Advanced State Estimation Techniques for Packed Bed Reactors

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Abstract: This work focuses on the evaluation of some of the advanced recursive state estimation techniques applied to packed bed reactors. Tubular, packed or fixed bed reactors are typically modeled as infinite dimensional partial differential equations, also called Distributed Parameter Systems (DPS). Discretization methods like orthogonal collocation or any other polynomial approximation can be used to convert these DPS into a set of Ordinary Differential Equations (ODE) or Differential Algebraic Equations (DAE), that are more suitable for application of the estimation algorithms. Here we demonstrate the superior performance of the Ensemble Kalman Filter over its other variants (EKF and UKF) for a tubular reactor model. This work also includes the evaluation of the constrained forms of these algorithms for the same tubular reactor model and the results show that the Constrained EnKF which is a nondeterministic approach is able to estimate the states accurately and is less susceptible to numerical errors unlike the Constrained UKF and Constrained EKF which encounter the problem of the covariance matrix becoming negative definite.

Keywords: Packed Bed Reactors, Distributed Parameter Systems, State Estimation, Kalman Filters, Constrained State Estimation

1. INTRODUCTION

Many chemical engineering processes use tubular reactors of various types such as plug flow reactors, fixed/packed-bed reactors, and fluidized-bed reactors. These reactors ability to perform effectively over a wide range of operating conditions as well as their good conversion rate per unit mass of the catalyst against any other catalytic reactor make them the most preferred choice. The other factors that make these reactors a vital part of the chemical industry are low maintenance, low operating cost and long residence time owing to the near complete reaction. In most of the cases, the reactions that take place in these reactors are exothermic in nature. The model equations for these reactors are obtained by mass and energy balances resulting in Partial Differential Equations (PDE). The PDEs which are infinite dimensional are called distributed parameter systems.

Generation of optimal estimates of critical states in a process unit is important from the perspectives of monitoring, control and safe operation as the measurements of all such states cannot be obtained either due to low availability and high cost of reliable sensors or due to measurement errors and excessive time delays required for online analysis. In this sense, several methods for estimation of states in a process system were developed. This can be either inferential estimation in which unmeasured states are estimated by the conjunction of secondary measurements with a suitable dynamic model of the system or normal estimation of the measured states to improve the measurement reliability. For systems defined by linear dynamic models, the Kalman Filter (KF) developed by Kalman in 1960, provides optimal state estimates assuming the measurement and state uncertainties as Gaussian in nature. Many physical systems however show nonlinear dynamics and sometimes need to satisfy constraints that characterize the system states, as a result different types of suboptimal nonlinear estimators have been developed. Most of them are based on the recursive approach proposed in the KF.

In order to implement the KF approach which is recursive as well as easy to realize for nonlinear systems, extensions were sought to the approach by linearising the nonlinear model resulting in a formulation called the Extended Kalman Filter (EKF). These Jacobian calculations, as they approximate the nonlinear model to a first order linear model, fail to account for the fully nonlinear dynamics and are therefore prone to numerical errors. This may even lead to divergence and sometimes biased estimates. This necessitated the need for development of derivative free approaches unlike the analytical approximation of EKF. The Unscented Kalman Filter (UKF) uses a technique called unscented transformation (UT) in which a set of deterministically chosen sample points called as sigma points are used to approximate the prior probability densities. The UKF assumes the estimation error, state and measurement noises to be Gaussian which can be incorrect if the prior distribution is multimodal or follows some other random distribution.

The Ensemble Kalman Filter (EnKF), on the other hand incorporates a Monte-Carlo sampling approach which requires no Gaussian assumption while calculating the covariance information. EnKF belongs to the class of derivative free filters that can accommodate multimodal and non-Gaussian distributions. Though EnKF eliminates the
deficiencies in the earlier proposed estimation algorithms, it still cannot handle constraints. These constraints can be included into the EnKF by modifying the update step and the resulting algorithm in a formulation termed as the Constrained Ensemble Kalman Filter (CEnKF).

The state estimation of distributed parameter systems is usually based on an approach called early lumping. In this method the infinite dimensional PDE model is converted to a set of ODEs that are valid at certain axial points (discretization points) using Orthogonal Collocation or any other polynomial approximation method. However, the boundary conditions which are also present in the model when converted along with the PDEs become algebraic in nature and thus the reduced model becomes a set of Differential Algebraic Equations (DAE) rather than simple ODEs. The state estimation problem of such DAEs has not been studied extensively. In this work we have investigated the performance of some of the advanced state estimators for a differential algebraic system, viz. tubular reactor estimation problem. The necessary modifications required in the estimator algorithms to account for the distributed parameter model structure of tubular reactor are also presented. We studied the unconstrained and constrained forms of the algorithms mentioned above with the tubular reactor model by modifying the algorithm to be applicable to the distributed parameter nature of the system model. Estimation results including relative analysis of different algorithms for the task of concentration profile estimation in the tubular reactor is presented.

2. AUTO-THERMAL TUBULAR REACTOR MODEL

The present study concerns an auto-thermal tubular chemical reactor with an external heat exchanger (Berezowski et al., 2000).

FIGURE 1: Schematic representation of an auto-thermal reactor (Berezowski et al., 2000)

In addition to the external heat exchanger, the reactor is cooled with a medium of constant temperature as can be seen from the schematic of the reactor in FIGURE 1. It is assumed that the dynamics of the external heat exchanger are negligible compared with the reactor dynamics. The dynamic model is pseudo homogeneous and is analogous to the standard diffusion-convection-reaction model.

The dimensionless balance equations are shown below. \( \alpha, \theta \) are the dimensionless concentration and temperature.

\[
\frac{\partial \alpha}{\partial \tau} = \frac{1}{P e_M} \frac{\partial^2 \alpha}{\partial \xi^2} - \frac{\partial \alpha}{\partial \xi} + \phi(\alpha, \theta) \\
\frac{\partial \theta}{\partial \tau} = \frac{1}{P e_T} \frac{\partial^2 \theta}{\partial \xi^2} - \frac{\partial \theta}{\partial \xi} + \phi(\alpha, \theta) + \delta(\theta - \theta_0) \\
(1)
\]

The boundary conditions are:

\[
\xi = 0: \frac{\partial \theta}{d \xi} + \eta \theta(1) = \theta(0); \alpha(0) = \frac{1}{P e_M} \frac{\partial \alpha}{d \xi} = 0 \\
\xi = 1: \frac{\partial \alpha}{d \xi} = 0; \frac{\partial \theta}{d \xi} = 0
\]

where, \( \eta \) is the thermal recycle coefficient defining the heat exchanger efficiency. The kinetics of the process, for a reaction of the type \( A \rightarrow B \) of any order, is given by

\[
\phi(\alpha, \theta) = Da(1-\alpha) \exp\left(\frac{-\beta \theta}{1+\beta \theta}\right).
\]

The significance of the various parameters used in the model can be found in Berezowski et al., 2000.

The discretization of the model in equations (1) and (2) using orthogonal collocation results in a set of DAE containing the system state model and measurement model can be represented in a more general form (continuous time model) as

\[
x(t) = f(x(t), z(t), u(t), t) \\
g(x(t), z(t), u(t), t) = 0
\]

where, the vector of differential states is \( x = [\alpha_2 \ldots \alpha_n, \theta_2 \ldots \theta_n]^T \) (where \( x \in \mathbb{R}^n \)), the vector of algebraic states is \( z = [\alpha_1, \alpha_\nu, \theta_1, \theta_\nu]^T \) (where \( z \in \mathbb{R}^\nu \)), the vector of known inputs is \( u \) (where \( u \in \mathbb{R}^m \)) and the vector of measurements (outputs) is \( y \) (where \( y \in \mathbb{R}^p \)). Here we considered the measurements coming from differential states and algebraic states and necessary modifications to the estimation algorithms are presented later. In the continuous model of equation (3), \( f \) is the nonlinear mapping of the differential states, \( g \) is the mapping of the algebraic states and \( h \) is the mapping of the states to the output. The discrete time representation of the DAE model in equation (3) is presented in equation (4) which is under the assumption that the state and measurement noises are additive and the manipulated inputs are piece-wise constant over the sampling period \( \Delta t \) (when \( \Delta t \) is chosen to be small compared to the system).

\[
x_k = x_{k-1} + \int_{(k-1)\Delta t}^{k\Delta t} f(x(\tau), z(\tau), u_{k-1})d\tau + w_k \\
= F(x_{k-1}, z_{k-1}, u_{k-1}) + w_k \\
g(x(t), z(t), u(t)) = 0 \\
y_k = h(x_k) + v_k \\
(4)
\]
\( w \in \mathbb{R}^{n_w} \) and \( v \in \mathbb{R}^{n_v} \) are independent uncorrelated random variables following the Gaussian distributions \( p(w) \sim N(0, Q) \) and \( p(v) \sim N(0, R) \) respectively. \( Q_{k-1} \) and \( R_{k-1} \) are state and measurement noise covariance matrices at time instant \((k-1)\). The parameter \( k \) represents the discrete time steps only at which measurements are assumed to be available.

3. EXTENDED KALMAN FILTER

Becerra et al. (2001) has studied the applicability of EKF to DAE systems by considering a system represented by DAE model and reducing the model to an ODE by linearization of the nonlinear model. As an extension to this, Mandela et al. (2010) modified this algorithm to allow measurements coming from both differential and algebraic states in the measurement model which is achieved by the augmentation of differential states with algebraic states. Though EKF has the above mentioned flaws, the predictor-corrector method and the recursive nature makes it the most viable technique for online implementation.

In order to keep these merits of EKF and also to make it suitable for handling algebraic constraints or bound constraints on the states, the Recursibe Nonlinear Dynamic Data Reconciliation (RNDDR) technique which is an improvement to the moving window based Nonlinear Dynamic Data Reconciliation (NDDR) was developed (Vachhani et al., 2005). This RNDDR which is largely based on the EKF incorporated a modified update step that can impose algebraic constraints or bound constraints on the state estimates. This modification does not alter the recursive nature and at the same time constraints are satisfied. However, the covariance is still calculated without taking into account the nonlinearity and so the Jacobian calculations are necessary.

4. UNSCENTED KALMAN FILTER

In UKF, the sigma points which are deterministically chosen to approximate the probability distribution of initial random variable are propagated through the nonlinear function individually. The mean and covariance of the transformed random variable are calculated by the weighted mean and weighted covariance of these transformed sigma points. This formulation is suitable only to models represented by ODE and many studies showing the performance of UKF can be found for ODE systems (Julier, 2002; Vachhani et al., 2006). Mandela et al. (2010) presented an approach which extends the UKF for semi-explicit index-1 DAE systems. The approach follows the predictor-corrector approach and also incorporates algebraic states in the measurement model.

Asumed that at time instant \((k-1)\), we have the filtered state estimate \( \hat{x}_{k-1|k-1} \) and its error covariance matrix \( P_{k-1|k-1} \). Unlike in UKF, where the step sizes were considered to be equal to \( n + \kappa \), here the step sizes are calculated as follows:

\[
\theta_{j,k-1} = \min(\Theta)
\]

\[
\Theta_{(i,j)} = \begin{cases} 
\sqrt{(n+\kappa)}, & \text{if } s_{(i,j)} = 0, \\
\min(\sqrt{(n+\kappa)}), & \text{if } s_{(i,j)} > 0, \\
\min(\sqrt{(n+\kappa)}), & \text{if } s_{(i,j)} < 0,
\end{cases}
\]

\[
s = [ (P_{k-1|k-1})^{1/2} - (P_{k-1|k-1})^{1/2} ]
\]

For \( x_i \leq x \leq x_{i+1} \), \( i = 1,...,n \) and \( j = 1,...,2n \) the sigma points chosen in this manner are not equidistant from \( \hat{x}_{k-1|k-1} \). Similar to the UKF, the first sigma point \( \hat{x}_{k-1|k-1,0} \) is chosen to be equal to \( \hat{x}_{k-1|k-1} \). The sigma points selection is as follows:

\[
\hat{x}_{k-1|k-1,0} = \hat{x}_{k-1|k-1}
\]

\[
\hat{x}_{k-1|k-1,j} = \hat{x}_{k-1|k-1} + \theta_{j,k-1}(P_{k-1|k-1})^{1/2}
\]

\[
\hat{x}_{k-1|k-1,n+j} = \hat{x}_{k-1|k-1} - \theta_{j,n+k-1}(P_{k-1|k-1})^{1/2}
\]

The sum of weights of all sigma points is equal to ‘1’ and weights are calculated as follows:

\[
w_j = a\theta_{j,k-1} + b
\]

where, \( j = 0,...,2n \)

\[
a = \frac{2\kappa - 1}{2(n+\kappa)(S_0 - (2n+1)(\sqrt{n+\kappa}))}
\]

\[
b = \frac{1}{2(2n+\kappa)} - \frac{2\kappa - 1}{2(2n+\kappa)(S_0 - (2n+1)(\sqrt{n+\kappa}))}
\]

\[
S_0 = \sum_{j=1}^{2n} \theta_{j,k-1}
\]

Before propagating these sigma points, algebraic states \( \hat{z}_{k-1|k-1,j} \) consistent with differential state sigma points are calculated using the relation \( g(\hat{x}_{k-1|k-1,j}, \hat{z}_{k-1|k-1,j}) = 0 \). Now these sigma points are propagated through the nonlinear DAE model to obtain the transformed sigma points \( \hat{x}_{k|k-1,j} \).

The weighted mean and covariance of the transformed set of sigma points calculated give the mean \( \hat{x}_{k|k-1} \) and error covariance \( P_{k|k-1} \) of the predicted state estimate. The effect of state noise covariance \( Q_{k-1} \) on the predicted state error covariance calculated necessitates the re-calculation of sigma
points and weights corresponding to these sigma points. The modified optimization based update step for URNDDR is given below

\[
\begin{align*}
\min & \quad (x_{k,k,j}^{\text{aug}} - \hat{x}_{k,k-1,j})^T (P_{k,k-1})^{-1} (x_{k,k,j}^{\text{aug}} - \hat{x}_{k,k-1,j}) + (y_j - h(x_{k,k,j}^{\text{aug}}))^T (R_k)^{-1} (y_j - h(x_{k,k,j}^{\text{aug}})) \\
\text{subjected to} & \quad g(\hat{x}_{k,k,j}^{\text{aug}}, 0) = 0, \\
\hat{x}_{k}^{\text{aug}} & \leq x_{k,k,j}^{\text{aug}} \leq \hat{x}_{k}^{\text{aug}}, \\
I(\hat{x}_{k,k,j}^{\text{aug}}) & \leq 0, \\
d(\hat{x}_{k,k,j}^{\text{aug}}) & = 0
\end{align*}
\]

(11)

The updated mean and error covariance of the state estimate are calculated using the following equations:

\[
\begin{align*}
\hat{x}_{k,k} & = \sum_{j=0}^{2n} w_j \hat{x}_{k,k,j}, \\
P_{k,k} & = \frac{1}{2(n + \kappa)} \sum_{j=0}^{2n} (\hat{x}_{k,k,j} - \hat{x}_{k,k})(\hat{x}_{k,k,j} - \hat{x}_{k,k})^T
\end{align*}
\]

(13)

(14)

Finally the algebraic states are calculated using the equation \(g(\hat{x}_{k,k}^{\text{aug}}, z_{k,k}) = 0\).

When the covariance becomes non-positive semi definite, a modified form of covariance calculation can be incorporated making sure that the covariance is positive semi definite.

\[
P_{k,k} = \frac{1}{N} \sum_{i=1}^{N} \left( x_{k,k}^{\text{aug}(i)} - \hat{x}_{k,k} ight) (x_{k,k}^{\text{aug}(i)} - \hat{x}_{k,k})^T
\]

(15)

Remark: In this algorithm, the selection of the sigma points and their weights depend not only on the tuning parameter \(\kappa\), but also on the state error covariance (see equations (5)-(10)). Now choosing a value of \(\kappa\) which would give weights that do not make the error covariance matrix non positive definite, would be very critical. Furthermore, the selection of \(\kappa\) cannot necessarily ensure that the error covariance matrix is always positive definite, as the weights depend also on the prior covariance matrix whose effect cannot be defined in advance. This aspect of non-positive semi definite covariance is a numerical issue associated with the UKF as will be shown later, leads to a bias in the estimate when the alternative form defined in equation (15) is used.

5. ENSEMBLE KALMAN FILTER

The EnKF which was originally proposed by Evensen (1994) is a sequential data assimilation method belonging to particular class of particle filters. EnKF uses a Monte Carlo sampling technique that makes the approach applicable to all kinds of distributions which are not necessarily Gaussian. In the prediction step of the algorithm, a set of \(N\) sample points (\(N\) is a heuristic choice) as discussed earlier with mean equal to the mean of the initial probability distribution of state estimate given are generated randomly using a Monte Carlo sampling technique. Here sampling for differential states \(z_{k,k-1}^{(i)}\) is done and the algebraic states \(z_{k,k-1}^{(i)}\) are calculated from the algebraic relation \(g(x_{k,k-1}^{(i)}, z_{k,k-1}^{(i)}) = 0\). At each time step random \(N\) samples of process and measurement noise \(w_k\) and \(v_k\) are also drawn from their corresponding distribution. These particles are then propagated forward through the nonlinear DAE model, solution of which gives the transformed ensemble sample points.

\[
\begin{align*}
\chi_{k,k-1}^{(i)} & = F(x_{k,k-1}^{(i)}, z_{k,k-1}^{(i)}, u_{k-1}) \\
g(\chi_{k,k-1}^{(i)}, z_{k,k-1}^{(i)}, u_{k-1}) & = 0
\end{align*}
\]

(16)

The effect of the process noise is felt by adding \(w_k\) (\(w_{k}^{(i)}, i = 1, 2, \ldots, N\)).

\[
x_{k,k-1}^{(i)} = \chi_{k,k-1}^{(i)} + w_{k}^{(i)}
\]

(17)

The algebraic states are made consistent with the differential states by re-computing them using the algebraic relation \(g(x_{k,k-1}^{(i)}, z_{k,k-1}^{(i)}, u_{k-1}) = 0\).

The predicted estimates of state and measurement distribution are calculated using the following equations by augmentation of the differential states with the algebraic states.

\[
\begin{align*}
x_{k,k-1}^{\text{aug}} & = \frac{1}{N} \sum_{i=1}^{N} x_{k,k-1}^{(i)} \\
y_{k}^{(i)} & = \frac{1}{N} \sum_{i=1}^{N} y_{k}^{(i)} \\
y_{k}^{(i)} & = h(x_{k,k-1}^{(i)}, z_{k,k-1}^{(i)}) + v_{k}^{(i)}
\end{align*}
\]

(18)

(19)

(20)

In the equation (20), to simulate the effect of measurement noise \(v_{k}^{(i)}\) \((i = 1, 2, \ldots, N)\) is added. The Kalman gain calculations are as follows

\[
K_{k}^{\text{aug}} = P_{xy}^{\text{aug}} (P_{yy}^{\text{aug}})^{-1}
\]

(21)

where,

\[
\begin{align*}
P_{xy}^{\text{aug}} & = \frac{1}{N-1} \sum_{i=1}^{N} [e_{k,k-1}^{(i)}] [e_{k,k-1}^{(i)}]^T \\
P_{yy}^{\text{aug}} & = \frac{1}{N-1} \sum_{i=1}^{N} [e_{k,k-1}^{(i)}] [e_{k,k-1}^{(i)}]^T \\
e_{k,k-1}^{(i)} & = x_{k,k-1}^{(i)} - x_{k,k-1}^{\text{aug}(i)} \\
e_{k,k-1}^{(i)} & = y_{k}^{(i)} - y_{k}^{\text{aug}(i)}
\end{align*}
\]

(22)

(23)

(24)

(25)

The ensemble sample points are updated using the Kalman standard update step applied to each ensemble point.

\[
\begin{align*}
x_{k,k}^{\text{aug}(i)} & = x_{k,k-1}^{\text{aug}(i)} + K_{k}^{\text{aug}} (y_{k} - y_{k}^{\text{aug}(i)}) \\
x_{k,k}^{\text{aug}(i)} & = \frac{1}{N} \sum_{i=1}^{N} x_{k,k}^{\text{aug}(i)}
\end{align*}
\]

(26)

(27)

The algebraic ensemble points are calculated using the same algebraic relation which has been used earlier \(g(x_{k,k}^{(i)}, z_{k,k}^{(i)}) = 0\) and in case of a linear algebraic
relation between the differential and algebraic states mean of the algebraic states is obtained using $g_i(\hat{x}_{k/k}, \hat{z}_{k/k}) = 0$.

Constrained EnKF algorithm for DAE systems

Many of the modified algorithms proposed for constrained estimation either require high computational effort or exhibit the flaws associated with EKF and UKF. Prakash et al. (2008) proposed a modified approach to EnKF termed as CEnKF which incorporates bounds on the state variables. In their CEnKF approach, a modified update step which is similar to that of NDDR was proposed along with a method to sample initial ensemble points using truncated distribution of initial state (Prakash et al., 2008).

In order to select the initial particles or ensemble samples that lie within bounds, a method called truncated distribution is used (Prakash et al., 2008).

Each of these ensemble points are forecasted through the DAE model and then the predicted state estimate and measurement estimate are calculated using the equations (16)-(20). The error covariance of the predicted state estimates is calculated using the following equation

$$P_{k/k-1}^i = \frac{1}{N-1} \sum_{i=1}^{N} [\hat{e}_{k/k-1}^i] [\hat{e}_{k/k-1}^i]^T \tag{28}$$

The update step in CEnKF approach is

$$\Delta x_{k/k}^i = (x_{k/k}^i - \hat{x}_{k/k-1}) (P_{k/k-1}^{-1})(x_{k/k}^i - \hat{x}_{k/k-1})$$

$$+ [(y_k - y_{k}^{aug(i)})^T R_k^{-1} (y_k - y_{k}^{aug(i)})] \tag{29}$$

subjected to $g_i(\hat{x}_{k/k}^i) = 0$ and

$$\Delta x_L \leq \hat{x}_{k/k} \leq \Delta x_H$$

$$h(\hat{x}_{k/k}) \leq 0 \tag{30}$$

$$d(\hat{x}_{k/k}) = 0$$

Given the ensemble states obtained from the above step, the final estimate is calculated using equation (27). The algebraic estimates are obtained using the same procedure mentioned in unconstrained EnKF at the end of the algorithm.

6. RESULTS AND DISCUSSIONS

The discretization of the PDE model is done with 10 internal collocation points. The following are the various important parameters in the system model used for simulations.

$$Da = 0.15; \beta = 1.4; \gamma = 10; \delta = 2; \eta = 0.3$$

$$Pe_T = 100; Pe_M = 100; \theta_H = 0; \ell = 2$$

The collocation points are located at $[0 \ 0.01304 \ 0.0674 \ 0.1602 \ 0.2832 \ 0.4255 \ 0.5744 \ 0.7166 \ 0.8396 \ 0.9325 \ 0.9869 \ 1]$ when considered a unit length of reactor. So the dimension of the differential states is 20 consisting 10 concentrations and 10 temperatures corresponding to the internal collocation points. The algebraic states dimension is 4 consisting the concentration and temperature at the entry and exit of the reactor. The process and measurement noises are assumed to Gaussian White Noise with zero mean and covariance matrices $Q=diag[0.001^2]_{n_x}, R = diag[0.01^2]_{n_y}$ respectively.

The initial state error covariance matrix is also assumed to consist only diagonal elements given by $P_{0/k} = diag[0.1^2]_{n_x}.$

The initial state error covariance of the predicted state $\tilde{x}_{0/0} = \begin{bmatrix} 0 \ 0 \ \ldots \ 0 \end{bmatrix}_{n_x}$ and for the true system simulation $x_{0/0} = \begin{bmatrix} 0 \ 0 \ \ldots \ 0 \end{bmatrix}_{n_x}$. The lower and upper bounds on the states are $x_L = \begin{bmatrix} 0 \ 0 \ \ldots \ 0 \end{bmatrix}_{n_x}$ and $x_U = \begin{bmatrix} 1 \ 1 \ \ldots \ 1 \end{bmatrix}_{n_x}$. Measurements are assumed to be available from dimensionless temperature $\theta$ and are also assumed to be measured at all collocation points along the length of the reactor making the measurement vector dimension 10. When the measurements are coming from algebraic temperatures, the size of the measurement vector is 12. And when both the differential and algebraic states are considered, the augmented state vector is of size 24 as both the differential and algebraic states are included in it.

An ensemble size of 45 is used for sampling in both the EnKF and the CEnKF. The sampling time (dimensionless) considered for simulations is 0.05. In all the cases the problem at hand is inferential estimation of dimensionless concentration (conversion of reactant) by considering dimensionless temperature measurements. Here the estimation error is defined as the difference between the estimated state and the true state which is available from system simulations. All these simulations are performed using MATLAB 7.8.0 (R2009a) software in windows-7 operating system. ODE15s of MATLAB is used for the solution of the DAE model. [For solving the NLP problem of update step in constraints algorithm, “fmincon” optimizing function of MATLAB is used]. The relative performance of unconstrained EKF, UKF and EnKF is shown in the FIGURE 2 and 3. As it can be seen the performance of EnKF is superior to UKF and EKF. Though UKF performs better than EKF, it is less efficient than EKF.

FIGURE 2: The RMSE of the concentration at different collocation points
The estimate of conversion at collocation point 10 using the modified update step of URNDDR mentioned in equation (27) is shown in FIGURE 4 which clearly shows bias. The performance of CEnKF at the same collocation point for estimation of conversion is shown in FIGURE 5 which show the superior performance of CEnKF approach. The RNDDR approach failed to perform well for this system as the estimates are observed to diverge resulting in non positive semi definite covariance matrix.

The simulations when the URNDDR is directly implemented showed the occurrence of non positive semi definite covariance matrix. The RNDDR also showed similar problems with state covariance matrix becoming non positive semi definite. Thus the modified covariance calculation step is considered but it introduced bias in the estimates of URNDDR. Also this modification has shown no effect in case of RNDDR. These numerical issues do not exist in the case of the CEnKF where the covariance matrix does not become non positive semi definite since the calculation of covariance does not depend on the weights and also that the samples are taken non deterministically.

7. CONCLUSIONS

In this work we evaluated the three advanced state estimation algorithms for DAE systems exemplified by the packed bed reactor. It is observed that the non-deterministic sampling approaches EnKF and CEnKF are observed to perform very well in comparison with EKF, UKF and the constrained forms of these algorithms. It is also observed that apart from the deterministic nature of UKF, it can also turn out to be sensitive for systems having more states because the selection of sigma points becomes important and could lead to non-positive semi definite covariance matrix. We show that numerical errors could preclude the application of the CUKF and the CEKF where the non deterministic version CEnKF is seem to perform in a superior manner.

8. REFERENCES


