Analytic Local Linearization Particle Filter for Bayesian State Estimation in Nonlinear Continuous Process

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Abstract: - State estimation is a prerequisite for monitoring, control and fault diagnosis of many processes. Dynamic model based state estimation techniques are used for monitoring the state variables. Particle filter have been widely used to estimate the state of nonlinear and non-Gaussian system. Particle filters require a proposal distribution but the choice of proposal distribution is the key design issue. In this paper, the extended Kalman filter (EKF) which is based on analytic local linearization is used to generate a proposal distribution for the particle filter. The efficacy of this local linearization particle filter (LLPF) is demonstrated via application to a simulated nonlinear continuous stirred tank reactor (CSTR) and the results are compared with the sampling importance resampling (SIR) particle filter.

Key-Words: - State estimation; Particle filter; Non-Gaussian; Proposal distribution; Local linearization particle filter; Sampling importance resampling.

1 Introduction

The estimation of states of the system using a sequence of measurements made on the system is an important problem in the process engineering because knowledge of such states can enhance the control performance. State estimation can be considered as an optimal filtering problem within a Bayesian framework [1]. The state vector contains all relevant information required to describe the system under investigation. The system considered in this paper is described by a set of differential equations that are usually discretized to a set of difference equations. These difference equations can be regarded as a general state space model, with the difference variables defining the states.

The Kalman filter (KF) is generally used to estimate the state of the linear system. It is an optimal solution to the state estimation problem. The KF assumes that the posterior density function at every time step is Gaussian [2,3,21]. In many situations of interest, these assumptions do not hold and therefore approximations are necessary. The extended Kalman filter (EKF) is one of the approximate nonlinear Bayesian filter which can be used to deal with the nonlinear state estimation problem [4,5]. The EKF always approximates the posterior density to be Gaussian and adopts Taylor approximation. If the state equation is highly nonlinear and the posterior density is also non-Gaussian (e.g., multimodal distribution), then EKF directly cannot be used for the state estimation problem because it may give a high estimation error and thereby leading to convergence problems [6].

Sequential Monte Carlo (SMC) is an algorithm that makes it possible to recursively construct the posterior probability density of the state variables, with respect to all available measurements, through a random exploration of the states by entities called 'particle'. The particle filter based on the SMC method can deal with both the nonlinear and non-Gaussian sate estimation problem [7]. The basic idea of particle filter is that a large number of particles are generated using SMC methods to approximate the posterior probability of the states [8,22]. A brief review of applications of particle filtering in computer vision, target tracking, robotics, digital communication, machine learning and speech recognition are presented in [9]. The sequential importance sampling (SIS) algorithm is a Monte Carlo method that forms the basis for most SMC filters but a common difficulty associated here is the occurrence of degeneracy [10,11]. The drawback in SIS filter is overcome through implementation of resampling technique [12]. The sampling importance resampling (SIR) particle filter can be applied to deal with most of the recursive Bayesian filtering problems because it outperforms the nonlinear sate estimation algorithms like EKF

and unscented Kalman filter (UKF) [19]. Sometimes, the performance of the SIR filter may diverge since the assumptions required to design this filter are very weak [13]. The local linearization algorithm such as EKF is used to construct the suboptimal approximations to the importance density in the particle filter [10,15]. Such a nonlinear Bayesian filter combines the advantage of both EKF and particle filter. Successful implementation of particle filters to chemical batch reactors have been reported in [6,14].

In this paper, the particle filter based on analytic local linearization technique is demonstrated by application to a simulated CSTR and are observed to exhibit improved performance over the SIR particle filter for the estimation of the product concentration and reactor temperature.

2 Sequential Bayesian State Estimation Problem

Consider the following nonlinear form of state space model:

$$\mathrm{x}_k = \mathrm{g}(\mathrm{x}_{k-1}, \mathrm{v}_{k-1}) \quad (1)$$

$$\mathrm{y}_k = \mathrm{h}(\mathrm{x}_k, \mathrm{n}_k) \quad (2)$$

where k is the time step, x is the state vector and y is the measurement vector. g and h are nonlinear state and measurement functions respectively. Process noise, v represents disturbances, all unmodelled dynamics and any mismatch between the process and model. Measurement noise, n captures the inaccuracy in the measuring system namely sensor.

The objective of state estimation is to sequentially estimate the state vector x_k from the measurement y_k. One of the main advantage of state estimation technique is as much as possible states can be inferred from the limited measurements available. The aim of the sequential Bayesian estimation is to compute the conditional probability density function (PDF) which in this context is known as posterior density $p(\mathrm{x}_k \mid \mathrm{y}_{1:k})$ from the posterior density at the previous time step $p(\mathrm{x}_{k-1} \mid \mathrm{y}_{1:k-1})$. Generally, the posterior density is estimated in two stages namely prediction and update. In the prediction step, $p(\mathrm{x}_{k-1} \mid \mathrm{y}_{1:k-1})$ is propagated to the next time step through the transition density as follows:

$$p(\mathrm{x}_k \mid \mathrm{y}_{1:k-1}) = \int p(\mathrm{x}_k \mid \mathrm{x}_{k-1})\, p(\mathrm{x}_{k-1} \mid \mathrm{y}_{1:k-1}) \mathrm{dx}_{k-1} \quad (3)$$

$p(\mathrm{x}_k \mid \mathrm{x}_{k-1})$ is the transition density defined by the system function (1). The Bayes' rule is applied in the update step as follows:

$$p(\mathrm{x}_k \mid \mathrm{y}_{1:k}) = \frac{p(\mathrm{y}_k \mid \mathrm{x}_k)\, p(\mathrm{x}_k \mid \mathrm{y}_{1:k-1})}{p(\mathrm{y}_k \mid \mathrm{y}_{1:k-1})} \quad (4)$$

The propagation of the prior density $p(\mathrm{x}_k \mid \mathrm{y}_{1:k-1})$ to the posterior density $p(\mathrm{x}_k \mid \mathrm{y}_{1:k})$ is described by (4). The normalizing factor $p(\mathrm{y}_k \mid \mathrm{y}_{1:k-1})$ depends on the likelihood function $p(\mathrm{y}_k \mid \mathrm{x}_k)$, defined by the measurement function (2). The posterior density function of the state is the optimal solution from a Bayesian perspective to the state estimation problem.

In general, the posterior probability function cannot be determined analytically and hence approximations are required. The suboptimal filters which are the approximate nonlinear Bayesian filters are used to provide the suboptimal solutions. Some of the well known suboptimal filters are EKF and particle filter [13]. The EKF is commonly used to estimate the state of the nonlinear system by linearizing about an estimate of the current mean and covariance [16, 23]. It may perform poorly for highly nonlinear system because of the first-order Taylor series approximation of nonlinear function. A higher order EKF takes in to account the higher order terms in the Taylor series expansion, but the calculation of Jacobians provides additional complexity which has prohibited its wide spread use. An alternative approach is through particle filter which will yield an improvement in performance in comparison to EKF.

3 Particle Filtering Methods

SMC methods are a set of simulation based methods which provide a convenient and attractive approach for computing the posterior distributions [17, 18]. Particle filters perform SMC estimation based on particle representation of probability densities. It approximates the multidimensional integration involved in prediction and update steps using Monte Carlo sampling. It can very well deal with non-Gaussian conditional density functions for estimating the state of the nonlinear system [19].

The following description of particle filter is based on the tutorial of Arulampalam et al. [13].

The fundamental idea of particle filter is to approximate the posterior density $p(\mathrm{x}_k \mid \mathrm{y}_{1:k})$ using a set of random samples also called particles $\{\mathrm{x}_k^i, i = 1,..., N\}$ with associated weights $\{w_k^i, i = 1,..., N\}$. The posterior density is given by:

$$p(\mathrm{x}_k \mid \mathrm{y}_{1:k}) \approx \sum_{i=1}^{N} w_k^i \delta(\mathrm{x}_k - \mathrm{x}_k^i) \quad (5)$$

where $\delta(\mathrm{x})$ is an indicator function. The weights are normalized such that $\sum_{i=1}^{N} w_k^i = 1$. It can be shown that as $N \to \infty$ the approximation (5) approaches the true posterior density. The weights are chosen using the principle of importance sampling. The first step in importance sampling is to define an importance density function $\pi(\mathrm{x}_k \mid \mathrm{y}_{1:k})$, from which samples x_k^i can be drawn. Thus the weights are defined as

$$w_k^i \propto \frac{p(\mathrm{x}_k^i \mid \mathrm{y}_{1:k})}{\pi(\mathrm{x}_k^i \mid \mathrm{y}_{1:k})} \quad (6)$$

If the importance density is only relying on the current measurement, y_k and the previous state, x_{k-1}, the weights can be updated as

$$w_k^i \propto w_{k-1}^i \frac{p(\mathrm{y}_k \mid \mathrm{x}_k^i) p(\mathrm{x}_k^i \mid \mathrm{x}_{k-1}^i)}{\pi(\mathrm{x}_k^i \mid \mathrm{x}_{k-1}^i, \mathrm{y}_k)} \quad (7)$$

Therefore the importance sampling method is used to obtain the particles and associated weights from which the state vector $\hat{\mathrm{x}}_k$ can be estimated. A common problem encountered in this method is the degeneracy phenomenon. Degeneracy is where, after a few iterations, only one particle has significant weight. It has been shown that the variance of the importance weights increases over time, and thus, it is impossible to avoid the degeneracy. Such a problem can make the contribution of the particles to the approximation of $p(\mathrm{x}_k \mid \mathrm{y}_{1:k})$ almost negligible. The effective sample size N_{eff} is computed to give a measure of degeneracy of the algorithm as follows:

$$N_{eff} = \frac{1}{\sum_{i=1}^{N} (w_k^i)^2} \quad (8)$$

where w_k^i is the normalized weight obtained using (7).Hence, by proper selection of importance density, the N_{eff} can be minimized.

3.1 Sampling Importance Resampling (SIR) Particle Filter

Resampling method is used whenever a significant degeneracy is observed. Resampling eliminates those particles with smaller weights and replaces particles with large weights [12]. Thus a new particle set is generated by sampling with replacement from the original set $\{\mathrm{x}_k^i, i = 1,..., N\}$.

In summary, the SIR particle filter algorithm for the time step k is as follows:

(1) For $i = 1: N$

- Draw a sample $\mathrm{x}_k^i \sim p(\mathrm{x}_k \mid \mathrm{x}_{k-1}^i)$
- Compute weight $w_k^i = p(\mathrm{y}_k \mid \mathrm{x}_k^i)$

End

(2) Normalize w_k^i such that they sum to 1

(3) Resample to get an updated particle set $\{\mathrm{x}_k^i\}_{i=1}^N$

The output of the algorithm is the mean of the particle set that can be computed as follows:

$$\hat{\mathrm{x}}_k = \frac{1}{N} \sum_{i=1}^{N} \mathrm{x}_k^i \quad (9)$$

In the algorithm discussed here, the transitional prior $p(\mathrm{x}_k \mid \mathrm{x}_{k-1})$ is chosen to be the importance density. As the importance density is independent of the current measurement, the state space is explored without any knowledge of the measurement data. Hence, this filter can be inefficient and is sensitive to outliers.

3.2 Analytic Local Linearization Particle Filter

The importance density in the particle filter algorithm can be approximated by incorporating the most recent measurement y_k through an EKF [10]. When EKF is used to generate a proposal distribution for the particle filter, then the resulting filter is known as extended Kalman particle filter

(EKPF). This particle filter is also called as analytic local linearization particle filter because the EKF considered is based on analytic local linearization. In this type of particle filter, each particle is updated with EKF to generate and propagate a Gaussian importance distribution. The importance density is given by:

$$\pi(\mathrm{x}_k^i \mid \mathrm{x}_{k-1}^i, \mathrm{y}_k) = \mathcal{N}(\mathrm{x}_k^i; \hat{\mathrm{x}}_k^i, \mathrm{P}_k^i) \tag{10}$$

where $\hat{\mathrm{x}}_k^i$ and P_k^i are the estimate of the mean and covariance respectively. The notation $\mathcal{N}$ represents the Normal distribution. The EKF algorithm used to compute the importance density in this type of particle filter for the time step k is as follows:

(1) Predicted state: $\hat{\mathrm{x}}_{k|k-1} = \mathrm{g}(\hat{\mathrm{x}}_{k-1}, 0)$

(2) Predicted estimate covariance:
$\mathrm{P}_{k|k-1} = \mathrm{G}_k \mathrm{P}_{k-1} \mathrm{G}_k^T + \mathrm{Q}_k$
where the state transition matrix,
$\mathrm{G}_k = \left.\frac{\partial \mathrm{g}}{\partial \mathrm{x}}\right|_{\hat{\mathrm{x}}_{k-1}}$ and Q_k is the process noise covariance.

(3) Innovation or measurement residual:
$\mathrm{z}_k = \mathrm{y}_k - \mathrm{h}(\hat{\mathrm{x}}_{k|k-1}, 0)$

(4) Measurement covariance:
$\mathrm{S}_k = \mathrm{H}_k \mathrm{P}_{k|k-1} \mathrm{H}_k^T + \mathrm{R}_k$
where the observation matrix,
$\mathrm{H}_k = \left.\frac{\partial \mathrm{h}}{\partial \mathrm{x}}\right|_{\hat{\mathrm{x}}_{k|k-1}}$ and R_k is the measurement noise covariance.

(5) Kalman gain: $\mathrm{K}_k = \mathrm{P}_{k|k-1} \mathrm{H}_k^T \mathrm{S}_k^{-1}$

(6) Updated state estimate: $\hat{\mathrm{x}}_k = \hat{\mathrm{x}}_{k|k-1} + \mathrm{K}_k \mathrm{z}_k$

(7) Updated estimate covariance:
$\mathrm{P}_k = (\mathrm{I} - \mathrm{K}_k \mathrm{H}_k) \mathrm{P}_{k|k-1}$

In summary, the analytic local linearization particle filter for the time step k is as follows:

(1) For $i = 1:N$

- Run EKF
  $[\hat{\mathrm{x}}_k^i, \mathrm{P}_k^i] = \mathrm{EKF}[\mathrm{x}_{k-1}^i, \mathrm{P}_{k-1}^i, \mathrm{y}_k]$
- Draw a sample $\mathrm{x}_k^i \sim \mathcal{N}(\mathrm{x}_k^i; \hat{\mathrm{x}}_k^i, \mathrm{P}_k^i)$
- Compute weight
  $$w_k^i = \frac{p(\mathrm{y}_k \mid \mathrm{x}_k^i)\, p(\mathrm{x}_k^i \mid \mathrm{x}_{k-1}^i)}{\pi(\mathrm{x}_k^i \mid \mathrm{x}_{k-1}^i, \mathrm{y}_k)}$$

End

(2) Normalize w_k^i such that they sum to 1

(3) Resample to get an updated particle set $\{\mathrm{x}_k^j, i^j\}_{j=1}^N$, where j refers to the index of the particle after resampling. Here, the updated relationship is denoted as $\text{parent}(j) = i$.

(4) For $j = 1:N$

- Assign Covariance: $\mathrm{P}_k^j = \mathrm{P}_k^{i^j}$

End

The output of the algorithm is the mean of the particle set that can be computed as follows:

$$\hat{\mathrm{x}}_k = \frac{1}{N} \sum_{i=1}^{N} \mathrm{x}_k^i \tag{11}$$

The analytic local linearization method for approximation of importance density propagates the particles towards the likelihood function and thereby making such type of particle filter to perform better than the SIR filter.

4 Simulation Results

The performance of the extended Kalman particle filtering algorithm is illustrated through its application to a simulated nonlinear CSTR. The results of the SIR particle filter are presented for comparison.

4.1 Nonlinear CSTR

The system comprises of two state variables namely product concentration and reactor temperature. The reactor temperature is maintained by manipulating the coolant flow rate. The CSTR process and its operating conditions have been taken from [20]. The governing equations used to model the process are as follows:

$$\frac{dC_A}{dt} = \frac{q}{V}\left(C_{Af} - C_A\right) - K_0 C_A e^{\left(\frac{-E}{RT}\right)} \tag{12}$$

$$\frac{dT}{dt} = \frac{q}{V}\left(T_f - T\right) - \frac{\left(-\Delta H\right) K_0 C_A}{\rho C_p} e^{\left(\frac{-E}{RT}\right)} + \frac{\rho_c C_{pc}}{\rho C_p V} q_c \left\{1 - e^{\left(\frac{-\mathrm{hA}}{q_c \rho C_p}\right)}\right\}\left(T_c - T\right) \tag{13}$$

Table 1
Steady state operating data

Process variable	Steady state operating condition
Product concentration (C_A)	0.0795 mol/L
Reactor temperature (T)	443.4566 K
Coolant flow rate (q_c)	97 L/min
Process flow rate (q)	100 L/min
Feed concentration (C_{Af})	1 mol/L
Feed temperature (T_f)	350 K
Inlet coolant temperature (T_c)	350 K
CSTR volume (V)	100 L
Heat transfer term (hA)	7 x 10^5 cal/(min K)
Reaction rate constant (K_0)	7.2 x 10^{10} min^{-1}
Activation energy term (E/R)	1 x 10^4 K
Heat of reaction $(-\Delta H)$	-2 x 10^5 cal/mol
Liquid density (ρ, ρ_c)	1 000 g/L
Specific heats (C_p, C_{pc})	1 cal/(g K)

The nominal operating data for the CSTR process is given in Table 1.

The problem at hand is to generate estimates of state variables starting from the given initial estimates and with the knowledge of sensor measurements available at every sampling instant. For the two state benchmark problem presented here, the reactor temperature is the only measurement made but with that limited information both the temperature as well as the product concentration can be estimated as states of the system. The state estimation algorithm serves this purpose. In all the simulation runs of this section, the process is simulated using the nonlinear first principle model as given in (12) and (13). The true state variables are computed by solving the nonlinear differential equations using ordinary differential equation solver in Matlab.

The nominal operating condition of the states as shown in Table 1 is chosen as the initial states for this problem. The random errors are assumed to be present in the process as well as in its measurements. The covariance matrices of process noise and measurement noise are assumed as

$$\mathrm{Q} = \begin{bmatrix} (0.00079)^2 & 0 \\ 0 & (0.443)^2 \end{bmatrix}$$

$$\mathrm{R} = \begin{bmatrix} (0.443)^2 \end{bmatrix}$$

However, the variance should not be increased more than one order of magnitude as it gives rise to large oscillations in the estimated states of the system.

4.2 Estimation Performance of Particle Filtering Algorithms for CSTR

Simulation study had been made on the CSTR process to analyze the performance of SIR filter and EKPF using the number of particles *N*=200. Fig. 1 shows that the process is maintained with the constant coolant flow rate, $q_c = 97$ L/min. It can be noticed that in Fig. 2 and 3, the EKPF estimates both the states much closer to the true state than the SIR filter when the process is operated with the constant coolant flow rate. Fig. 4 shows a step change provided in the q_c from 97 L/min to 109 L/min. It can be observed from Fig. 5 and 6, the EKPF follows the true process trajectory more closely than the SIR filter in spite of step change provided in the coolant flow rate.

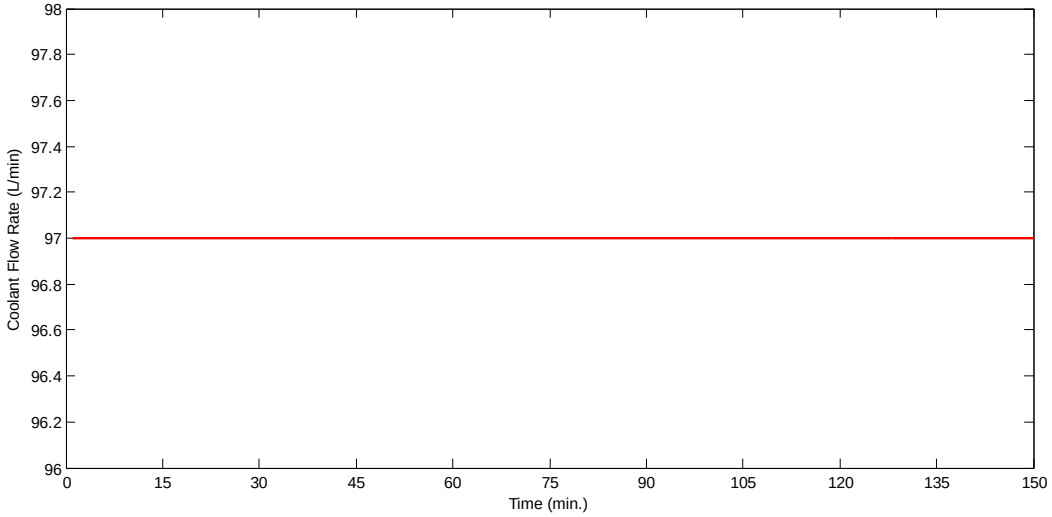

Fig. 1. Constant coolant flow rate for CSTR.

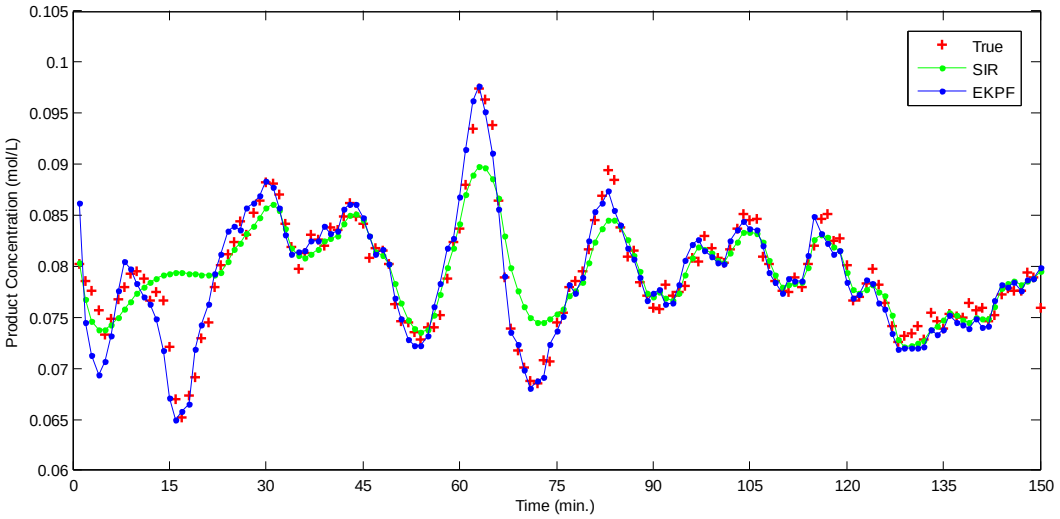

Fig. 2. Evolution of true and estimated product concentration of CSTR for fixed flow rate.

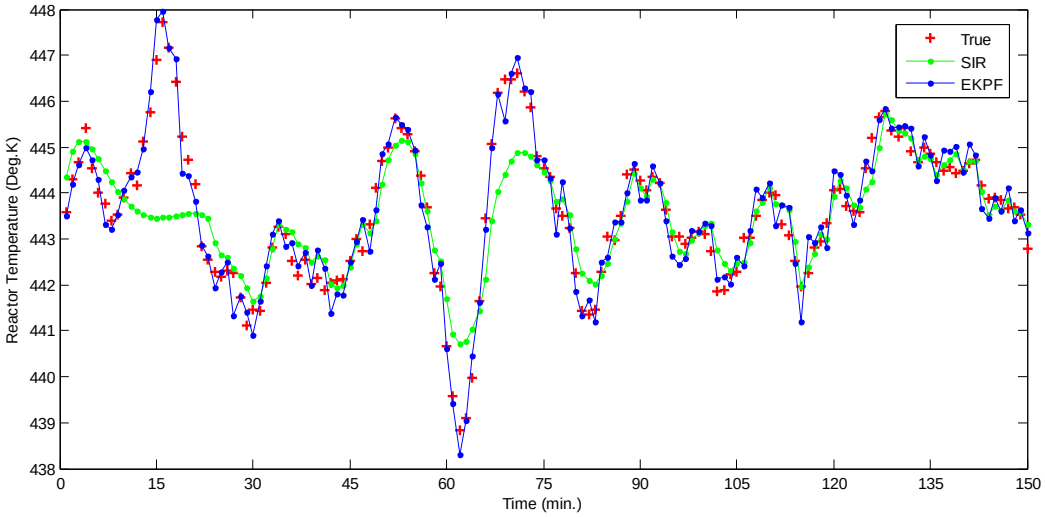

Fig. 3. Evolution of true and estimated reactor temperature of CSTR for fixed flow rate.

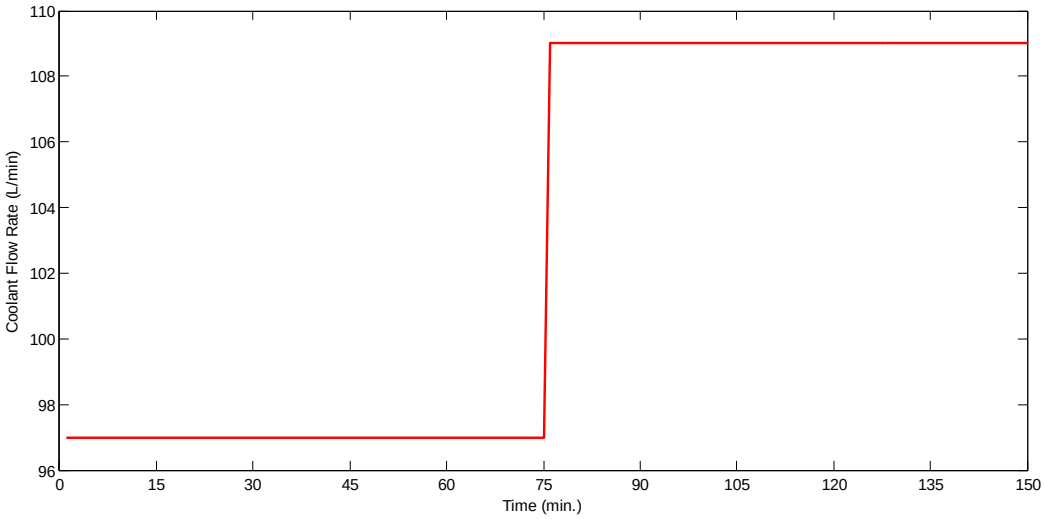

Fig. 4. Variation in coolant flow rate for CSTR.

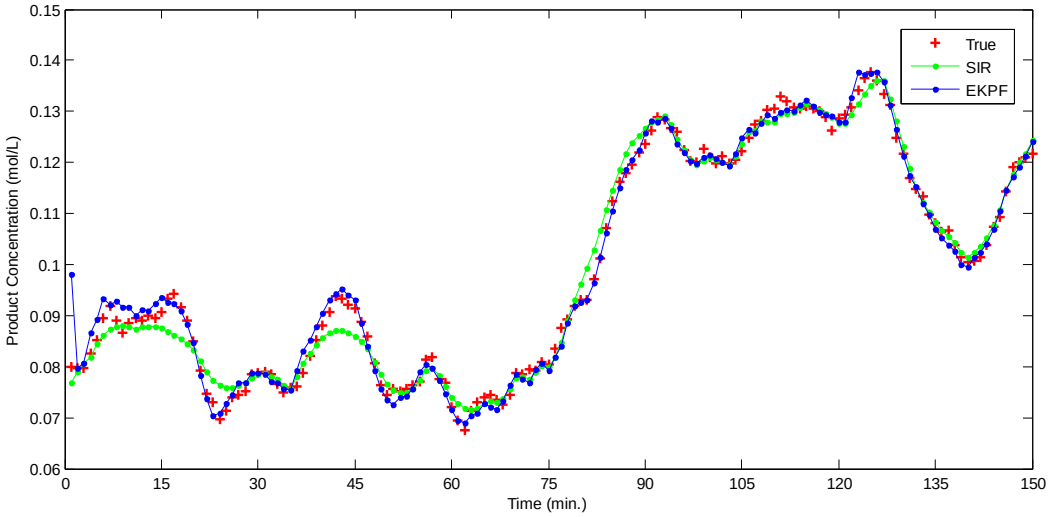

Fig. 5. Evolution of true and estimated product concentration of CSTR for a step change in flow rate.

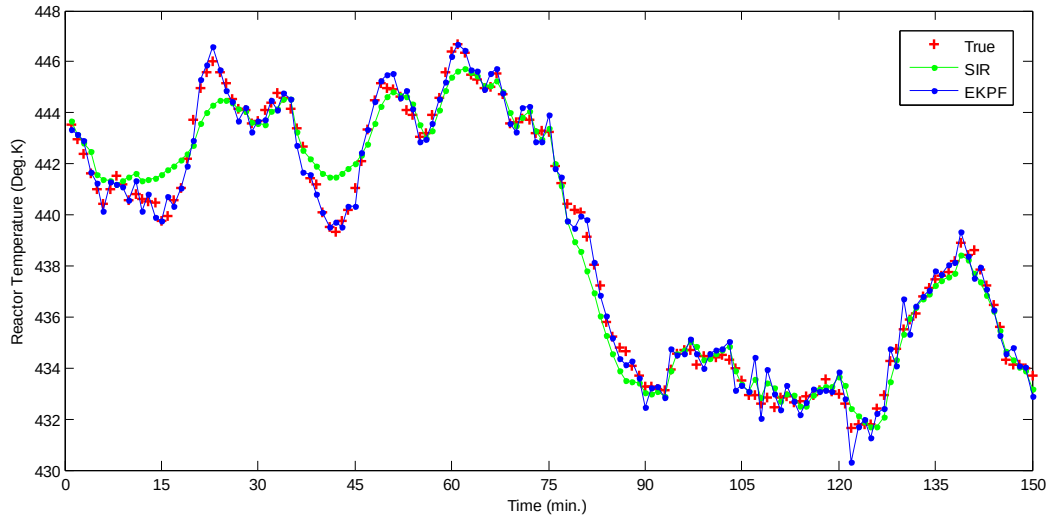

Fig. 6. Evolution of true and estimated reactor temperature of CSTR for a step change in flow rate.

The performance of these particle filters are compared using the root mean squared error (RMSE) over a simulation run which is defined by:

$$\text{RMSE}=\left(\frac{1}{T}\sum_{k=1}^{T}\left(\mathrm{x}_k-\hat{\mathrm{x}}_k\right)^2\right)^{1/2} \qquad (16)$$

where x_k and $\hat{\mathrm{x}}_k$ are true and estimated state at the instant k respectively and T indicates the total number of time steps.

Table 2
Estimation performance

Coolant flow rate (q_c)	Particle filtering algorithm	RMSE	
		Product concentration (C_A)	Reactor temperature (T)
Constant $(q_c = 97$ L/min)	SIR filter	0.0030	0.8847
	EKPF	0.0018	0.3654
Step change $(q_c = 97$ to 109 L/min)	SIR filter	0.0026	0.7012
	EKPF	0.0022	0.4460

The RMSE values of the estimated states of CSTR by the SIR filter and EKPF algorithm are reported in Table 2. From this table, it is clear that EKPF based on analytic local linearization outperforms the SIR filter.

The computational cost of the EKPF is higher than the SIR filter because the EKPF requires running an EKF in addition to particle filtering algorithm. Simulation study using this CSTR process clearly underscores that the computationally intensive EKPF performs better than SIR filter in order to deal with the nonlinear state estimation problem.

5 Conclusion

The application of particle filters for state estimation in a highly nonlinear CSTR process is presented. Particle filtering approximates the probability density as a finite number of particles. The nonlinear state estimation of CSTR is achieved by using SIR particle filter and EKPF. The simulation study on the performance of the particle filtering algorithms shows that EKPF can provide a relatively good tracking performance than SIR filter because the importance density in the EKPF algorithm is dependent on the current measurement but it is not so in the SIR filter. Hence, the choice made on the selection of importance density is critical, when designing a particle filter for a particular application. In addition, the RMSE values are also computed to show that the EKPF provides better estimation results than the SIR filter.

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