Comparative Assessment of a Chemical Reactor using Extended Kalman Filter and Unscented Kalman Filter

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Abstract
Continuous Stirred Tank Reactor is a typical chemical reactor system with complex nonlinear dynamic characteristics. The variables which characterize the quality of the final product in Continuous Stirred Tank Reactor are often difficult to measure in real-time and cannot be directly controlled using feedback configuration. In this work, a comparative study of the performance analysis of Extended Kalman Filter with respect to Unscented Kalman Filter for Continuous Stirred Tank Reactor that rely solely on concentration estimation of Continuous Stirred Tank Reactor via measured reactor temperature is done. The performance of these two filters is analyzed in simulation with Gaussian noise source under various operating conditions and model uncertainties. It is shown that in the presence of large model parameter mismatch and initial state mismatch, Unscented Kalman Filter is able to provide more reliable estimate, when compared to Extended Kalman Filter. However, under ideal conditions the performance of Extended Kalman Filter is found to be better.

1. Introduction
Online estimates of the state variables have been considered necessary in diverse applications such as process, controller performance monitoring and state feedback control. State observer can be designed to generate an

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estimate of the state by making use of the relevant process inputs, outputs and mathematical model of the system. The well-known Kalman filter [1] solves the general state estimation problem in stochastic linear system. For linear systems, Kalman filter generate optimal estimates of the state from observations. In addition, Kalman filter has become more useful even for very complicated real-time applications and has attracted the attention of chemical engineering community because of recursive nature of its computational scheme. However, for non-linear systems, Extended Kalman Filter (EKF) is a natural extension of the linear theory to the non-linear domain through local linearization. There are several variants of the basic EKF, which have been evaluated by various researchers [2]. Many studies in observer design for nonlinear system are based on EKF approach, which lead to complex nonlinear algorithm. In spite of good results, there is no a priori guarantee of the convergence and stability of the algorithms. Recently Simon J.Julier proposed an Unscented Kalman Filter (UKF) [3] for the nonlinear dynamic system. Its use for the state estimation of Continuous Stirred Tank Reactor (CSTR) has been reported in some literatures [4, 5]. Unlike EKF, it utilizes unscented transform which is a deterministic sampling approach to calculate the current mean and covariance of states and hence called derivative free filter. However, the UKF algorithm is more computationally intensive [8] than EKF.

The main contributions of this work is to implement EKF and UKF algorithms for the state estimation of CSTR and compare the performances under different operating conditions based on the performance index, Mean Square Error (MSE).

2. Mathematical model of CSTR

The first principle model of the continuous stirred tank system and the operating point data (Table 1) as specified in the Pottman and Seborg paper have been used in the simulation studies [6]. Highly nonlinear CSTR process is very common in chemical and petrochemical plants. In the process considered for simulation study as shown in Fig. 1, an irreversible, exothermic reaction \( A \rightarrow B \) occurs in constant volume reactor that is cooled by a single coolant stream.

\[
\frac{dC_A}{dt} = \frac{F}{V}(C_{Af} - C_A) - k_0 C_A \exp\left(\frac{-E}{RT}\right)
\]

\[
\frac{dT}{dt} = \frac{F}{V}(T_f - T) - \left(\frac{-\Delta H}{\rho C_p}\right)k_0 \exp\left(\frac{-E}{RT}\right)C_A + \frac{\rho C_p}{\rho C_p V} q_c \left(1 - \exp\left(\frac{-hA}{\rho C_p q_c}\right)\right)(T_{co} - T)
\]
Table 1. Steady state operating data of CSTR

| Process variable                        | Normal operating condition |
|-----------------------------------------|----------------------------|
| Measured Product Concentration ($C_0$)  | 0.08235 mol/L              |
| Reactor Temperature (T)                 | 441.81 K                   |
| Volumetric Flow rate (F)                | 100 L/min                  |
| Reactor Volume (V)                      | 100 L                      |
| Feed Concentration ($C_{af}$)           | 1 mol/L                    |
| Feed Temperature (Tf)                   | 350 K                      |
| Coolant Temperature ($T_{co}$)          | 350 K                      |
| Coolant Flow rate ($q_c$)               | 100 L/min                  |
| Heat of Reaction ($\Delta H$)           | 2e5 cal/mol                |
| Reaction rate constant ($k_0$)          | 7.2 e10 min$^{-1}$         |
| Activation energy term ($E/R$)          | 9980 K                     |
| Heat transfer term ($UA$)               | 7 e5 cal/(min.K)           |
| Liquid Density ($\rho$, $\rho_c$)       | 1000 g/L                   |
| Specific Heat Capacity ($C_p$, $C_{pc}$)| 1 cal/(g.K)                |

Fig. 3 and Fig. 4 show the temperature and concentration responses of the CSTR for the coolant flow rate variation as shown in Fig. 2. From the open loop response of the CSTR process shown in Fig. 3 and Fig. 4, it can be concluded that the dynamic behaviour of the CSTR process is not the same at different operating points and the process is indeed non-linear.
3. Extended Kalman Filter

The well-known Kalman filter [1] solves the state estimation problem in a stochastic linear system. The EKF is probably the most widely used nonlinear filter. For nonlinear problems, the Kalman Filter is not strictly applicable since linearity plays an important role in its derivation and performance as an optimal filter. The EKF attempts to overcome this difficulty by using a linearized approximation where the linearization is performed about the current state estimate. The basic framework for the EKF (and the UKF) involves the estimation of the states of a nonlinear dynamic system given by (1) and (2).

\[ x(k) = x(k-1) + \int_{t_{k-1}}^{t_k} F[x(\tau), u(k)d\tau] + w(k) \]  
\[ y(k) = H[x(k)] + v(k) \]

In the above equations, \( x(k) \) represents the unobserved state of the system, \( u(k) \) is a known exogenous input and \( y(k) \) is the only observed signal. We have assumed \( w(k) \) and \( v(k) \) as zero mean Gaussian white noise sequences with covariance matrices \( Q \) and \( R \) respectively. The symbols \( F \) and \( H \) represent an n-dimensional function vector and are assumed known. EKF involves the recursive estimation of the mean and covariance of the state under maximum likelihood condition. The function \( F \) can be used to compute the predicted state from the previous estimate and similarly the function \( H \) can be used to compute the predicted measurement from the predicted state. However, \( F \) and \( H \) cannot be applied to the covariance directly. Instead a matrix of partial derivatives (Jacobian) is computed at each time step with current predicted state and evaluated. This process essentially linearizes the non-linear function around the current estimate. The predicted state estimates are obtained as

\[ \hat{x}(k | k-1) = \hat{x}(k-1 | k-1) + \int_{t_{k-1}}^{t_k} F[x(\tau), u(k)d\tau] \]

The covariance matrix of estimation errors in the predicted estimates is obtained as

\[ P(k | k-1) = \Phi(k)P(k-1 | k-1)\Phi(k)^T + Q \]

Where \( \Phi(k) \) is the Jacobian matrix of partial derivatives of \( F \) with respect to \( \hat{A} \)

\[ \Phi(k) = \left[ \frac{\partial F}{\partial x} \right]_{\hat{x}(k-1 | k-1), u(k-1)} \]

Note that the EKF computes covariances using the linear propagation. The measurement prediction, computation of innovation and covariance matrix of innovation are as follows

\[ \hat{y}(k | k-1) = H[\hat{x}(k | k-1)] \]

\[ \gamma(k | k-1) = y(k) - \hat{y}(k | k-1) \]

\[ V(k) = C(k)P(k | k-1)C(k)^T + R \]

Where \( C(k) \) is the Jacobian matrix of partial derivatives of \( H \) with respect to \( x \).

\[ C(k) = \left[ \frac{dH}{\partial x} \right]_{\hat{x}(k-1), u(k-1)} \]

The Kalman gain is computed using the following equation

\[ K(k) = P(k | k-1)C(k)^TV^{-1}(k) \]

The updated state estimates are obtained using the following equation
\[ \hat{x}(k | k) = \hat{x}(k | k-1) + K(k)\gamma(K | k-1) \]

The covaraince matrix of estimation errors in the updated state estimates is obtained as

\[ P(k | k) = [I - K(k)C(k)]P(k | k-1) \]

4. Unscented Kalman Filter

The sigma points are not drawn at random, but they are deterministically chosen. As a result, high-order information about the distribution can be captured with a fixed and small number of points. UKF filter uses the unscented transform [3] to pick a minimal set of sample points (called sigma points) around the mean. These sigma points are then propagated through the nonlinear functions and the covariance of the estimate is then determined. The result is a filter which more accurately captures the true mean and covariance [7]. A set of 2L + 1 sigma points, \( x(k|k,i) \) with the associated weights \( W(i) \) are chosen symmetrically about \( \hat{x}(k | k) \) as given below

\[
X_i = \bar{x} + \sqrt{(L+\lambda)P_x}i,
\]

where \( i=1,\ldots, L \)

\[
X_i = \bar{x} + \sqrt{(L+\lambda)P_x}i-L,
\]

where \( i=L+1,\ldots, 2L \)

The weights for the state and covariance are as follows

\[
W_0^{(m)} = \frac{\lambda}{(L+\lambda)},
\]

\[
W_0^{(c)} = \frac{\lambda}{(L+\lambda)} + (1 - \alpha^2 + \beta),
\]

\[
W_0^{(i)} = \frac{\lambda}{(L+\lambda)} + (1 - \alpha^2 + \beta),
\]

where \( i = 1 \ldots 2L \)

where \( \lambda = \alpha^2(L+K)-L \) is a scaling parameter. \( \alpha \) determines the spread of the sigma points around mean and is usually set to a small positive value. \( K \) is a secondary scaling parameter which is usually set to 0 and \( \beta \) is used to incorporate prior knowledge of the distribution of \( x\sqrt{(L+\lambda)P_x} \)

A set of 2L+1 sigma points is derived from the augmented state and covariance where \( L \) is the dimension of the augmented state.

The sigma points are propagated through the transition function \( f \).

\[
X^{i}_{k-1|k-1} = f\left(X^{i}_{k-1|k-1}\right), \text{ where, } i=0 \ldots 2L
\]

The weighted sigma points are recombined to produce the predicted state and covariance.
\[
\hat{x}(k|k-1) = \sum_{i=0}^{2L} W_{(m)}^{i} X_{k|k-1}^{i}
\]
\[
P_{k|k-1} = \sum_{i=0}^{2L} W_{(c)}^{i} \left[ X_{k|k-1}^{i} - \hat{x}_{k|k-1} \right] \left[ X_{k|k-1}^{i} - \hat{x}_{k|k-1} \right]^T
\]

(22)

(23)

The weighted sigma points are recombined to produce the predicted measurement and predicted measurement covariance.

\[
\hat{y}_k = \sum_{i=0}^{2L} W_{(m)}^{i} Y_k
\]
\[
P_{y_k|y_k} = \sum_{i=0}^{2L} W_{(c)}^{i} \left[ Y_k^{i} - \hat{y}_k \right] \left[ Y_k^{i} - \hat{y}_k \right]^T
\]

(24)

(25)

The state-measurement cross-variance matrix,

\[
P_{x_k|y_k} = \sum_{i=0}^{2L} W_{(c)}^{i} \left[ X_{k|k-1}^{i} - \hat{x}_{k|k-1} \right] \left[ Y_k^{i} - \hat{y}_k \right]^T
\]

(26)

UKF Kalman filter gain is calculated from the above two covariance matrices as follows:

\[
K_k = P_{x_k|y_k} P_{y_k|y_k}^{-1}
\]

(27)

As like EKF, the update state is the predicted state plus the innovation weighted by the Kalman gain,

\[
\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k \left( y_k - \hat{y}_k \right)
\]

(28)

The updated covariance is the predicted covariance minus the predicted measurement covariance, weighted by the Kalman gain

\[
P_{k|k} = P_{k|k-1} + K_k P_{y_k|y_k} K_k^T
\]

(29)

5. Simulation results

In all the simulation runs, the process is simulated using the non-linear first principle model and the true state variables are computed by solving the non-linear differential equations using differential equation solver in MATLAB. Fig. 5 shows the block diagram of the proposed method for the CSTR process. It is assumed that feed temperature and concentration are constants, and coolant flow rate and feed flow rate are given as input parameters. The other parameters such as activation energy, heat of reaction, coolant temperature etc., are taken as constants, because certain assumptions are considered like perfect mixing, constant volume, constant parameter values and constant physical properties. The tuning parameters values of EKF and UKF are listed in Table 2.

Keeping in mind the realistic conditions, simulation studies have been carried out under the following conditions:

- Normal Operating Conditions
- Model parameter mismatch
- Initial state mismatch

Table 2. Tuning parameters used in EKF and UKF algorithms
### Noise covariance matrices used in EKF and UKF

\[
Q = \text{Diag}(0.0025, 0.0025) \\
R = 0.0025
\]

### Initial state error covariance matrices

\[
P = 1000 \cdot I_{2 \times 2}
\]

### Other UKF tuning parameters

\[
\alpha = 0.001; \beta = 2; \quad K = 0
\]

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#### 5.1. Normal operating conditions

Fig. 6 and Fig. 7 show the EKF and UKF estimated reactor concentration in CSTR for step changes in the coolant flow rate and random errors in the measurement.

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Fig. 8 and Fig. 9 show the EKF and UKF estimated reactor temperature in CSTR for step changes in the coolant.

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5.2. Model parameter mismatch

Due to inaccuracy in measurements and variation in operating conditions, parameters of process and model will not be identical, leading to poor estimation and hence poor control. Simulation studies are made considering both the above mentioned situations. Since the feed flow rate affects both temperature and concentration of the reactants simultaneously, it is chosen as the parameter of mismatch between the model and process. 10%, 20% and 30% model mismatches are considered and are applied to both EKF and UKF. The responses are compared on the basis of MSE. Fig. 10 and Fig. 11 show the EKF and UKF estimated reactor concentration and Fig. 12 and Fig. 13 show the reactor temperature in CSTR for 30% model mismatch.

5.3. Initial state mismatch

Simulation studies are performed with different initial state values and it is observed that the performances of the filters are affected mainly due to the difference in initial values between the process and model. Accordingly, simulations are carried out for different initial settings.
Moreover, the filter estimation is started at different instances after the process has been started. The process is simulated with initial temperature mismatch and also initial concentration mismatch. Initial state mismatches are given at 200, 400 and 600th sampling instants. Fig. 14 and Fig. 15 show the EKF and UKF estimated reactor concentration and Fig. 16 and Fig. 17 show the reactor temperature in CSTR for initial state mismatch applied at 600th instant.

5.4. Comparison of performance index

MSE is used as the performance index to evaluate the performance of EKF and UKF algorithm under different operating conditions. Table III, IV and V show the comparative study.

| Performance index | Concentration | Temperature |
|-------------------|---------------|-------------|
| MSE               | 0.6386 * 10^{-7} | 0.2880 * 10^{-4} |
| MSE               | 0.6325 * 10^{-7} | 0.1186 * 10^{-7} |

| Performance index | Percentage variation in feed flow rate | EKF | UKF |
|-------------------|----------------------------------------|-----|-----|
| MSE               | 30%                                    | 30% |     |
| MSE               | Concentration                          | 31.4227 | 0.0001 |
| MSE               | Temperature                            | 0.8669 | 0.0262 |

| Performance index | Sampling instants | EKF | UKF |
|-------------------|-------------------|-----|-----|
| MSE               | Concentration     | 27.2927 | 0.3627*10^{-1} |
| MSE               | Temperature       | 0.6275 | 0.0002*10^{-3} |

From Table 3, MSE value of EKF has been found lesser than UKF. So it is clear that EKF shows better performance than UKF under ideal conditions. But when model mismatch is introduced, EKF fails to estimate the true states. UKF algorithm is able to track the true states even in the presence of model mismatch with reasonable error which is shown in Table 4. Similarly for initial state mismatch conditions UKF gives less error than EKF as shown in Table 5.
6. Conclusion

The two filters namely EKF and UKF have been developed. A comprehensive simulation study in MATLAB has been carried out for state estimation, more specifically for the estimation of concentration and temperature of a Continuous Stirred Tank Reactor.

Simulation studies are conducted at different operating conditions. From the results, it can be inferred that for normal operating conditions specifically under low and medium level uncertainties EKF gives better state estimates than UKF. It can be concluded that EKF still remains as best choice compared to UKF for inferential control of CSTR. For extreme conditions like large parameter uncertainties, UKF estimates are more reliable than EKF. This indicates that there is enough scope for the use of derivative free filter in advanced process control applications if its performance can be improved using methods such as adaptive weight change.

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