only in case of linear dynamic systems and this algorithm propagates the mean and covariance of the probability distribution function of the model state in an optimal way. In the EKF, the pdf is propagated through a linear approximation of the system around the operating point at each time instant. In doing so, the EKF needs the Jacobian matrices which may be difficult to obtain for higher order systems, especially in the case of time-critical applications. Further, the linear approximation of the system at a given time instant may introduce errors in the state which may lead the state to diverge over time.

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Problem description:**Nonlinear process control reactor (continuous stirred tank reactor):**

CSTR is a vat or back mix reactor, common ideal reactor type in processing unit in chemical and polymer industry. In a CSTR one or more fluid reagents are introduced into a tank equipped with an impeller and the reactance are continuously added and withdrawn with the help of mechanical and hydraulic agitation to achieve uniform composition and temperature while the reactor effluent is removed. The impeller stirs the reagents to ensure proper mixing and to achieve the specific output. Proper knowledge of manipulating the equations for control of the CSTR is tantamount to the successful operation and production of desired products.

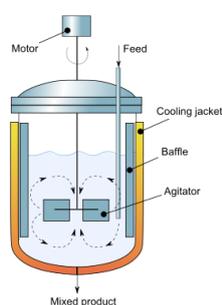


Fig. 1: Schematic Diagram of CSTR.

Because the compositions of mixtures leaving a CSTR are those within the reactor, the reaction driving forces usually the reactant concentrations are necessarily low. When high conversions of reactants are needed, several CSTRs in series can be used. Continuous Stirred Tank Reactors in series are simpler and easier to design for various temperature operations than are tubular reactors. Reactions with narrow operating temperature ranges or those requiring close control of reactant concentrations for optimal selectivity benefit from series arrangements. If severe heat transfer requirements are imposed, heating or cooling zones can be incorporated within or external to the CSTR. The impellers or centrally mounted draft tubes circulate liquid upward, and then download through vertical heat exchanger tubes. The heat transfer fluid is pumped through agitation nozzles that circulate the fluid through jacket at a high velocity. The coolant can be chilled water, ethylene glycol/water mixture or a proprietary mixture of hydrocarbons. Chemical kinetics and reactor design are at the heart of processing almost all industrial chemicals. The selection of a reaction system that operates in the safest and most efficient manner can be the key to the success or failure of a chemical plant.

Nonlinear Mathematical Modelling of Continuous Stirred Tank Reactor:

The process control industries require a nonlinear process control reactor (Continuous Stirred

Tank Reactor) as a main key constituent. The detailed diagram of CSTR is presented in the figure no.1. A cooling jacket provision has been arranged in CSTR to reduce the heat created due to thermal reaction in the system which will be carrying out the Vander Vusse reaction scheme described by the following reactions.

To ensure the successful operation of a continuous stirred tank reactor it is necessary to understand their dynamic characteristics. A good understanding will ultimately enable effective control design. To describe the dynamic behaviour of a CSTR mass, component and energy balance equations must be developed. This requires an understanding of the functional expressions that describe the chemical reaction.

Complicated mathematical models that have many considerations such as (i). A priori information (ii). Subjective information (iii). Complexity (iv). Training (v). Model evaluation (vi). Fit to empirical data (vii). Scope of the model (viii). Philosophical considerations



When the input A reacts and creates the desired product B by an exothermic reaction, but the B product is degraded to undesired product C and due to the successive high order parallel reaction A is converted into byproduct D.

The reaction rate constants are k_1 , k_2 and k_3 .

The modeling of nonlinear process control reactor is detailed as four set of Ordinary Differential Equations (ODE) which is derived from material and heat balances phenomenon inside the 4reactor.

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

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

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

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

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

In this differential equations,

t - time of operation in the reactor c - concentrations of the product in kmol m^{-3} T - temperatures in K c_p - specific heat capacities in $\text{kJ kg}^{-1} \text{K}^{-1}$ q - the volumetric flow rate Q_c - the heat removal rate V - the volume of the products in m^3

ρ - the densities in kg m^{-3} A_r - the heat exchange surface in m^2 U - the heat transfer coefficient in $\text{kJ min}^{-1} \text{m}^{-2} \text{K}^{-1}$.

The suffices $(.)_A$ and $(.)_B$ denotes the compounds A and B, $(.)_r$ given for the reactant mixture, $(.)_c$ denotes the cooling liquid and $(.)_0$ denotes the feed (inlet) values. The nonlinear modeling of the

Continuous Stirred tank Reactor is derived by taking the four parameters 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 as state variables.

CSTRs often have recirculation jacket fluid heat-transfer systems to improve the heat removal capability. For tighter control, and particularly for start-up and transition control, it is important to incorporate a split-range strategy; here, the jacket temperature controller output manipulates either a hot fluid valve or a cold fluid valve, depending on the range of the controller output. For most reactors it is desirable for the cold valve to fail open and the hot valve to fail closed.

The modelling is based on the rate of heat removal through a cooling coil or jacket as Q (J/s) and volumetric flow rate q. To develop a more realistic model of the system Q must be related to the flow rate through the coil or jacket. To develop the model a number of assumptions are made:

- The mixture density (ρ) and heat capacity (C_p) are assumed constant.
- Density and specific heat of the coolant are constant.
- Coolant dynamics are be ignored (they are assumed fast when compared to the temperature dynamics of the liquid in the CSTR).
- The area of the coil multiplied by the overall heat transfer coefficient is approximated as $A_c U = F_c^\beta \alpha$
Where α and β are appropriately defined constants
- The logarithmic mean temperature difference is approximately using an arithmetic mean.
- The reaction proceeds at the reaction rate associated with the final (output) concentration.
- The complex kinetics is not considered as single 1st order reaction as following, $-r_a = kC_A$

- The reacting mixture is assumed to be well mixed.
- The heat losses from the process to the atmosphere are negligible.
- The overall heat transfer coefficient is assumed constant.
- The liquid level in the reactor tank h is considered as constant and the flow of liquid into the tank Q1 and Q2 is assumed as equal
- The first order reaction with a temperature relation was carried out based on the Arrhenius law.
- The work in the shaft and the temperature increase in the coolant on the coil were neglected.

The values of the CSTR Parameters are given in the Table No 1. It is necessary to control the heat created in the reactor due to exothermic reaction which 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.

Arrhenius temperature dependence:

The effect of temperature on the reaction rate k is usually found to be exponential

$$k_j(T_r) = k_{0j} \cdot \exp\left(\frac{-E_j}{RT_r}\right), \text{ for } j = 1, 2, 3 \quad (7)$$

Where k_0 a pre exponential factor, E the activation energy, T is the reaction temperature and R the gas law constant.

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

$$h_r = h_1 k_1 c_A + h_2 k_2 c_B + h_3 k_3 c_A^2 \quad (8)$$

Where h_j means reaction enthalpies.

Table 1: Parameters of CSTR.

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

The Extended Kalman Filter deals with nonlinear process model and nonlinear observation

model. The nonlinear process model (from time k to time k+1) is described as

$$\mathbf{x}_{k+1} = \mathbf{f}(\mathbf{x}_k, \mathbf{u}_k) + \mathbf{w}_k \quad (9)$$

Extended Kalman Filter:

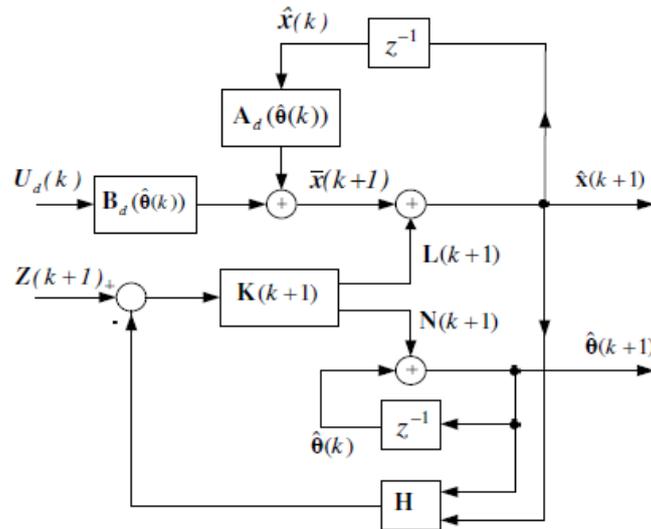


Fig. 2: Block Diagram of Extended Kalman Filter Design.

Where x_k, x_{k+1} are the system state vector at time $k, k+1$, f is the system transition function, u_k is the control, and w_k is the zero mean Gaussian process noise $w_k \sim N(0, Q)$ for state estimation problem, the true system state is not obtainable and requirements to be estimated. The initial state x_0 is assumed to follow a known Gaussian distribution $x_0 \sim N(\hat{x}_0, P_0)$.

The aim is to estimate the state at each time step of the process model and the observations.

The observation model at time $k+1$ is given by
$$z_{k+1} = h(x_{k+1}) + v_{k+1} \tag{10}$$

Here the observation function is denoted as h and v_{k+1} is the zero mean Gaussian Observation noise
$$v_{k+1} \sim N(0, R) \tag{11}$$

The knowledge on x_k at time k is
$$x_k \sim N(\hat{x}_k, P_k) \tag{12}$$

Then x_{k+1} at time $k+1$ follows
$$x_{k+1} \sim N(\hat{x}_{k+1}, P_{k+1}) \tag{13}$$

Where P_{k+1} can be computed by the following Extended Kalman Filter formula.

Predict using process model:
$$\hat{x}_{k+1} = f(\hat{x}_k, u_k) \tag{14}$$

$$\hat{P}_{k+1} = \nabla f_x P_k \nabla f_x^T + Q \tag{15}$$

where the Jacobian of function is denoted as ∇f_x , f with respect to x evaluated at x_k .

Update using observation:
$$\hat{x}_{k+1} = \hat{x}_{k+1} + K(z_{k+1} - h(\hat{x}_{k+1})) \tag{16}$$

$$P_{k+1} = \hat{P}_{k+1} - KSK^T \tag{17}$$

Where S is the innovation covariance (here $z_{k+1} - h(\hat{x}_{k+1})$ is called innovation) and the Kalman gain K is derived as

$$S = \nabla h \hat{P}_{k+1} \nabla h^T + R \tag{18}$$

$$K = \hat{P}_{k+1} \nabla h^T S^{-1} \tag{19}$$

Here the Jacobian of function is denoted as ∇h , h evaluated at x_{k+1} .

Linearization of Process model:

The Extended Kalman filter is designed to solve the estimation of nonlinear process model. The linearization of the process model is carried out at the current estimate x_k using the first order Taylor series expansion,

$$x_{k+1} \approx f(\hat{x}_k, u_k) + \nabla f_x (x_k - \hat{x}_k) + w_k \tag{20}$$

The Jacobian of function is denoted as ∇f_x , f with respect to x evaluated at \hat{x}_k . In this equation, all the higher order terms are ignored since the x_k is close \hat{x}_k .

The linear process model
$$x_{k+1} \approx F x_k + U_k + w_k \tag{21}$$

with $F = \nabla f_x$ and
$$U_k = f(\hat{x}_k, u_k) - \nabla f_x \hat{x}_k \tag{22}$$

Deriving the EKF prediction formula

Now applying the linear EKF prediction formulae using a linear process model,
$$\hat{x}_{k+1} \approx F \hat{x}_k + U_k = \nabla f_x \hat{x}_k + f(\hat{x}_k, u_k) - \nabla f_x \hat{x}_k = f(\hat{x}_k, u_k) \tag{23}$$

$$\hat{P}_{k+1} = F P_k F^T + Q = \nabla f_x P_k \nabla f_x^T + Q \tag{24}$$

EKF Update:

The EKF update formula can be attained by linearizing the observation model and applying the KF update formula

Linearization of observation model:

The current estimate of the state after the prediction step is $\hat{\mathbf{x}}_{k+1}$. The linearized observation model at the current estimate $\hat{\mathbf{x}}_{k+1}$ using first order Taylor series expansion.

$$\mathbf{z}_{k+1} \approx \mathbf{h}(\hat{\mathbf{x}}_{k+1}) + \nabla \mathbf{h}(\mathbf{x}_{k+1} - \hat{\mathbf{x}}_{k+1}) + \mathbf{v}_{k+1} \quad (25)$$

The Jacobian of function is denoted as $\nabla \mathbf{h}$, \mathbf{h} is evaluated at $\hat{\mathbf{x}}_{k+1}$. The higher order terms are ignored since the \mathbf{x}_{k+1} is close to $\hat{\mathbf{x}}_{k+1}$.

The linear observation model

$$\mathbf{Z}_{k+1} \approx \mathbf{H}\mathbf{x}_{k+1} + \mathbf{v}_{k+1} \quad (26)$$

where $\mathbf{H} = \nabla \mathbf{h}$ and $\mathbf{Z}_{k+1} = \mathbf{z}_{k+1} - \mathbf{h}(\hat{\mathbf{x}}_{k+1}) + \nabla \mathbf{h}\hat{\mathbf{x}}_{k+1}$ (27)

Deriving the EKF update formula:

Now concerning the linear KF update formula using the linear observation model

$$\hat{\mathbf{x}}_{k+1} = \hat{\mathbf{x}}_{k+1} + \mathbf{K}(\mathbf{z}_{k+1} - \mathbf{H}\hat{\mathbf{x}}_{k+1}) \quad (28)$$

$$\hat{\mathbf{x}}_{k+1} = \hat{\mathbf{x}}_{k+1} + \mathbf{K}(\mathbf{z}_{k+1} - \mathbf{h}(\hat{\mathbf{x}}_{k+1}) + \nabla \mathbf{h}\hat{\mathbf{x}}_{k+1} - \nabla \mathbf{h}\hat{\mathbf{x}}_{k+1}) \quad (29)$$

$$\hat{\mathbf{x}}_{k+1} = \hat{\mathbf{x}}_{k+1} + \mathbf{K}(\mathbf{z}_{k+1} - \mathbf{h}(\hat{\mathbf{x}}_{k+1})) \quad (30)$$

and

$$\mathbf{P}_{k+1} = \hat{\mathbf{P}}_{k+1} - \mathbf{K}\mathbf{S}\mathbf{K}^T \quad (31)$$

Where \mathbf{S} denotes the innovation covariance and the \mathbf{K} denotes the Kalman gain

$$\mathbf{S} = \mathbf{H}\hat{\mathbf{P}}_{k+1}\mathbf{H}^T + \mathbf{R} = \nabla \mathbf{h}\hat{\mathbf{P}}_{k+1}\nabla \mathbf{h}^T + \mathbf{R} \quad (32)$$

$$\mathbf{K} = \hat{\mathbf{P}}_{k+1}\mathbf{H}^T\mathbf{S}^{-1} = \hat{\mathbf{P}}_{k+1}\nabla \mathbf{h}^T\mathbf{S}^{-1} \quad (33)$$

This Kalman filter linearized about the current estimated state. Thus the system must be represented by continuously differentiable functions.

Prediction:

In the nonlinear case the dynamic matrix \mathbf{F} is a function of the state to be estimated. So the predicted state is calculated by solving the differential equations in the form

$$\dot{\mathbf{x}}^-(t) = \mathbf{f}(\mathbf{x}^-(t)) \quad (34)$$

By deriving this equation by a Taylor series with respect to \mathbf{x} at the predicted state $\mathbf{x}^-(t_i)$ And assuming that the higher order terms can be neglected, the dynamic matrix $\mathbf{F}(t_i)$ can be calculated with

$$\mathbf{F}(t_i) = \frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \text{ for } \mathbf{x} = \mathbf{x}^-(t_i) \quad (35)$$

And now the other steps of the prediction can be calculated. The used matrices are not constant as like a linear case, but depend on the time step.

$$\frac{d}{dt} \boldsymbol{\varphi}_{ti-1}^{ti} = \mathbf{F}(t_i) \cdot \boldsymbol{\varphi}_{ti-1}^{ti} \quad (36)$$

$$\mathbf{P}^-(t_i) = \boldsymbol{\varphi}_{ti-1}^{ti} \mathbf{P}(t_{i-1}) (\boldsymbol{\varphi}_{ti-1}^{ti})^T + \int_{t_{i-1}}^{t_i} \mathbf{Q}(t) dt \quad (37)$$

Correction:

The nonlinear observation equations are linearized with the Taylor series about the predicted state

$$\underline{\mathbf{x}}^-(t_i) \text{ and higher order terms are neglected.}$$

Thus the observation matrix is given by

$$\mathbf{H}(t_i) = \frac{\partial \mathbf{h}(\underline{\mathbf{x}})}{\partial \underline{\mathbf{x}}} \text{ for } \underline{\mathbf{x}} = \underline{\mathbf{x}}^-(t_i) \quad (38)$$

In that case the predicted measurement $\underline{\mathbf{l}}^-(t_i)$ for calculating the measurement residual $(\mathbf{l}(t_i) - \underline{\mathbf{l}}^-(t_i))$ is $\underline{\mathbf{l}}^-(t_i) = \mathbf{h}(\underline{\mathbf{x}}^-(t_i))$

Further on, it can be use the same formulas to calculate the corrected state and its covariance matrix like in the linear case but with time depended matrices.

$$\mathbf{x}(t_i) = \mathbf{x}^-(t_i) + \mathbf{K}(\mathbf{l}(t_i) - \underline{\mathbf{l}}^-(t_i)) \quad (39)$$

And

$$\mathbf{P}^+(t_i) = (\mathbf{I} - \mathbf{K}(t_i)\mathbf{H}(t_i))\mathbf{P}^-(t_i) \quad (40)$$

With

$$\mathbf{K}(t_i) = \mathbf{P}^-\mathbf{H}(t_i)^T (\mathbf{H}(t_i)\mathbf{P}^-\mathbf{H}(t_i)^T + \mathbf{R}(t_i))^{-1} \quad (41)$$

Simulation results:

The state estimation of nonlinear process control reactor (Continuous Stirred Tank Reactor) was carried out by Extended Kalman filter algorithm using MATLAB Software. The estimation of all four states of the nonlinear process control reactor Concentration A, Concentration B, Reactor Temperature and Coolant Temperature for the input-1 volumetric flow rate q was given in the Figure no 3. The actual and estimated state simulation for all the four states was compared which will show the efficient tracking capability of the extended Kalman filter.

The following assumptions are made while doing the simulations:

- The measurement update frequency of the KF coincides with the system discretization sampling frequency.
- The system model and the state estimator model are the same unless otherwise specified.
- Process noise and measurement noise are applied to the system. The noise is Gaussian with zero mean value.
- The tuning parameters (the initial covariance and process and measurement noise covariance's) are chosen for EKF.

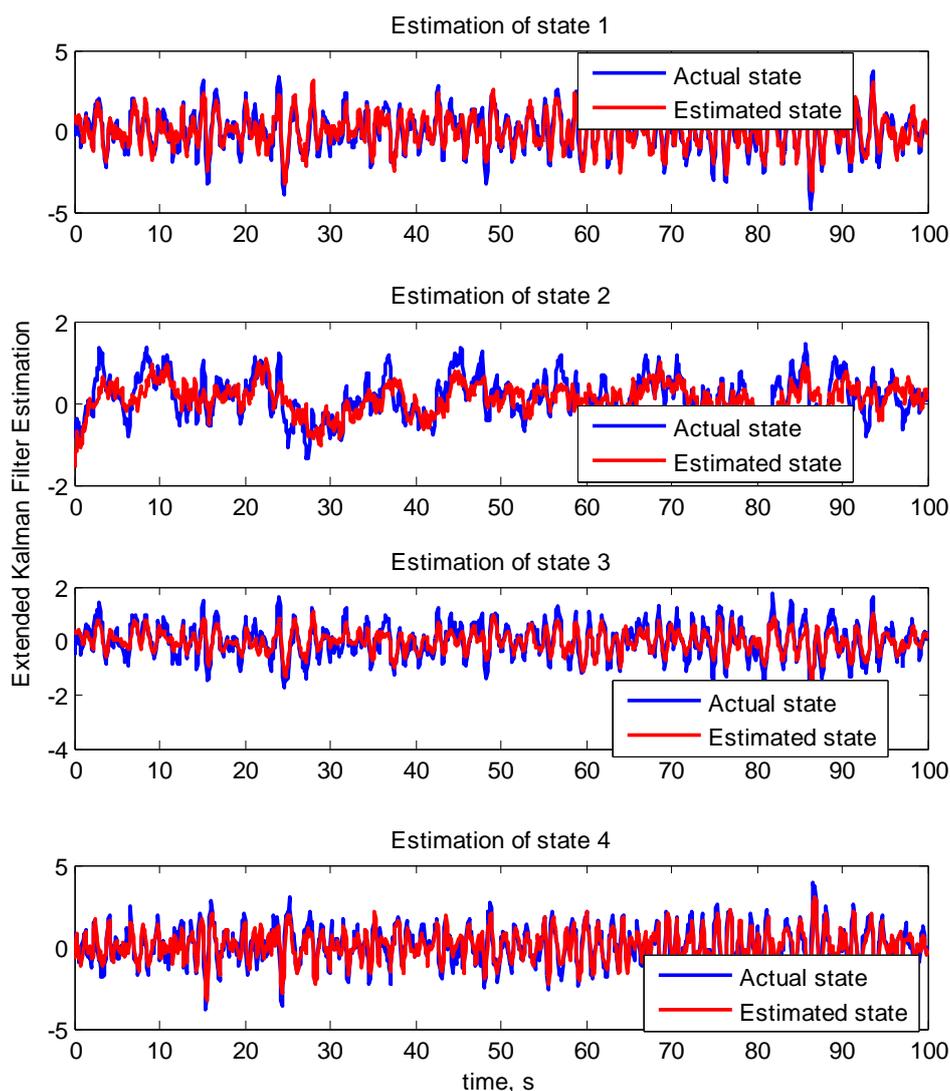


Fig. 3: Simulation Result of the Extended Kalman Filter Design

Conclusion:

In this paper, the estimation procedure using Extended Kalman filter theory was applied on highly nonlinear plants. The Extended Kalman filter is more accurate than Kalman filter, in order to reduce the error in estimations in which the noise variances are not known, Fading and novel adaptive methods of EKF has been presented in this paper. In novel adaptive method, variance matrices for both process and measurement noise signals were assumed unknown a priori and thus incrementally estimated and updated using a sliding time window paradigm within which an estimation of the noise variance is calculated and adaptively updated each time the window is shifted forward. The simulation results show the capability of the proposed novel adaptive method in performance monitoring of this nonlinear case study. Kalman filter algorithm attempts to propagate the mean and covariance of a system using a time update and a measurement update. If the system is linear, then the mean and covariance can be exactly updated with the Kalman filter. If the system

is nonlinear, then the mean and covariance can be approximately updated with the extended Kalman filter. The extended Kalman filter (EKF) is the most widely applied state estimation algorithm for nonlinear systems. However, the EKF can be difficult to tune and often gives unreliable estimates if the system nonlinearities are severe. This is because the EKF relies on linearization to propagate the mean and covariance of the state. The EKF propagates the pdf in a simple and effective way and it is accurate up to second order in estimating mean and covariance. The present paper focuses on using the EKF for nonlinear state estimation in process systems and the performance is evaluated in Continuous Stirred Tank Reactor.

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