Evaluation of Adaptive Extended Kalman Filter Algorithms for State Estimation in Presence of Model-Plant Mismatch

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Abstract: The occurrence of model-plant mismatch is a common problem in dynamic model based applications such as state estimation. The use of an inaccurate model results in biased estimates of the states. Hence, conventional state estimation algorithms are modified in various ways to compensate for model-plant mismatch. In this work, the performance of four adaptive state estimation algorithms is compared in the presence of a model plant mismatch arising due to random drifts in parameter values. The comparison is carried out through simulations on a benchmark non-isothermal CSTR problem. Simulation results demonstrate that online reidentification of the parameters susceptible to drift or change is the most effective approach to minimize the effect of model-plant mismatch on the state estimates.

Keywords: adaptive state estimation; extended Kalman filter; model-plant mismatch; state and parameter estimation

1. INTRODUCTION

In various chemical processes, online estimation of the process states forms an essential part of monitoring the process conditions and state-feedback based control. This is because processes are affected by various random disturbances and it is difficult to obtain regular and noisefree online measurements of many process states, such as concentrations, compositions, etc. The Bayesian state estimation approach is widely used because it provides a systematic and general approach to handle the effect of various random uncertainties on the process states and measurements. Bayesian state estimation algorithms use a first-principles based dynamic model and the statistical properties of the random disturbances and measurements to obtain the posterior distribution of the state estimates. The accuracy of the state estimation algorithms is, therefore, reliant on the accuracy of the dynamic model used to generate the state predictions (Chitralekha et al., 2010) and the statistical properties of the process disturbances and noise (Fitzgerald, 1971; Bavdekar et al., 2011).

The standard Bayesian state estimation algorithms available in the literature are developed under the assumption that the values of model parameters used are reasonably accurate (Patwardhan et al., 2012). In most cases, the model building exercise is carried out offline using batches of input-output data. The model structure and parameters obtained from this exercise are then deployed for online use. However, it is well known that due to changes in process or equipment conditions, certain parameters of a process or unit may change over time. For example, in

a catalytic reactor, the catalyst activity may change as time progresses due to various reasons, such as sintering, fouling, etc. Another example is the variation in the height equivalent to a theoretical plate (HETP) of a packed-bed distillation column due to changes in the available surface area of the packed-bed particles. This variation affects the final composition of the distillate and bottoms streams. Such random drifts introduce a time-varying model-plant mismatch (MPM), which deteriorates the accuracy of the model used to generate state predictions. Using a model without accurate parameters can lead to biased estimates of the unmeasured states, which can have further implications on applications such as state-feedback control, where the controlled variables are not directly measured. Hence, it becomes essential to modify the standard state estimation algorithms to compensate for the parametric model-plant mismatch.

Joint state and parameter estimation formulations (Gordon et al., 1993; Kitagawa, 1998; Tulsyan et al., 2013) are one of the most popular approaches used to compensate for model plant mismatch. In this approach, the parametric variations are modelled using a random walk model and the new parameter estimates are jointly obtained along with the state estimates using the Bayesian state estimation algorithm. However, one limitation of this approach is that the maximum number of parameters that can be uniquely estimated is equal to the number of measurements available (Pannocchia and Rawlings, 2003). Moreover, if the sensitivity matrix of the state-to-measurement equations is ill-conditioned, the parameter estimates obtained in such conditions are less accurate (Olivier et al., 2012). Kantas et al. (2009) provide a comprehensive

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overview of joint state and parameter estimation algorithms using particle filters and discuss the pros and cons associated with each of them. The dual state and parameter estimation approach (Gove and Hollinger, 2006; Moradkhani et al., 2005; Olivier et al., 2012) overcomes the limitation posed due to ill-conditioning of the sensitivity matrix of state-to-measurement equations by solving the state and parameter estimation problem, independently and in parallel to each other. Both– the joint and dual– state and parameter estimation approaches attempt to reduce the errors arising from model plant mismatch by online re-identification of the model parameters.

On the other hand, adaptive state estimation algorithms are proposed in the literature, that attempt to compensate for errors arising from model-plant mismatch through mechanisms other than re-identification of model parameters. These methods are based on the premise that the contribution towards the prediction error covariance of the states arises from two terms, namely the model dynamics of covariance propagation and the covariance of the process disturbances. A model-plant mismatch introduces extra error in propagation of the estimation error covariance, which is accounted for by tuning the value of the covariance of the process disturbances. Efe et al. (1999) have proposed an adaptive Kalman filter, which uses a scaling factor that is multiplied with the process noise covariance matrix. The scaling factor is a positive real number, which is computed based on the difference between the observed sum of squared error of the innovations and the trace of the innovations covariance matrix obtained from the state estimation algorithm. Thus, the scaling factor modifies the process noise covariance matrix in an adaptive manner. A high value of the scaling factor indicates a deterioration in the model predictions, thereby increasing the uncertainty associated with the predicted states.

Linder and Shafai (1997) have proposed a robust PI Kalman filter, which introduces artificial bias states, whose dynamics are modelled as an integrator. The bias term is then added to the state predictions in order to correct for the error introduced due to model-plant mismatch. The extent of the integral action is determined through the innovations and an adaptive integral gain, which is a function of the estimation error covariance matrices and the measurement noise covariance. The algorithm uses the steady state Kalman gain obtained from the standard Kalman filter algorithm and an empirical tuning method of the gain and integral terms to obtain a stable realisation of the filter. Bodizs et al. (2011) have developed the integral Kalman predictor (IKP) which is similar to the one developed by Linder and Shafai (1997). In their case, however, while the proportional term is fixed and can be tuned, the integral term is adaptive and its value is obtained through the solution of Riccati equations at every sampling instant. Shenoy (2010) has proposed the use of a proportional-integral Kalman filter (PI-KF), in which the error arising due to model-plant mismatch or linearisation is compensated by using a bias term, which is integrated over time based on the innovation sequence. While the concept of the PI-KF is similar to the IKP, there are two key differences. First, the IKP is implemented as a Kalman predictor. This implies that the IKP algorithm does not make used of the current measurements to update

the predicted value of the states. One the other hand, the implementation of the PI-KF is similar to that of the standard KF. The second difference is that the integral gain is computed adaptively in the IKP algorithm, while it is used as a tuning parameter in the PI-KF algorithm. In both algorithms, the number of integral states are equal to the number of measurements available.

In this work, simulation studies are carried out to compare the performance of the three adaptive state estimation algorithms– the adaptive extended Kalman filter (EKF) with covariance scaling, the PI-Kalman filter and the integral Kalman predictor– in the presence of a modelplant mismatch. The model-plant mismatch is introduced via a random drift in certain parameter values of the process and is, therefore, time-varying in nature. The benchmark CSTR case study (Marlin, 1995) is used to compare the state estimation algorithms. The performance of these three algorithms is also compared with the popular approach of joint state and parameter estimation (Gordon et al., 1993).

The remainder of the paper is organised as follows. The process model used for simulations and state estimation is described in Section 2. The state estimation algorithms that are compared in this study are described in Section 3. The simulation case used to compare the performance of the state estimators and the results obtained are described in detail in Section 4, followed by the concluding remarks in Section 5.

2. PROCESS MODEL

A general nonlinear process can be mathematically represented using the following equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{f} \left(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}, t \right)$$

$$\mathbf{y} \left(t \right) = \mathbf{h} \left(\mathbf{x}, t \right)$$
 (1)

where, $\mathbf{x} \in \mathbb{R}^n$ represents the process states, $\mathbf{u} \in \mathbb{R}^m$ represents the manipulated inputs, $\boldsymbol{\theta} \in \mathbb{R}^p$ represents the model parameters and $\mathbf{y} \in \mathbb{R}^r$ represents the process measurements. For the purpose of simulations and modelling for state estimation the process is discretised as follows

$$\mathbf{x}_{k} = \mathbf{x}_{k-1} + \int_{(k-1)T}^{kT} \mathbf{f} \left(\mathbf{x} \left(\tau \right), \mathbf{u}_{k-1}, \boldsymbol{\theta}_{k-1}, \tau \right) d\tau + \mathbf{w}_{k-1}(2)$$

$$= \mathbf{F} \left(\mathbf{x}_{k-1}, \mathbf{u}_{k-1}, \boldsymbol{\theta}_{k-1} \right) + \mathbf{w}_{k-1}$$
(3)

$$\mathbf{y}_{k} = \mathbf{h}\left(\mathbf{x}_{k}\right) + \mathbf{v}_{k} \tag{4}$$

where, $\mathbf{w}_{k-1} \sim \mathcal{N}(\bar{\mathbf{0}}, \mathbf{Q})$ represents the random unmodelled process disturbances and $\mathbf{v}_k \sim \mathcal{N}(\bar{\mathbf{0}}, \mathbf{R})$ is the measurement noise. The process disturbances can be modelled to enter through the inputs or as additive in the state dynamics. Further, it is assumed that \mathbf{w}_{k-1} and \mathbf{v}_k are mutually independent random signals.

3. STATE ESTIMATION IN PRESENCE OF MPM

The adaptive state estimation algorithms that are compared in this work are described briefly in this section.

3.1 Joint EKF

The most popular approach to account for random changes in the parameter is to model the parametric variations as an integrated white noise process and simultaneously estimate the process states and parameters using the EKF. The joint EKF algorithm, henceforth abbreviated to as J-EKF, is as follows

$$\hat{\mathbf{x}}_{k|k-1} = \mathbf{F}\left(\hat{\mathbf{x}}_{k-1|k-1}, \mathbf{u}_{k-1}, \hat{\boldsymbol{\theta}}_{k-1|k-1}\right)$$
(5)

$$\boldsymbol{\theta}_{k|k-1} = \boldsymbol{\theta}_{k-1|k-1} \tag{6}$$

Define the following augmented vectors and matrices

$$\hat{\mathbf{x}}^{a} = \begin{bmatrix} \hat{\mathbf{x}} & \hat{\boldsymbol{\theta}} \end{bmatrix} \quad \mathbf{Q}^{a} = \begin{bmatrix} \mathbf{Q} & \mathbf{0} \\ \mathbf{\bar{0}} & \mathbf{Q}_{\theta} \end{bmatrix}$$
(7)

where, \mathbf{Q}_{θ} refers to the covariance of the noise in $\boldsymbol{\theta}$. The Kalman gain is computed as follows

$$\mathbf{P}_{k|k-1} = \mathbf{\Phi}_a \mathbf{P}_{k-1|k-1} \mathbf{\Phi}_a^T + \mathbf{\Gamma}_a \mathbf{Q}^a \mathbf{\Gamma}_a^T \tag{8}$$

$$\mathbf{K}_{k} = \mathbf{P}_{k|k-1} \mathbf{C}_{a}^{T} \left(\mathbf{C}_{a} \mathbf{P}_{k|k-1} \mathbf{C}_{a}^{T} + \mathbf{R} \right)^{-1}$$
(9)

where,
$$\Phi_a = \begin{bmatrix} \Phi & \Phi_c \\ \bar{\mathbf{0}} & \mathbf{I}_p \end{bmatrix}$$
, $\Phi = \frac{\partial \mathbf{F}}{\partial \mathbf{x}}\Big|_{\hat{\mathbf{x}}_{k-1|k-1}}$, $\Phi_c = \frac{\partial \mathbf{F}}{\partial \mathbf{x}}\Big|_{\hat{\mathbf{x}}_{k-1|k-1}}$, $\Phi_c = \frac{\partial \mathbf{F}}{\partial \mathbf{x}}\Big|_{\hat{\mathbf{x}}_{k-1|k-1}}$

 $\begin{array}{l} \frac{\partial \mathbf{F}}{\partial \boldsymbol{\theta}}|_{\boldsymbol{\hat{\theta}}_{k-1|k-1}}; \ \boldsymbol{\Gamma}_{a} = \begin{bmatrix} \mathbf{I}_{w}^{w} & \mathbf{J} \\ \bar{\mathbf{0}} & \mathbf{I}_{p} \end{bmatrix}, \ \boldsymbol{\Gamma} \ \text{is the partial differential} \\ \text{of } \mathbf{F} \ \text{based on the source of the process noise. E.g., if} \\ \text{noise enters through inputs, } \mathbf{\Gamma} = \frac{\partial \mathbf{F}}{\partial \mathbf{u}}|_{\mathbf{u}_{k-1}}. \ \text{If process} \\ \text{noise is modelled as additive in state dynamics, } \mathbf{\Gamma} = \mathbf{I}_{r}. \\ \mathbf{C} = \frac{\partial \mathbf{h}}{\partial \mathbf{x}}|_{\hat{\mathbf{x}}_{k|k-1}} \ \text{and } \mathbf{C}_{a} = [\mathbf{C} \ \bar{\mathbf{0}}]. \end{array}$

The updated values of the joint states and their covariance matrix are obtained as

$$\hat{\mathbf{x}}_{k|k}^{a} = \hat{\mathbf{x}}_{k|k-1}^{a} + \mathbf{K}_{k} \left(\mathbf{y}_{k} - \hat{\mathbf{y}}_{k|k-1} \right)$$
(10)

$$\mathbf{P}_{k|k} = (\mathbf{I}_{n+p} - \mathbf{KC}_a) \,\mathbf{P}_{k|k-1} \tag{11}$$

Finally, $\hat{\mathbf{x}}_{k|k} = \hat{\mathbf{x}}^a_{k|k}(1:n)$ and $\hat{\boldsymbol{\theta}}_{k|k} = \hat{\mathbf{x}}^a_{k|k}(n+1:n+p)$.

3.2 EKF with covariance scaling

The adaptive Kalman filter with covariance scaling proposed by Efe et al. (1999) is described in this section. The prediction step is given by

$$\hat{\mathbf{x}}_{k|k-1} = \mathbf{\Phi} \hat{\mathbf{x}}_{k-1|k-1} + \mathbf{\Gamma}_u \mathbf{u}_{k-1}$$
(12)

$$\hat{\mathbf{y}}_{k|k-1} = \mathbf{C}\hat{\mathbf{x}}_{k|k-1} \tag{13}$$

The predicted and innovation covariance matrices are obtained as

$$\mathbf{P}_{k|k-1} = \mathbf{\Phi} \mathbf{P}_{k-1|k-1} \mathbf{\Phi}^T + \Omega_{k-1} \mathbf{\Gamma}_d \mathbf{Q} \mathbf{\Gamma}_d^T$$
(14)

$$\mathbf{P}_{ee,k} = \mathbf{C}\mathbf{P}_{k|k-1}\mathbf{C}^T + \mathbf{R}$$
(15)

$$= \mathbf{C} \mathbf{\Phi} \mathbf{P}_{k-1|k-1} \mathbf{\Phi}^T \mathbf{C}^T + \Omega_{k-1} \mathbf{C} \mathbf{\Gamma}_d \mathbf{Q} \mathbf{\Gamma}_d^T \mathbf{C}^T (16)$$

where, Ω denotes the scaling factor, which is used to modify the covariance matrix in the presence of modelplant mismatch. Let β , γ and δ denote the trace of $\mathbf{P}_{ee,k}$, $\mathbf{C} \Phi \mathbf{P}_{k-1|k-1} \Phi^T \mathbf{C}^T$ and $\mathbf{C} \Gamma_d \mathbf{Q} \Gamma_d^T \mathbf{C}^T$ respectively. Further, let ν denote the sum of squares of the observed innovations vector $(\mathbf{y}_k - \hat{\mathbf{y}}_{k|k-1})$. The value of Ω is obtained as follows

$$\Upsilon_k = a\Omega_0 + b\Omega_{k-1} + c\left(\frac{\nu_k - \gamma_k}{\delta_k}\right) \tag{17}$$

$$\Omega_k = \max\left(\Upsilon_k, 0\right) \tag{18}$$

If $\nu_k = \beta_k$

$$\Upsilon_k = a\Omega_0 + (b+c)\,\Omega_{k-1} \tag{19}$$

$$\Omega_k = \max\left(\Upsilon_k, 0\right) \tag{20}$$

where, a, b, c are constants such that a + b + c = 1 and Ω_0 is the value of the scaling factor at k = 0 and is normally chosen as $\Omega_0 = 1.0$.

The updated estimates of the states and the covariance matrix are obtained as follows

$$\mathbf{K}_k = \mathbf{P}_{k|k-1} \mathbf{C}^T \mathbf{P}_{ee,k}^{-1} \tag{21}$$

$$\hat{\mathbf{x}}_{k|k} = \hat{\mathbf{x}}_{k|k-1} + \mathbf{K}_k \left(\mathbf{y}_k - \hat{\mathbf{y}}_{k|k-1} \right)$$
(22)

$$\mathbf{P}_{k|k} = (\mathbf{I}_n - \mathbf{K}_k \mathbf{C}) \, \mathbf{P}_{k|k-1} \tag{23}$$

It should be noted that although the above algorithm is proposed for linear systems with a Kalman filter, it can be easily modified for nonlinear systems with an EKF, henceforth abbreviated as A-EKF.

3.3 Proportional-integral Kalman filter

The proportional-integral Kalman filter (PI-KF) (Shenoy, 2010) integrates the errors arising due to linearization and model-plant mismatch and adds this error to the predicted values of the states.

$$\hat{\mathbf{x}}_{k|k-1} = \mathbf{\Phi} \hat{\mathbf{x}}_{k-1|k-1} + \mathbf{\Gamma}_u \mathbf{u}_{k-1} + \mathbf{P}_i \boldsymbol{\upsilon}_{k-1} \qquad (24)$$

$$\hat{\mathbf{y}}_{k|k-1} = \mathbf{C}\hat{\mathbf{x}}_{k|k-1} \tag{25}$$

where, $\mathbf{P}_i \in \mathbb{R}^{n \times n}$ is analogous to the gain in a PIcontroller. $\boldsymbol{v}_{k-1} \in \mathbb{R}^n$ is the error term, obtained as

$$\boldsymbol{v}_{k} = \boldsymbol{v}_{k-1} + \mathbf{K}_{i} \left(\mathbf{y}_{k-1} - \hat{\mathbf{y}}_{k-1|k-2} \right)$$
(26)

where, \mathbf{K}_i can be viewed as a "forgetting factor" that influences the impact of the past measurements on the accumulated error. The remainder of the algorithm is identical to the standard Kalman filter.

$$\mathbf{P}_{k|k-1} = \mathbf{\Phi} \mathbf{P}_{k-1|k-1} \mathbf{\Phi}^T + \mathbf{\Gamma}_d \mathbf{Q} \mathbf{\Gamma}_d^T$$
(27)

$$\mathbf{K}_{k} = \mathbf{P}_{k|k-1}\mathbf{C}^{T} \left(\mathbf{C}\mathbf{P}_{k|k-1}\mathbf{C}^{T} + \mathbf{R}\right)^{-1}$$
(28)

$$\hat{\mathbf{x}}_{k|k} = \hat{\mathbf{x}}_{k|k-1} + \mathbf{K}_k \left(\mathbf{y}_k - \hat{\mathbf{y}}_{k|k-1} \right)$$
(29)

$$\mathbf{P}_{k|k} = (\mathbf{I}_n - \mathbf{K}_k \mathbf{C}) \, \mathbf{P}_{k|k-1} \tag{30}$$

While the algorithm has been proposed for a linear system, it can be easily modified and extended for state estimation of nonlinear systems, using the EKF (PI-EKF).

3.4 Integral Kalman predictor

Bodizs et al. (2011) have proposed an integral Kalman predictor (IKP), in which an integral term is added to the predicted states. While the proportional gain of the integral states can be tuned to achieve desired performance, the integral gain is computed in an adaptive manner.

$$\mathbf{e}_{k-1} = \mathbf{y}_{k-1} - \hat{\mathbf{y}}_{k-1} \tag{31}$$

$$\hat{\mathbf{x}}_k = \mathbf{\Phi} \hat{\mathbf{x}}_{k-1} + \mathbf{\Gamma}_u \mathbf{u}_{k-1} + \mathbf{K}_x \mathbf{e}_{k-1} + \mathbf{K}_i \boldsymbol{\alpha}_{k-1} \quad (32)$$

$$\boldsymbol{\alpha}_k = \boldsymbol{\alpha}_{k-1} + \mathbf{K}_{\alpha} \mathbf{e}_{k-1} \tag{33}$$

$$\hat{\mathbf{y}}_k = \mathbf{C}\hat{\mathbf{x}}_k \tag{34}$$

$$\mathbf{K}_{x} = \left(\mathbf{\Phi}\mathbf{P}_{k-1|k-2}\mathbf{\Phi}^{T} + \mathbf{K}_{i}\mathbf{P}_{x\alpha}^{T}\mathbf{C}^{T}\right) \times \left(\mathbf{C}\mathbf{P}_{k|k-1}\mathbf{C}^{T} + \mathbf{R}\right)^{-1}$$
(35)

$$\mathbf{K}_{\alpha} = \mathbf{P}_{x\alpha}^{T} \mathbf{C}^{T} \left(\mathbf{C} \mathbf{P}_{k|k-1} \mathbf{C}^{T} + \mathbf{R} \right)^{-1}$$
(36)

$$\bar{\mathbf{P}}_{k|k-1} = \bar{\mathbf{\Phi}}\bar{\mathbf{P}}_{k-1|k-2}\bar{\mathbf{\Phi}}^T + \bar{\mathbf{Q}} - \bar{\mathbf{\Phi}}\bar{\mathbf{P}}_{k-1|k-2} \times \\ \bar{\mathbf{C}}^T \left(\bar{\mathbf{C}}\bar{\mathbf{P}}_{k|k-1}\bar{\mathbf{C}}^T + \mathbf{R}\right)^{-1}\bar{\mathbf{C}}\bar{\mathbf{P}}_{k-1|k-2}\bar{\mathbf{\Phi}}^T (37)$$

where, $\alpha \in \mathbb{R}^r$ represents the integral states, $\mathbf{K}_i \in \mathbb{R}^{n \times r}$ represents the integral gain.

$$\bar{\mathbf{\Phi}} = \begin{bmatrix} \mathbf{\Phi} & \mathbf{K}_i \\ \bar{\mathbf{0}}_{r \times n} & \mathbf{I}_r \end{bmatrix} \qquad \bar{\mathbf{C}} = \begin{bmatrix} \mathbf{C} & \bar{\mathbf{0}}_r \end{bmatrix}$$
(38)

and

$$\bar{\mathbf{P}}_{k|k-1} = \begin{bmatrix} \mathbf{P}_{k|k-1} & \mathbf{P}_{x,\alpha} \\ \mathbf{P}_{x,\alpha}^T & \mathbf{P}_{\alpha} \end{bmatrix} \qquad \bar{\mathbf{Q}} = \begin{bmatrix} \mathbf{Q} & \bar{\mathbf{0}} \\ \bar{\mathbf{0}} & \bar{\mathbf{0}} \end{bmatrix}$$
(39)

4. CASE STUDY: CSTR

A first-order, catalytic and non-isothermal reaction taking place in a CSTR can be described by the following differential equations (Marlin, 1995)

$$r_A = C_d k_0 \exp\left(-\frac{E}{RT_r}\right) C_A \tag{40}$$

$$V\frac{dC_A}{dt} = F\left(C_{A,in} - C_A\right) - Vr_A \tag{41}$$

$$V\rho C_{p}\frac{dT_{r}}{dt} = \rho C_{p}F\left(T_{in} - T_{r}\right) - \frac{aF_{c}^{b+1}}{F_{c} + \frac{aF_{c}^{b}}{2\rho_{c}C_{pc}}}\left(T - T_{c,in}\right)$$

$$+ \left(-\Delta H_{rxn}\right) V r_A \tag{42}$$

where, $\mathbf{x} = \begin{bmatrix} C_A & T_r \end{bmatrix}^T$ are the process states. C_A is the reactant concentration, T_r is the reactor temperature. The manipulated inputs are the reactant flow rate Fand coolant flow rate F_c . The reactor temperature (T_r) is the only available measurement. The catalyst activity is denoted by C_d and its value is $0 < C_d \leq 1$. The process parameters and steady conditions are given in Table 1. The sampling time for this process is chosen as T = 0.4 min. To simulate the conditions of process disturbances, the manipulated inputs are corrupted with a zero-mean Gaussian white noise and the measurement noise is simulated by adding a zero-mean Gaussian white noise to the measurement of T_r . The covariance matrices of the process disturbances (\mathbf{Q}) and measurement noise (\mathbf{R}) are given in Table 1. It is well-known that catalyst activity (C_d) changes with time. To simulate this drift in the catalyst activity, the parameter C_d is modelled using a random walk model

$$C_{d,k} = C_{d,k-1} + w_{c,k-1} \tag{43}$$

where, $w_c \sim \mathcal{N}(0, q_c)$ is the random noise in the catalyst activity.

The scenario of a model-plant mismatch was created by introducing the change in catalyst activity (Eq. 43) only in the process, while the model for the state estimators begins with the nominal value of C_d . The adaptive state estimation algorithms used in this work are expected to compensate for the changes in C_d based on the mechanism proposed in their algorithms.

Table 1. Operating conditions

Param.	Value	Param.	Value
V	$1 m^3$	$C_{A,in}$	$2 \text{ kmol}/m^3$
C_p	1 cal/(g K)	ρ	$10^{6} { m g}/m^{3}$
C_{pc}	1 cal/(g K)	$ ho_c$	$10^{6} { m g}/m^{3}$
T_{in}	323 K	$T_{c,in}$	365 K
C_d	0.8	k_0	$1.25 \times 10^{10} min^{-1}$
$\frac{E}{R}$	8830.1 K	$-\Delta H_{rxn}$	$130 \times 10^6 \text{ cal/kmol}$
$C_{A,ss}$	$0.265 \; {\rm kmol}/m^3$	$T_{r,ss}$	394 K
F_{ss}	$1 m^3/\min$	$F_{c,ss}$	$15 m^3/\min$
Q	$10^{-4} \times diag[0.25 \ 9.0]$	R	0.0225
q_c	2×10^{-6}		

4.1 Results

The results of performances of the J-EKF, A-EKF, PI-EKF and IKP for state estimation of the CSTR are presented here. Simulations are carried out for the CSTR for 1000 sampling instants (400 min.). The variation in the catalyst activity, C_d , is shown in Fig. 1. This identical variation is used with all state estimation algorithms. This is done in order to have a fair comparison of the performance of the state estimation algorithms. The CSTR process was excited by subjecting the two inputs, F and F_c to a pseudo random binary sequence (PRBS) signal. The amplitude of the PRBS in F was 0.2 m^3 /min with switching frequency $[0 \ 0.025 \ \omega_N]$, where ω_N is the Nyquist frequency. The amplitude of the PRBS was 2 m^3 /min with switching frequency $[0 \ 0.038 \ \omega_N]$. The manipulated inputs were corrupted with a zero-mean Gaussian noise with covariance **Q**, given in Table 1. Similarly the measurements of the temperature were corrupted with a zero-mean Gaussian noise with covariance \mathbf{R} given in Table 1. Identical realisations of the input and measurement noise were used with all the state estimation algorithms. It should be noted that the input signals sent to the process are corrupted with noise, while those sent to the state estimators are not. The root mean squared error (RMSE) of the state estimates is used as a metric to compare the performance of each state estimation algorithm. For every state, the RMSE is defined as

$$RMSE = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \left(\mathbf{x}_{i,j} - \hat{\mathbf{x}}_{i,j|j} \right)^2}$$
(44)

where, the subscript i refers to the i^{th} element of the state vector.

The tuning parameters used in each algorithm are as follows. For the J-EKF, the variance of the noise, q_c , in the process parameter is used to tune the algorithm, and its value is given in Table 1. For the A-EKF, the parameters a, b, c given in Eq. 17 and Eq. 19 are tuning parameters. The values used in this work are a = 0.45, b = 0.25 and c = 0.3. For the PI-EKF, the values $\mathbf{P}_i = \text{diag } [0.05 \ 1]$ and $\mathbf{K}_i = 10^{-3} \times [5 \ 0.2]^T$ are used for the integral states. In the IKP algorithm, the value of $\mathbf{K}_i = [0.002 \ 0.5]^T$ is used as the integral gain. The results reported in this work are based on these values of the tuning parameters being used



Fig. 1. CSTR: Random variation in catalyst activity, C_d

in their respective algorithms. For a part of the data, the estimates of C_A obtained using the four state estimators are shown in Fig. 2 and Fig. 3, while the estimates of T_r are shown in Fig. 4 and Fig. 5. The RMSE values obtained for both the states, using the different state estimators are given in Table 2. From the table, it can be seen that the J-EKF has the least value of the RMSE, especially for the unmeasured state, C_A . The RMSE values for C_A obtained using the other adaptive state estimators are between 4 to 20 times of that obtained using the J-EKF. Similarly, for T_r , the RMSE values obtained using the other adaptive state estimators are 1.3-50 times the RMSE value obtained using the J-EKF. While the figures are not able to clearly differentiate the performance of the A-EKF and PI-EKF, they clearly demonstrate the unsatisfactory performance of the IKP. One of the reasons behind this is that while the rest of the state estimators utilise the current measurement for correcting the predictions of the process states, the IKP algorithm does not make this correction. From the table of the RMSE values, it is clear that online re-identification of the parameters through algorithms like the J-EKF is the most effective method to compensate for model-plant mismatch.



Fig. 2. CSTR: comparison of estimates of C_A obtained using the J-EKF and A-EKF



Fig. 3. CSTR: comparison of estimates of C_A obtained using the PI-EKF and IKP



Fig. 4. CSTR: comparison of estimates of T_r obtained using the J-EKF and A-EKF



Fig. 5. CSTR: comparison of estimates of T_r obtained using the PI-EKF and IKP

5. CONCLUSIONS

A comparative study of four adaptive state estimation algorithms was conducted in this work. The aim of this

 Table 2. RMSE of state estimates: Comparison of estimator performance

Estimator	C_A	T_r
J-EKF	0.0032	0.1337
A-EKF	0.0124	0.1674
PI-EKF	0.0142	0.2251
IKP	0.0689	6.2936

study was to gauge the performance of these adaptive state estimation algorithms in the presence of a modelplant mismatch occurring due to a random drift in the values of certain process parameters. The three adaptive state estimation algorithms, namely the EKF with covariance scaling (A-EKF), the PI-EKF and the IKP were compared with the conventional method of joint state and parameter estimation (J-EKF). The comparison was carried out through simulations on the benchmark CSTR problem. The results of the simulation studies indicate that the J-EKF has the best performance in terms of the RMSE values of the state estimates, particularly for the unmeasured state. Further, the results also demonstrate that while the A-EKF and PI-EKF are able to reduce the bias in the measured state, they are unable to do the same for the unmeasured state. The performance of the IKP was the worst amongst all estimators and the IKP did not aid in reducing bias from both, the measured as well as unmeasured states. This is because the IKP does not use the current measurement to correct the error in the prediction of the states. While the A-EKF, PI-EKF and IKP seek to correct for the model prediction error through external mechanisms such as covariance scaling or addition of bias terms, the J-EKF attempts to rectify the prediction error by changing the model parameters used. Thus, while the J-EKF alters the model dynamics to minimise the errors due in model predictions, the other estimators do not alter the model. The results of the simulation case study demonstrate that the most effective approach to reduce the bias occurring due to a parametric model-plant mismatch is to re-identify those model parameters, which are deemed to be susceptible to change or drift. This work assumes that the parameters whose values are changing with time are known. However, one of the key challenges in adaptive state and parameter estimation is to develop methods that can detect such parameter changes so as to re-estimate only that subset of the parameters whose values are changing.

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REFERENCES

- V. A. Bavdekar, A. P. Deshpande, and S. C. Patwardhan. Identification of process and measurement noise covariance for state and parameter estimation using extended Kalman filter. J. Process Contr., 21(4):585–601, 2011.
- L. Bodizs, B. Srinivasan, and D. Bonvin. On the design of integral observers for unbiased output estimation in the presence of uncertainty. J. Process Contr., 21(3): 379–390, 2011.

- S. B. Chitralekha, J. Prakash, H. Raghavan, R. B. Gopaluni, and S. L. Shah. A comparison of simultaneous state and parameter estimation schemes for a continuous fermentor reactor. *J. Process Contr.*, 20(8):934–943, 2010.
- M. Efe, J. A. Bather, and D. P. Atherton. An adaptive Kalman filter with sequential rescaling of process noise. In *Proceedings of the American Control Conference*, volume 6, pages 3913–3917, 1999.
- R. J. Fitzgerald. Divergence of the Kalman filter. IEEE Trans. Automat. Contr., 16(6):736–747, 1971.
- N. J. Gordon, D. J. Salmond, and A. F. M. Smith. Novel approach to nonlinear/non-Gaussian Bayesian state estimation. *IEE Proceedings on Radar and Signal Processing*, 140(2):107–113, 1993.
- J. H. Gove and D. Y. Hollinger. Application of a dual unscented Kalman filter for simultaneous state and parameter estimation in problems of surface-atmosphere exchange. *Journal of Geophysical Research D: Atmospheres*, 111(8), 2006.
- N. Kantas, A. Doucet, S.S. Singh, and J.M. MacIejowski. An overview of sequential monte carlo methods for parameter estimation in general state-space models. In *Proceedings of the 15th IFAC Symposium on System Identification*, volume 15, pages 774–785, 2009.
- G. Kitagawa. A self-organizing state-space model. Theory and Methods, Journal of the American Statistical Association, 93(443):1203–1215, 1998.
- S.P. Linder and B. Shafai. Rejecting disturbances to flexible structures using PI Kalman filters. In *Control Applications, 1997., Proceedings of the 1997 IEEE International Conference on*, pages 475–477, 1997.
- T. E. Marlin. Process Control: Designing Processes and Control Systems for Dynamic Performance. McGraw-Hill Inc., New York, 1995.
- H. Moradkhani, S. Sorooshian, H. V. Gupta, and P. R. Houser. Dual state-parameter estimation of hydrological models using ensemble Kalman filter. *Advances in Water Resources*, 28:135–147, 2005.
- L. E. Olivier, B. Huang, and I. K. Craig. Dual particle filter for state and parameter estimation with application to run-of-mine ore mill. J. Process Contr., 22:710–717, 2012.
- G. Pannocchia and J. B. Rawlings. Disturbance model for offset-free model predictive control. AIChE J., 49(2): 426–437, 2003.
- S. C. Patwardhan, S. Narasimhan, J. Prakash, R. B. Gopaluni, and S. L. Shah. Nonlinear Bayesian state estimation: a review of recent developments. *Control Eng. Pract.*, 20:933–953, 2012.
- A. V. Shenoy. Unconstrained nonlinear state estimation for chemical processes. Master's thesis, University of Alberta, Edmonton, AB, Canada, 2010.
- A. Tulsyan, B. Huang, R. B. Gopaluni, and J. F. Forbes. On simultaneous on-line state and parameter estimation in non-linear state-space models. *Journal of Process Control*, 23(4):516–526, 2013.