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# Comparison of unconstrained nonlinear state estimation techniques on a MMA polymer reactor ⋆

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**Abstract:** Estimation theory finds a wide variety of applications in process engineering. Most chemical processes exhibit highly nonlinear dynamics, and the extended Kalman filter (EKF) has been widely used to solve the estimation problem in chemical processes. However, it is claimed that the EKF performs poorly when the noise sequences are non-Gaussian(NG). Owing to high nonlinearity of chemical process dynamics, it is likely that innovation sequences are non-Gaussian. Nonlinear estimators such as the unscented Kalman filter (UKF) and particle filters (PF) have been developed to address the theoretical limitations of the EKF. In this paper, we study the effect of filter assumptions on their practical performance. Different estimation algorithms are applied onto a methyl methacrylate (MMA) continuous stirred tank reactor (CSTR) under different scenarios of state and measurement noise and plant-model mismatch.

*Keywords:* Nonlinear estimation, EKF, UKF, PF, MMA polymerization.

## 1. INTRODUCTION

State estimation is a fundamental problem in most fields of science and engineering. It is a method of combining the information from measurement sensors with a dynamic model of the system under consideration to predict its states. The need for increased estimation accuracy has led to the development of numerous algorithms based on various mathematical fundamentals. Fig. 1 provides a schematic of the different estimation techniques developed to date. In process industries, estimation is widely used to infer accurate measurements from noisy sensor data, as a soft sensor to predict variables that are not measurable online, estimate parameters to obtain accurate dynamic process models and for model predictive control. This not only provides improved control, but assists in fault detection and process monitoring.

It is well known that the Kalman filter provides an optimal solution to the state estimation problem for linear stochastic systems. It is however important to note that most chemical processes exhibit non-linear dynamics. The development of an estimator that provides an exact optimal solution to all nonlinear stochastic systems remains an open problem. The EKF is the most traditional and widely used estimator in chemical processes (Kiparissides et al. (2002),McAuley and MacGregor (1991)). While the EKF has been successfully used to solve many industrial problems, it has been demonstrated to perform poorly in the case of non-Gaussian posterior estimates obtained when state equations are non-linear (Daum (2005)). The EKF requires that the local linearization of the dynamic model to which the Kalman Filter is applied remains good over the entire operating region of the process, which may not hold true in all cases. Moreover, it requires that the nonlinear function vectors be smooth and once differentiable, which is not exhibited by many hybrid systems that involve continuous and discrete states (Patwardhan et al. (2007)). Therefore, though the EKF works well in many cases, there are scenarios where an alternate estimator needs to be applied to provide a better solution to the estimation problem. Estimation algorithms like the UKF and PF which rely on fitting an approximate solution to the dynamic equations rather than solving the linear equations obtained by approximating the system dynamics (like EKF), may be of use in scenarios where the EKF might exhibit poor performance. The literature relating application of these filters in chemical process engineering is recent. Imtiaz et al. (2006) applied the PF to a two state CSTR. Chen et al. (2005) used PF for state and parameter estimation in batch processes. Romanenko and Castro (2004) demonstrated the superiority of the UKF over the EKF in a simulated CSTR. In this paper, we study the use of three estimators in different scenarios for chemical processes. We attempt to address the need for different estimation algorithms in chemical processes. EKF, UKF and PF algorithms have been applied onto a MMA polymerization CSTR under different cases of measurement noise, state noise and plant-model mismatch. All estimators have been studied under similar tuning rules. Section 2 describes the filters that have been chosen for this study. Section 3 introduces the MMA model under consideration. In section 4, the case studies for different scenarios of noise and plant-model mismatch have been

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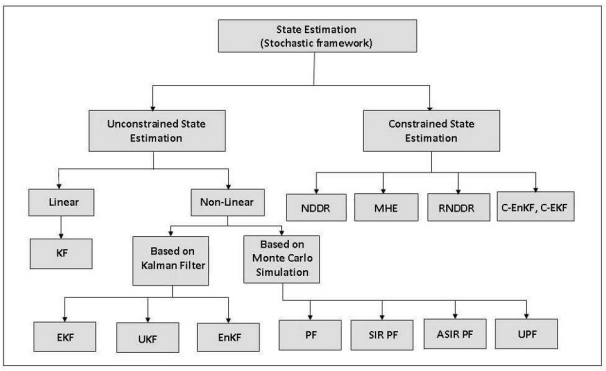



Fig. 1. Estimation : Classification chart of estimation methods

discussed. Section 5 summarizes the results of the case studies.

## 2. ESTIMATION METHODS

Consider the following nonlinear state space model :

$$x_k = f(x_{k-1}, u_{k-1}) + w_k \quad (1)$$

$$y_k = g(x_k) + v_k \quad (2)$$

The objective of state estimation is to sequentially calculate the state vector $x_k$ given the measurement $y_k$ at each time instant. Sometimes, not all the states are measureable online (hidden states) , hence the estimator would not only filter out the noise $v_k$, but also provide estimates of the hidden states (soft-sensing ability).

In our study, the traditional EKF, the unscented transform based UKF and the Bayesian Sequential Monte Carlo estimator SIR-PF(Sequential Importance Resampling) have been used. The algorithms for these estimators are described in the following sections.

### *2.1 Extended Kalman Filter*

The EKF is the most widely used estimator in chemical processes. It involves application of the traditional linear Kalman filter to the linearized system model at each time instant. The EKF works well when local linear models accurately represent the dynamics of the process. The EKF algorithm as explained by Lee and Ricker (1994) is summarized below.

The EKF algorithm requires an initial guess of the state vector, and state and disturbance covariances.

$$\hat{x}_0 = E[x_0] \quad (3)$$

$$P_0 = E[(x_0 - \hat{x}_0)(x_0 - \hat{x}_0)^T] \quad (4)$$

Time update:

The prior estimates are obtained by propagating the estimates from the previous time step through the nonlinear differential equations. The Jacobian of the nonlinear dynamics is used to estimate the prior covariance matrices.

$$\hat{x}_{k/k-1} = F(x_{k-1}, u_{k-1}, w) \quad (5)$$

$$A_{k-1} = \frac{\partial F(x, u_{k-1}, w)}{\partial x} \mid_{\hat{x}_{k-1}} \quad (6)$$

$$P_{x_{k/k-1}} = A_{k-1} P_{x_{k-1}} A_{k-1}^T \quad (7)$$

Measurement update:

The state vector and state covariance matrices are updated using the available measurement. The Kalman gain is the variable that defines the extent to which the estimator trusts the measurement or the estimates. For high magnitudes of measurement innovations, the Kalman gain accquires low values, indicating more trust in the state estiamtes. Low measurement innovations result in a high Kalman gain indicating complete trust in the measurements.

$$C_k = \frac{\partial G(x, w)}{\partial x} \mid_{\hat{x}_{k-1}} \quad (8)$$

$$\mathcal{K}_k = P_{x_{k/k-1}} C_k^T (C_k P_{x_{k/k-1}} C_k^T + R_n)^{-1} \quad (9)$$

$$\hat{x}_k = \hat{x}_{k/k-1} + \mathcal{K}_k [y_k - H(\hat{x}_{k/k-1}, w)] \quad (10)$$

$$P_{x_k} = (I - \mathcal{K}_k C_k) P_{x_{k/k-1}} \quad (11)$$

Eq. 10 is solved recursively at each time step thus making it a recursive minimum mean squared error estiamtor (MMSE). The EKF is computationally expensive for higher order systems as it requires calculation of the Jacobain at each time step. Bad initial state estimates or high plant-model mismatch might cause the filter to diverge. However, the EKF exhibits superior performance in scenarios where its underlying assumptions hold good.

### *2.2 Unscented Kalman Filter*

The UKF is based on the unscented transform (UT), which provides a deterministic sampling technique to approximate a distribution using a minimum number of points (sigma points) around the mean. As described by Julier and Uhlmann (1997) , the UT is based on approximating a Gaussian distribution, which is considered easier than approximating a nonlinear function or transformation. Wan and van der Merwe (2000) give a comprehensive review of the algorithm used in the UKF.

The UKF requires an initial guess of the state and covariance matrices, as represented by Eq. 3 and Eq. 4. In the following algorithm, the variable $x$ represents the augmented states, i.e. system states and the disturbance which is also modelled as a state.

Calculation of sigma points:

Sigma points along with their corresponding weights provide a deterministic method of representing the state distribution. $\mathcal{X}$ represents the sigma points, while W represents the weights.

$$\mathcal{X}_{k-1} = [\hat{x}_{k-1} \quad \hat{x}_{k-1} \pm \sqrt{(L+\lambda) P_{k-1}}] \quad (12)$$

$$W_0^{(m)} = \lambda/(L+\lambda) \quad (13)$$

$$W_0^{(c)} = \lambda/(L+\lambda) + (1 - \alpha^2 + \beta) \quad (14)$$

$$W_i^{(m)} = W_i^{(c)} = 1/(2(L+\lambda)) \quad i = 1, ..., 2L \quad (15)$$

L represents the number of states. $\lambda = \alpha^2(L+\kappa) - L$ is a scaling parameter where $\kappa$ (generally set to 0) and $\beta$ (incorporates knowledge of prior distribution of x) are secondary scaling parameters. The number of sigma points is 2L + 1.

Time update:

This step involves calculation of the prior estimates, obtained by propagating the sigma points through the nonlinear system dynamics.

$$\mathcal{X}_{k/k-1} = F(\mathcal{X}_{k-1}) \quad (16)$$

$$\mathcal{Y}_{k/k-1} = G(\mathcal{X}_{k/k-1}) \tag{17}$$

$$\hat{x}_{k/k-1} = \sum_{i=0}^{2L} W_i^{(m)} \mathcal{X}_{i,k/k-1} \tag{18}$$

$$P_{k/k-1} = \sum_{i=0}^{2L} W_i^{(c)} [\mathcal{X}_{i,k/k-1} - \hat{x}_{k/k-1}][\mathcal{X}_{i,k/k-1} - \hat{x}_{k/k-1}]^T \tag{19}$$

$$\hat{y}_{k/k-1} = \sum_{i=0}^{2L} W_i^{(m)} \mathcal{Y}_{i,k/k-1} \tag{20}$$

Measurement update:

The measurement update in the UKF is similar to the Kalman update except that the cross-covariances are used rather than the auto-covariance. It has however been shown that there is an increased efficiency of the measurement update step in the case of the UKF (Kandepu et al. (2008)). Posterior estimates of the state are calculated by using the Kalman gain to weight the measurement innovations with the state estimates.

$$\mathcal{K} = P_{x_k y_k} P_{y_k y_k}^{-1} \tag{21}$$

$$\hat{x}_{k/k} = \hat{x}_{k/k-1} + \mathcal{K}(y_k - \hat{y}_{k/k-1}) \tag{22}$$

$$P_k = P_{k/k-1} - \mathcal{K} P_{y_k y_k} \mathcal{K}^T \tag{23}$$

The UKF estimates are said to be accurate upto $3^{rd}$ order statistics for Gaussian distributions and upto $2^{nd}$ order statistics for non-Gaussian distributions (Julier and Uhlmann (1997)). The true mean and covariance estimates of the UKF are more accurate than those obtained through the EKF. In addition, it does not require computation of the Jacobian, thereby reducing the computational complexity of the problem.

### *2.3 Particle Filter*

Particle filtering is a method of recursive Bayesian filtering of Monte Carlo simulations. The algorithm is based on calculating the entire posterior distribution of the state rather than finding a single estimate at each sampling instant. Random samples (particles) are obtained from a distribution which are then propagated through the nonlinear differential equations to give prior particles. The measurement information which is then available is fused with this prior distribution of particles to generate the posterior distribution. The particle filtering algorithm is variously known as bootstrap filtering or condensation algorithm (Arulampalam et al. (2002) and Gordon et al. (1993)). Various algorithms have been developed by extending the generic PF. In our study , the SIR-PF, which resolves the degeneracy problem of generic PFs, has been used. It includes an importance resampling step which ensures that particles formed are of equal weights (each of 1/N), thus avoiding having particles of lower weights during computation.

To calculate the estimate at time step k, first random samples are generated from $p(x_{k-1}|y_{k-1})$, i.e $p(x_{k-1}|y_{k-1})$ is approximated by a set of N (fixed) particles $x_k^i, i = 1, ..., N$ with associated weights $w_k^i, i = 1, ..., N$. The weights are normalized such that $\sum_{i=1}^{N} w_k^i = 1$. These particles are propagated through the nonlinear differential equations to obtain prior particles which represent the density $p(x_k|y_{k-1})$.

The key step in the importance sampling algorithm is to define an importance density $q(x_{k-1}|y_{k-1})$, drawing samples from which would be equivalent to drawing samples from the posterior distribution. The weights of the particles from the importance distribution would be

$$w_{k-1}^i \propto \frac{p(x_{k-1}^i|y_{k-1})}{q(x_{k-1}^i|y_{k-1})} \tag{24}$$

The SIR-PF makes an assumption that the prior is an approximation of the posterior, i.e. the prior is the importance density (Arulampalam et al. (2002)). The importance weights would then be obtained from the likelihood. From the derivation from Bayes rule as stated below, the prior density is fused with the measurement density at time step k ($p(y_k|x_k^i)$) to obtain the posterior distribution of the state.

$$Posterior \propto likelihood \times prior \tag{25}$$

$$p(x_k|y_k) = p(y_k|x_k) \times p(x_k|y_{k-1}) \tag{26}$$

The estimated state vector is calculated as the mean of $p(x_k|y_k)$. The particle filter algorithm does not make any assumptions about the distribution of the states. It is claimed to work much better than the other estimators where noise distributions are non-Gaussian. The challenges in PF lie in reducing its computational complexity and choice of its importance density.

## 3. PROCESS DESCRIPTION

A free-radical MMA polymerization process has been used for this study. Polymerization takes place in a CSTR with azo-bis-isobutyronitrile (AIBN) as an initiator and toluene as a solvent. Fig. 2 describes the reactor. The reactions are exothermic and a cooling jacket is used to remove the heat of reaction. The details of the model can be obtained from Silva and Flores (1999).The reaction mechanism for MMA free-radical polymerization is as follows:

Initiation:
$I \xrightarrow{k} R^{\cdot}$
$R^{\cdot} + M \xrightarrow{k_I} P_1^{\cdot}$

Propagation:
$P_i^{\cdot} + M \xrightarrow{k_p} P_{i+1}^{\cdot}$

Monomer Transfer:
$P_i^{\cdot} + M \xrightarrow{k_{fm}} P_i^{\cdot} + D_i$

Addition Termination:
$P_i^{\cdot} + P_j^{\cdot} \xrightarrow{k_{tc}} D_{i+j}$

Disproportionation Termination:
$P_i^{\cdot} + P_j^{\cdot} \xrightarrow{k_{td}} D_i + D_j$

A mathematical model of the process is developed based on the following assumptions: (a) constant volume of the reactor, (b) reactor contents are perfectly mixed, (c) no gel effect, (d) uniform cooling fluid temperature, (e) heat capacity and density of cooling fluid and reactor mixture remain constant. The mass and energy balance equations are as follows:

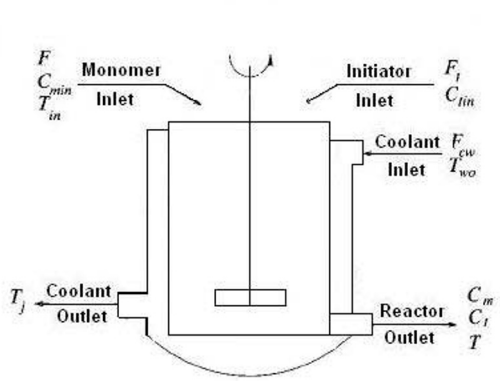



Fig. 2. MMA polymerization reactor flow sheet

$$\frac{dC_m}{dt} = -(k_p + k_{fm})C_m P_0 + \frac{F(C_{min} - C_m)}{V} \quad (27)$$

$$\frac{dC_I}{dt} = -k_I C_I + \frac{(F_I C_{Iin} - F C_I)}{V} \quad (28)$$

$$\frac{dT}{dt} = \frac{(-\Delta H)k_p C_m P_0}{\rho C_p} - \frac{UA}{\rho C_p V}(T - Tj) + \frac{F(T_{in} - T)}{V} \quad (29)$$

$$\frac{dD_0}{dt} = (0.5k_t c + k_t d)P_0^2 + k_{fm} C_m P_0 - \frac{FD_0}{V} \quad (30)$$

$$\frac{dD_1}{dt} = Mm(k_p + k_f m)C_m P_0 - \frac{FD_1}{V} \quad (31)$$

$$\frac{dTj}{dt} = \frac{F_{cw}(T_{w0} - T_j)}{V_0} + \frac{UA}{\rho_w C_{pw} V_0}(T - T_j) \quad (32)$$

$$P_o = \sqrt{\frac{2f^* C_I k_I}{k_{td} + k_{tc}}} \quad (33)$$

Table 1 lists the design and operating parameters. $f^*$ is the initiator efficiency. The temperatures $(T_j, T)$ are the measured states, while the reactor concentrations $(C_m, C_I)$ and polymer moments $(D_0,\ D_1)$ are considered as the hidden states (to be estimated). A parameter estimation problem can be considered for any of the kinetic parameters $(k_i, k_p, k_{fm}, k_{tc}, k_{td})$.

Table 1. Operating Parameters

| | |
|---|---|
| $F = 1.0m^3/h$ | Mm = 100.12 $kg/kgmol$ |
| $F_I = 0.0032m^3/h$ | f* = 0.58 |
| $F_{cw} = 0.1588m^3/h$ | R = 8.314 $kJ/(kgmol.K)$ |
| $C_{min} = 6.4678kgmol/m^3$ | $-\Delta$ H = 57800 $kJ/kgmol$ |
| $C_{Iin} = 8.0kgmol/m^3$ | $E_p = 1.8283 \times 10^4 kJ/kgmol$ |
| $T_{in} = 350K$ | $E_I = 1.2877 \times 10^5 kJ/kgmol$ |
| $T_{w0} = 293.2K$ | $E_{fm} = 7.4478 \times 10^4 kJ/kgmol$ |
| $U = 720kJ/(h.K.m^2)$ | $E_{tc} = 2.9442 \times 10^3 kJ/kgmol$ |
| $U = 2.0m^2$ | $E_{td} = 2.9442 \times 10^3 kJ/kgmol$ |
| $V = 0.1m^3$ | $A_p = 1.77 \times 10^9 m^3/(kgmol.h)$ |
| $V_0 = 0.02m^3$ | $A_I = 3.792 \times 10^{18} l/h$ |
| $\rho = 866kg/m^3$ | $A_{fm} = 1.0067 \times 10^{15} m^3/(kgmol.h)$ |
| $\rho_w = 1000kg/m^3$ | $A_{tc} = 3.8223 \times 10^{10} m^3/(kgmol.h)$ |
| $C_p = 2.0kJ/(kg.K)$ | $A_{td} = 3.1457 \times 10^{11} m^3/(kgmol.h)$ |
| $C_{pw} = 4.2kJ/(kg.K)$ | $A_{td} = 3.1457 \times 10^{11} m^3/(kgmol.h)$ |

## 4. CASE STUDIES

The model is tested for various scenarios of Gaussian and non-Gaussian state and measurement noise sequences, and plant-model mismatch. Using these case studies, we establish the scenarios in which significant difference in filter performance is exhibited. In each case study, same noise sequences and filter tuning parameters have been used for all filters. Measurement noise has been considered on the reactor and coolant temperatures. State noise is added to the system dynamic equations of the monomer and initiator concentrations. The polymer moments have not been used to compare filter performance as they are unobservable states.

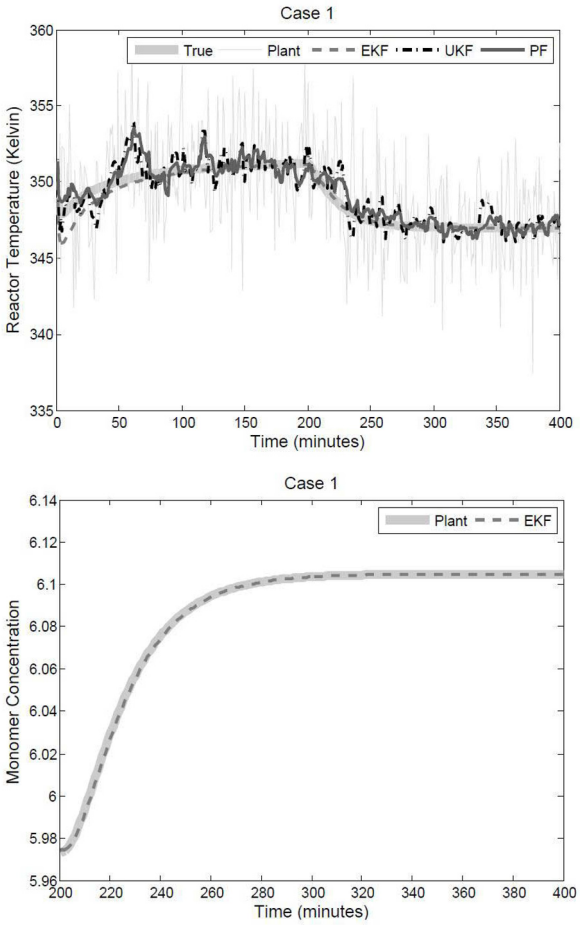


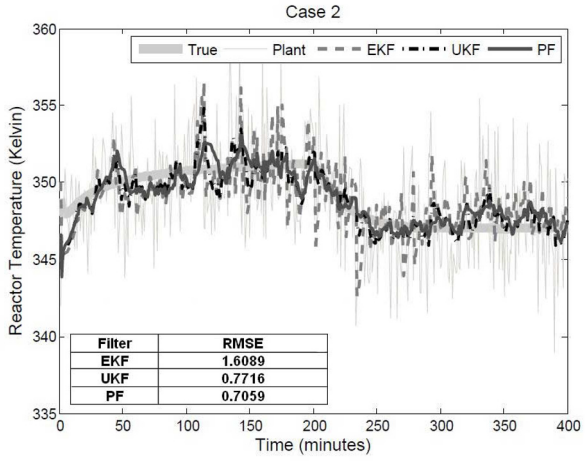

Fig. 3. No state noise. Gaussian measurement noise. 10% Positive step in cold water flow rate.

### *4.1 Case 1*

This case represents the simulation for Gaussian noise on the measurements (temperatures). Fig. 3 indicates that the EKF works extremely well when the estimator is used to filter the measurement noise. It also tracks the concentrations (hidden states). It is important to note that there is an exact match of plant and model in this case. Analysis of this case reveals that the Kalman gain goes to zero thereby trusting the model estimates completely. This shows the importance of good process models in estimation.

### *4.2 Case 2*

In addition to Gaussian measurement noise on the temperatures, Gaussian state noise is introduced on the concentrations. Fig. 4 indicates the superiority of the PF and UKF performance over the EKF. The Kalman gain goes to zero no more, thus weighting the measurement innovations and the estimates. The soft-sensing ability of the



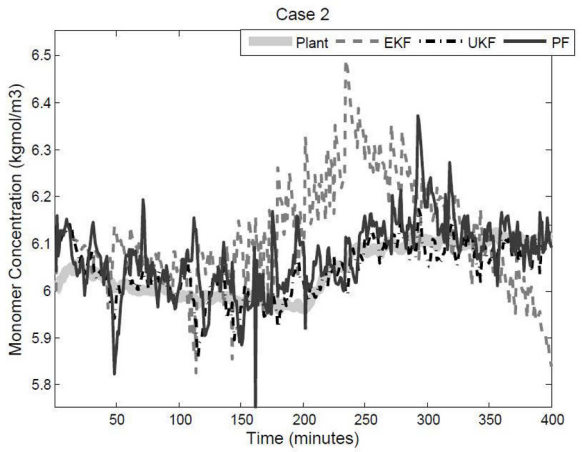




Fig. 4. Gaussian state and measurement noise. 10 % positive step in cold water flow rate.

EKF is limited as it diverges completely in concentration estimation.

### *4.3 Case 3*

Non-Gaussian measurement and non-Gaussian state noise is introduced into the system. Fig. 5 indicates that the results are similar to that of Case 2. This demonstrates that any Gaussian state noise transforms into non-Gaussian form after passing through the non-linear dynamics.

### *4.4 Case 4*

Non-Gaussian measurement noise is introduced. No state noise is introduced. It is seen that the EKF works extremely well in tracking the true measurement (Fig. 6). This reiterates what was concluded in case 1, that for any measurement noise and exact plant-model match, the EKF gives good estimates.

### *4.5 Case 5*

Plant-model mismatch is introduced in the termination rate constant. There is no state noise, but non-Gaussian measurement noise is introduced. The model uses a fixed value of the termination rate constant while the parameter is made to vary in the plant equations. A plot of the measured reactor temperature indicates that the EKF gives biased estimates unlike the UKF and PF (Fig. 7).

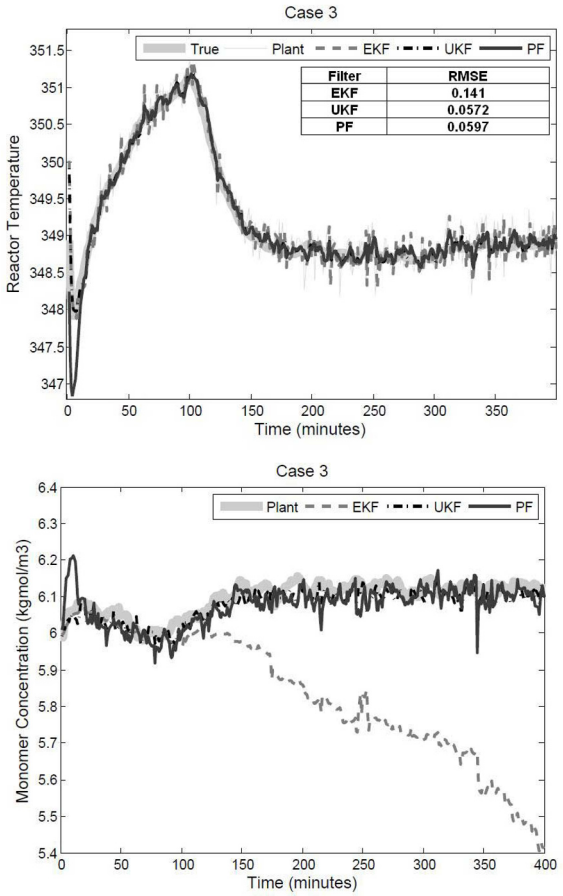



Fig. 5. Non-Gaussian state and measurement noise. 10 % positive step in monomer flow rate.

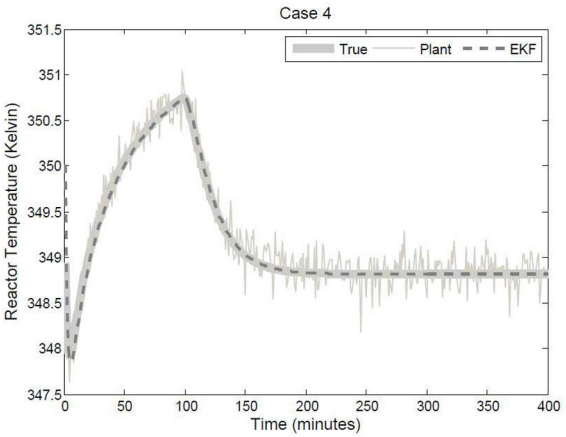



Fig. 6. Non-Gaussian measurement noise. 10 % positive step in monomer flow rate.

### *4.6 Case 6*

In this case, we try to capture the plant-model mismatch by estimating the unknown kinetic parameter. The initiation rate constant has been used for this study as the reactor is highly sensitive to this parameter. Small changes of this parameter causes wide variations in the monomer and initiator concentrations, in turn affecting the polymer moments. Fig. 8 indicates the superiority of the UKF and PF over the EKF. Though the RMSE values are small, it can be argued that small changes in this parameter value could affect the system in a large way.

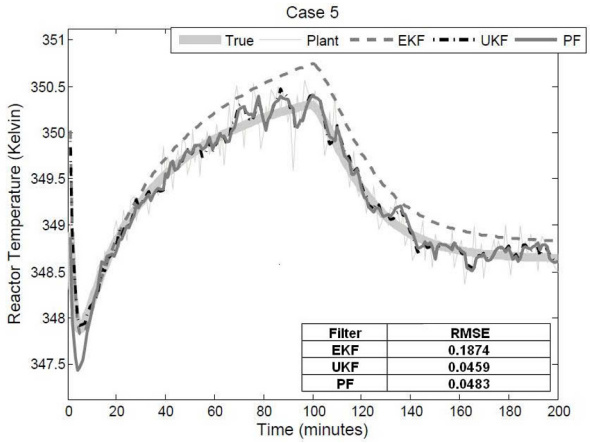



Fig. 7. Plant model mismatch through termination kinetic rate constant. 10 % step in cold water flow rate.

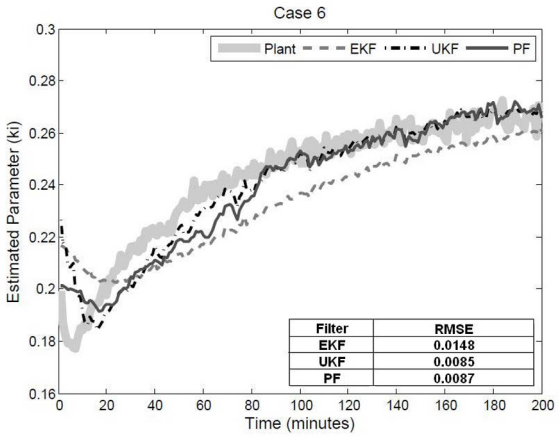



Fig. 8. Parameter Estimation for initiation rate constant.

## 5. CONCLUSION

Table 2 summarizes the case studies. There is no plant-model mismatch when the model captures the system dynamics including the state noise sequences. For perfect plant-model match, the EKF is capable of providing good estimates. This is because the Kalman gain approaches zero, thus trusting the model estimates completely (Cases 1 & 4). Any state noise translates into non-Gaussian form after passing through the non-linear dynamics causing the EKF to perform poorly (Cases 2 & 3). For plant-model mismatch, UKF and PF perform better than the EKF. It can however be seen that the EKF works well when the linear approximation of system equations represent system dynamics and performs poorly during sudden jump in process variables (Case 5). Parameter estimation can be treated as a form of plant-model mismatch, and the UKF and PF work better than the EKF (Case 6).

The UKF and PF seem to be similar in performance behavior, however, for extreme non-Gaussian behavior, difference in estimator performance may be seen. Estimator performance varies based on degree of non-linearity of system dynamics, state and measurement noise levels and degree of plant-model mismatch. The above analysis shows that for chemical processes, the UKF and PF exhibit superior performance over the EKF. This is because the linearization approximation of the EKF does not capture highly nonlinear process dynamics accurately. Highly non-linear dynamics is exhibited when noise covariances are high, there is a sudden jump in process variables and for large state systems. In these scenarios, it is important to consider the UKF and PF as choice of estimators.

Table 2. Tabulation of case studies *(G = Gaussian ; NG = Non-Gaussian)*

| Case | Measurement Noise | State Noise | Plant-Model Mismatch | Conclusion (choice of filter) |
|---|---|---|---|---|
| 1 | G | - | - | EKF, UKF, PF |
| 2 | G | G | - | UKF,PF |
| 3 | NG | NG | - | UKF,PF |
| 4 | NG | - | - | EKF UKF, PF |
| 5 | NG | - | In parameter | UKF, PF |
| 6 | NG | - | Parameter Estimated | UKF,PF |

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