Nonlinear State Estimation of Differential Algebraic Systems

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Abstract: Kalman filter and its variants have been used for state estimation of systems described by ordinary differential equation (ODE) models. Moving Horizon Estimation (MHE) has been a popular approach in chemical engineering community for the estimation of both ODE and differential algebraic equation (DAE) systems but is computationally demanding. There has been some work on applying Extended Kalman filter for state estimation of DAE systems with measurements as functions of only the differential states. This work describes the estimation of nonlinear DAE systems with measurements being a function of both the differential and algebraic states. An Unscented Kalman filter (UKF) formulation is also derived for semi-explicit index 1 DAE systems. The utility of these formulations are demonstrated through a case study.

1. INTRODUCTION

Differential algebraic equation (DAE) models naturally arise in several chemical/physical systems, where some rate processes are much faster than the others and admit quasi steady-state approximations. Common examples of these can be found in separation and reaction systems. Many chemical engineering systems can be modeled as DAE systems. Examples of algebraic equations include mole fraction summations, vapor-liquid equilibrium relationships and so on. The algebraic equations can be either linear or nonlinear. Other areas where DAE models arise are mechanical systems, electrical systems and biological systems. A DAE system is characterized by the index of the system. The index of a DAE system is defined as the number of differentiations that are required to convert the DAE system into an explicit ODE system. It is not always possible and easy to convert DAE into ODE systems [Petzold, 1988]. In this paper. the focus is on estimation of nonlinear index one DAE systems that are common in chemical engineering.

The Kalman filter (KF) is an optimal estimator for linear dynamical systems in the presence of state and measurement uncertainties [Gelb, 1988, Sorenson, 1985]. Extended Kalman filter (EKF) is an extension of the Kalman filter for nonlinear systems described by a class of ordinary differential equations. Simultaneous parameter and state estimation is achieved in KF and EKF by augmenting the states [Jazwinski, 1970].

The KF has been used by several researchers for state estimation of systems describing linear DAE models [Nikoukhah et al., 1992, Chisci and Zappa, 1992]. The state estimation of nonlinear DAEs has already been studied by Albuquerque and Biegler [1997] using Moving -horizon estimation technique. Moving-horizon estimation (MHE) is considered as an efficient optimization based method for state estimation. Moving-horizon estimation can also be extended to parameter estimation of nonlinear DAEs [Tjoa and Biegler, 1991].

Moving-horizon estimator can handle constraints and bounds at every sampling instant [Rao et al., 2003]. However, questions remain about the computational complexity for on-line implementation of MHE estimators. The main advantage of the EKF lies in their predictor-corrector recursive form that has the potential for online deployment [Muske and Edgar, 1997].

There has been some work on the application of EKF for nonlinear DAE systems. One of the first attempts at this can be found in Becerra et al. [1999]. Becerra et al. [2001] extend this work further and demonstrate their approach on an experimental case study. They also explore the use of square root formulation of the EKF which has better numerical stability than the standard EKF [Park and Kailath, 1995]. However, the measurements available to the estimator are all assumed to be functions of differential states. In this paper, we extend Becerra et al. [2001] approach to cases where the measurements are functions of both the differential and algebraic states. Further, we develop an approach for the use of Unscented Kalman filter (UKF) for estimation in index 1 nonlinear DAE systems.

The paper is organized as follows. Section 2 provides an introduction to DAE systems. EKF and UKF algorithms

for DAE systems are discussed in section 3 and section 4 respectively. Simulation results with discussions are presented in section 5 followed by conclusions in section 6.

2. DIFFERENTIAL ALGEBRAIC SYSTEMS

As discussed in the previous section, DAE systems consist of both differential and algebraic equations. DAE systems are characterized by the index of the system. The index of the DAE system is defined as the number of differentiations required to convert the DAE into an ODE. As a simple example, consider

$$\dot{y_2}(t) = y_1(t) + \lambda_1(t) \tag{1}$$
$$0 = y_2(t) + \lambda_2(t) \tag{2}$$

Differentiating the algebraic equation 2 once, we get
$$0 = \dot{y_2}(t) + \dot{\lambda_2}(t) \tag{3}$$

Differentiating the algebraic equation 3 once more yields
$$0 = \ddot{y_2}(t) + \ddot{\lambda_2}(t) \tag{4}$$

Putting these equations together we now get an ODE as shown in equation .

$$\dot{y_2}(t) = y_1(t) + \lambda_1(t)$$
$$\dot{y_1}(t) = -\dot{\lambda_1}(t) - \ddot{\lambda_2}(t) \tag{5}$$

Since the equations had to be differentiated twice this is an index 2 DAE system. While there are DAE systems of orders higher than 1 in chemical engineering, index 1 DAE systems are common as seen in electrochemistry, reactive distillation and biochemical engineering applications. As mentioned before, this work considers index 1 DAE systems.

3. EKF FOR DAE SYSTEMS

While EKF has been studied extensively for ODE systems, the application of EKF approaches to DAE systems are not many. Becerra et al. [2001] developed an EKF estimation approach for for nonlinear index 1 DAEs. The EKF approach follows the same predictor-corrector form with some modifications. In the prediction step, a DAE solver is used for propagating the prior state through the system model. This is in contrast to the use of an ODE solver in standard EKF. The covariance matrix of the differential states are propagated by linearizing the system model. The correction step is performed only for the differential states through a linearization of the measurement model. This is possible because it is assumed that the measurements are functions of differential states alone. Once the corrected differential states are available, the corrected algebraic states are calculated using the algebraic portion of the system model. The corrected covariance matrix for the differential states is calculated using the standard EKF procedure. The mathematical details of the algorithm are explained below. The nonlinear DAE system is considered with discrete measurements sampled at regular intervals with sampling period Δt

$$x_{k+1} = x_k + \int_{(k)\Delta t}^{(k+1)\Delta t} f(x(\tau)), z(\tau)) \, d\tau + w_{k+1} \tag{6}$$

$$g(x_{k+1}, z_{k+1}) = 0 \tag{7}$$

$$y_{k+1} = h(x_{k+1}) + v_{k+1} \tag{8}$$

where w_{k+1} and v_{k+1} are assumed to be independent Gaussian white noise processes with known covariance matrix Q_{k+1} and R_{k+1}

For a fixed input, the linearized equation is given by

$$\dot{x} = Ax \tag{9}$$

where

$$A = (J_1 - J_2 J_4^{-1} J_3) \tag{10}$$

$$\begin{bmatrix} J1 & J2 \\ J3 & J4 \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f}{\partial x} & \dfrac{\partial f}{\partial z} \\ \dfrac{\partial g}{\partial x} & \dfrac{\partial g}{\partial z} \end{bmatrix} \tag{11}$$

Following are the steps involved in the algorithm

- The differential states are propagated by integrating the DAE model from time t_k to t_{k+1}. The predicted state estimate $\hat{x}_{k+1/k}$ is obtained with u_k, which is the constant input between sampling intervals.
- The predicted covariance matrix in differential states is propagated using

$$P_{k+1/k} = \bar{A}_k P_{k/k} \bar{A}_k^T + Q_k \tag{12}$$

  where $\bar{A} = exp(A\Delta t)$
- The kalman gain is computed using

$$K_{k+1} = P_{k+1/k} G_{k+1}^T (G_{k+1} P_{k+1/k} G_{k+1}^T + R_{k+1})^{-1} \tag{13}$$

  where G_{k+1} is the linearized measurement model and the actual measurement model is a function of only differential states.
- The updated differential estimates are obtained from kalman update equation

$$\hat{x}_{k+1/k+1} = \hat{x}_{k+1/k} + K_{k+1}(y_{meas} - h(\hat{x}_{k+1/k})) \tag{14}$$
- The updated estimate $\hat{z}_{k+1/k+1}$ is obtained from the set of algebraic equations defining the DAE system once differential state estimate $\hat{x}_{k+1/k+1}$ is obtained
- The updated covariance matrix is computed as

$$P_{k+1/k+1} = (I - K_{k+1}G_{k+1})P_{k+1/k} \tag{15}$$

  In this method, $\hat{z}$ is computed only from the $\hat{x}$ using algebraic equation and there is no dependence or use of prior estimates of z (algebraic states). This method cannot be applied to cases where there is an availability of algebraic states measurements.

4. PROPOSED APPROACH: EXTENDED KALMAN FILTER FOR DAE SYSTEMS

In DAE systems, the measurements can, in general, be a function of both the differential and algebraic states. In the proposed work, we extend the EKF approach to this case. The algorithm deviates from the work of Becerra et al. [2001] in that the EKF works with an augmented system (with both the differential and algebraic states). A linearized ODE model involving both differential and

algebraic states (augmented) is derived. This linearized ODE model is used for the covariance propagation of augmented state as opposed to just the differential states as in Becerra et al. [2001]. The gain matrix is calculated form the augmented predicted covariance matrix and the linearized measurement model which is a function of both the differential and algebraic measurements. The corrected augmented state is computed. From these corrected augmented states, only the differential states are retained. As the algebraic constraints are to be met, the algebraic states are calculated from the corrected differential states using algebraic equations. The details of the algorithm are explained below. The nonlinear DAE system is considered with discrete measurements sampled at regular intervals with sampling period Δt

$$x_{k+1} = x_k + \int_{(k)\Delta t}^{(k+1)\Delta t} f(x(\tau)), z(\tau))\, d\tau + w_{k+1} \quad (16)$$

$$g(x_{k+1}, z_{k+1}) = 0 \quad (17)$$

$$y_{k+1} = h(x_{k+1}) + v_{k+1} \quad (18)$$

where w_{k+1} and v_{k+1} are assumed to be independent Gaussian white noise processes with known covariance matrix Q_{k+1} and R_{k+1}

Linearizing the differential equations and algebraic equations of index 1 DAE system, we get

$$\dot{x} = Ax + Bz$$
$$0 = Cx + Dz \quad (19)$$

where

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f}{\partial x} & \dfrac{\partial f}{\partial z} \\ \dfrac{\partial g}{\partial x} & \dfrac{\partial g}{\partial z} \end{bmatrix} \quad (20)$$

Differentiating the linearized algebraic equation once , we get

$$0 = C\dot{x} + D\dot{z} \quad (21)$$

Then

$$\dot{z} = -D^{-1}C\dot{x} \quad (22)$$
$$\dot{z} = -D^{-1}CAx - D^{-1}CBx \quad (23)$$

Writing in matrix form

$$\begin{bmatrix} \dot{x} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} A & B \\ -D^{-1}CA & -D^{-1}CB \end{bmatrix} \begin{bmatrix} x \\ z \end{bmatrix} \quad (24)$$

The augmented form is

$$\dot{X}^{aug} = A^{aug} X^{aug} \quad (25)$$

The transition matrix is evaluated as

$$\phi = exp(A^{aug}\Delta t) \quad (26)$$

The algorithm consists of following steps

- Both differential and algebraic states are propagated using a DAE solver from t_k to t_{k+1} starting from the latest updated estimate $\hat{X}_k^{aug}$ and the latest input u_k.

- The predicted covariance matrix of the augmented states is computed as

$$P_{k+1/k}^{aug} = \phi P_{k/k}^{aug} \phi^T + \Gamma Q_{k+1}\Gamma^T \quad (27)$$

where

$$\Gamma = \begin{bmatrix} I \\ -D^{-1}C \end{bmatrix} \quad (28)$$

- The augmented Kalman gain is computed as

$$K_{k+1}^{aug} = P_{k+1/k}^{aug} G_{k+1}^T (G_{k+1} P_{k+1/k}^{aug} G_{k+1}^T + R_{k+1})^{-1} \quad (29)$$

where G_{k+1} is the linearised measurement model.

- The updated state estimate is given by

$$X_{k+1/k+1}^{aug} = X_{k+1/k}^{aug} + K_{k+1}^{aug}(y_{meas} - h(X_{k+1/k}^{aug})) \quad (30)$$

- As the algebraic constraints are to be met, differential terms (x) of the updated estimate are retained and the updated estimates of the algebraic states (z) are calculated from the algebraic equation of DAE system.

- The updated covariance matrix is calculated as

$$P_{k+1/k+1}^{aug} = (I - K_{k+1}^{aug} G_{k+1}) P_{k+1/k}^{aug} \quad (31)$$

5. UNSCENTED KALMAN FILTER FOR DAE SYSTEMS

Unscented Kalman filter (UKF) is an approach that was developed to improve on EKF. The UKF approach uses the idea of unscented transforms for predicting the mean and covariance when a random variable passes through a nonlinear transformation. In EKF, linearization of the nonlinear transformation is used to predict the mean and covariance of the transformed variable. Unscented transformation is a sampling technique where a small number of deterministic samples are chosen such that their weighted mean and covariance exactly equal the mean and covariance of the random variable undergoing the nonlinear transformation. The transformed sample points are used to calculate the *a posteriori* mean and covariance. This results in much better accuracy than the linearization approach [Julier et al., 2000].

UKF estimation for ODE systems is well developed and several application studies have appeared [Romanenko and Castro, 2004, Romanenko et al., 2004, van der Merwe et al., 2000, Julier, 2002, Wan et al., 2000, Wan and van der Merwe, 2000]. In this paper, we extend the UKF approach for semi-explicit index 1 DAE systems. The proposed approach also follows the predictor-corrector form. First, unscented samples are chosen for the differential states. The unscented samples for the algebraic states are generated from the algebraic equations. This makes all the sigma points consistent. These sigma points are propagated through the system through a DAE solver. Unscented samples for the differential and algebraic states are again generated using the propagated covariance matrix. The sample points for the measurements are calculated by passing the unscented differential and algebraic state samples through the measurement function. The sample covariances are used to calculate the Kalman gain. Using the Kalman gain, the corrected differential states are obtained. The corrected algebraic states are calculated using the algebraic equations in the system model. This algorithm of unscented Kalman filter for DAE systems is

explained below. The nonlinear DAE system is considered with discrete measurements sampled at regular intervals with sampling period Δt

$$x_{k+1} = x_k + \int_{(k)\Delta t}^{(k+1)\Delta t} f(x(\tau), z(\tau)) \, d\tau + w_{k+1} \quad (32)$$

$$g(x_{k+1}, z_{k+1}) = 0 \quad (33)$$

$$y_{k+1} = h(x_{k+1}, z_{k+1}) + v_{k+1} \quad (34)$$

where w_{k+1} and v_{k+1} are assumed to be independent Gaussian white noise processes with known covariance matrix Q_{k+1} and R_{k+1}

- The first step is the generation of sigma points. At the kth instant, $\hat{x}_{k/k}$ is the filtered estimate of differential states and $P_{k/k}$ is the covariance matrix associated with it. A set of 2n+1 sigma points $\hat{X}_{k/k,i}$ with associated weights are chosen symmetrically about $\hat{x}_{k/k}$ where n is the dimension of the state.

$$\hat{X}_{k/k,0} = \hat{x}_{k/k}; W_0 = \frac{\kappa}{(n+\kappa)} \quad (35)$$

$$\hat{X}_{k/k,i} = \hat{x}_{k/k} + (\sqrt{(n+\kappa)P_{k/k}})_i; W_i = \frac{1}{2(n+\kappa)} \quad (36)$$

$$\hat{X}_{k/k,i+n} = \hat{x}_{k/k} - (\sqrt{(n+\kappa)P_{k/k}})_i; W_{i+n} = \frac{1}{2(n+\kappa)} \quad (37)$$

where $(\sqrt{P_{k/k}})_i$ is the ith column of matrix square root of $P_{k/k}$ and W_i is the weight associated with the corresponding point. The parameter κ is a tuning parameter. The weights W_i add to one and the weighted mean of the set X is same as $\hat{x}_{k/k}$. The weighted covariance matrix of the sample is equal to $P_{k/k}$.

$$P_{k/k} = \sum_{i=0}^{2n} W_i(\hat{X}_{k/k,i} - \hat{x}_{k/k})(\hat{X}_{k/k,i} - \hat{x}_{k/k})^T \quad (38)$$

- Calculate $\hat{Z}_{k/k,i}$ from $g(\hat{X}_{k/k,i}, \hat{Z}_{k/k,i}) = 0$
- Propagate $\hat{X}_{k/k,i}$ and $\hat{Z}_{k/k,i}$ through DAE system to get $\hat{X}_{k+1/k,i}$ and $\hat{Z}_{k+1/k,i}$
  The predicted differential state estimate $\hat{x}_{k+1/k}$ is given by

$$\hat{x}_{k+1/k} = \sum_{i=0}^{2n} W_i\hat{X}_{k+1/k,i} \quad (39)$$

- Calculate $P_{k+1/k}^{xx}$

$$P_{k+1/k}^{xx} = \sum_{i=0}^{2n} W_i(\hat{X}_{k+1/k,i} - \hat{x}_{k+1/k}) (\hat{X}_{k+1/k,i} - \hat{x}_{k+1/k})^T + Q_{k+1} \quad (40)$$

- Do unscented sampling with $\hat{x}_{k+1/k}$ as mean and $P_{k+1/k}^{xx}$ as covariance matrix
- Recalculate $\hat{Z}_{k+1/k,i}$ from $g(\hat{X}_{k+1/k,i}, \hat{Z}_{k+1/k,i}) = 0$
- Form $\hat{X}_{k+1/k,i}^{aug}$ by augmenting $\hat{X}_{k+1/k,i}$ with $\hat{Z}_{k+1/k,i}$

- Calculate $\hat{x}_{k+1/k}^{aug}$

$$\hat{x}_{k+1/k}^{aug} = \sum_{i=0}^{2n} W_i\hat{X}_{k+1/k,i}^{aug} \quad (41)$$

- The predicted sigma points are propagated through the nonlinear measurement equation to obtain the predicted measurement as

$$Y_{k+1,i} = h(\hat{X}_{k+1/k,i}^{aug}) \quad (42)$$

Using the set of predicted measurements, the covariance matrix of innovations and the cross covariance between predicted state estimate errors and innovations are computed as

$$P_{\nu\nu,k+1} = \sum_{i=0}^{2n} W_i(Y_{k+1,i} - \hat{y}_{k+1}) (Y_{k+1,i} - \hat{y}_{k+1})^T + R_{k+1} \quad (43)$$

$$P_{x\nu,k+1} = \sum_{i=0}^{2n} W_i(\hat{X}_{k+1,i}^{aug} - \hat{x}_{k+1/k}^{aug})(Y_{k+1,i} - \hat{y}_{k+1})^T \quad (44)$$

where

$$\hat{y}_{k+1} = \sum_{i=0}^{2n} W_iY_{k+1,i} \quad (45)$$

- The Kalman gain matrix is computed as
$$K_{k+1} = P_{x\nu,k+1}(P_{\nu\nu,k+1})^{-1} \quad (46)$$
- The Kalman gain corresponding to differential states is K_{k+1}^{diff}
- The updated differential estimates are obtained using the linear update equation as in Kalman filter
$$\hat{x}_{k+1/k+1} = \hat{x}_{k+1/k} + K_{k+1}^{diff}(y_{k+1} - \hat{y}_{k+1}) \quad (47)$$
- The updated estimate $\hat{z}_{k+1/k+1}$ is obtained from the set of algebraic equations defining the DAE system once differential state $\hat{x}_{k+1/k+1}$ is obtained
- The covariance matrix of error in the updated differential estimates is computed using

$$P_{k+1/k+1} = P_{k+1/k} - K_{k+1}^{diff}P_{\nu\nu,k+1}K_{k+1}^{diff^T} \quad (48)$$

6. CASE STUDY

The utility of the proposed approaches is tested on an electrochemical case study. The case study considers the galvanostatic charge /open-circuit/ discharge processes of a thin film nickel hydroxide electrode [Celik et al., 2002]. The modeling equations are

$$\frac{\rho V}{W}\frac{dy_1}{dt} = \frac{j_1}{F} \quad (49)$$

$$j_1 + j_2 - i_{app} = 0 \quad (50)$$

where

$$j_1 = i_{01}[2(1-y_1)exp(\frac{0.5F}{RT}(y_2 - \phi_{eq,1})) - 2y_1 \times exp(\frac{-0.5F}{RT}(y_2 - \phi_{eq,1}))] \quad (51)$$

$$j_2 = i_{02}[exp(\frac{F}{RT}(y_2 - \phi_{eq,2})) - exp(\frac{-F}{RT}(y_2 - \phi_{eq,2}))] \quad (52)$$

The first equation is the species balance equation, the second equation is the charge balance equation and j_1 and j_2 are derived using the Butler-Volmer kinetics. For the purpose of demonstrating the utility of the proposed approaches we assume that the differential state is corrupted with process noise w_{k+1} and the algebraic equation is exact. The values of parameters used are $F = 96487$, $R = 8.314$, $T = 298.15$, $\phi_{eq,1} = 0.420$, $\phi_{eq,2} = 0.303$, $\rho = 3.4$, $W = 92.7$, $V = 1 \times 10^{-5}$, $i_{app} = 1 \times 10^{-5}$, $i_{01} = 1 \times 10^{-04}$, $i_{02} = 1 \times 10^{-08}$. The units of parameters and variables are omitted for the simplicity. y_1 is the mole fraction of Nickel hydroxide and y_2 is potential difference between at the solid-liquid interface. The initial guess to the estimator is $[x0, z0] = [0.5322, 0.4254]$ and the actual value is $[0.35024, 0.4071]$. The tuning parameters used in EKF are

The following parameters are used

$$\Delta t = 15$$
$$P_0 = \begin{bmatrix} 0.005 & 0 \\ 0 & 0.005 \end{bmatrix}$$
$$Q_{k+1} = 0.00001$$
$$R_{k+1} = 0.0001$$

where Δt is the sampling time , P_0 is the error covariance matrix of differential and algebraic states, Q_{k+1} is the process noise associated with differential states and R_{k+1} is the measurement covariance matrix. The measurement in this case study is y_2, which is the potential difference at the solid-liquid interface. The important point to note is that the augmented covariance matrix should be taken into consideration if the measurement model is a function of differential and algebraic states. Figure 1 and Figure 2 show the estimates for the mole fraction and potential difference.

Fig. 2. EKF estimates of potential difference for case study

4. The tuning parameters for the UKF are same as used in EKF implementation. Figure 5 shows the comparison of UKF and EKF estimates and the their performances are compared by computing the root mean square error (RMSE) of the two states. Table 6 shows the RMSE values of estimates of UKF and EKF. It can clearly be seen that the UKF performs better than the EKF for this case study. Further, the UKF also avoids linearization in the computation of the covariance matrices.

RMSE values of EKF and UKF		
Method	RMSE y_1	RMSE y_2
EKF	0.0305	0.0035
UKF	0.0035	0.0035

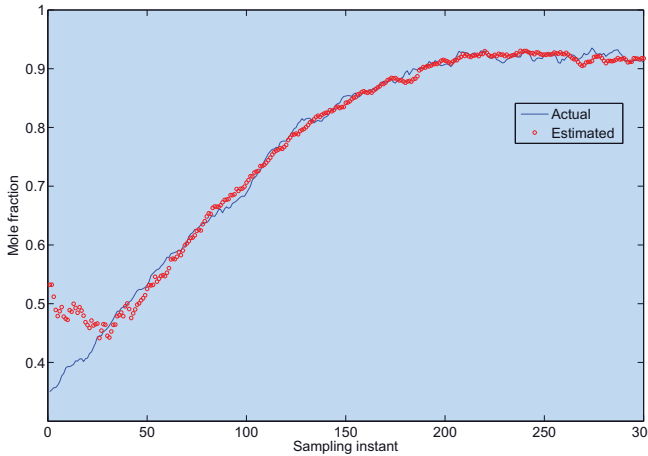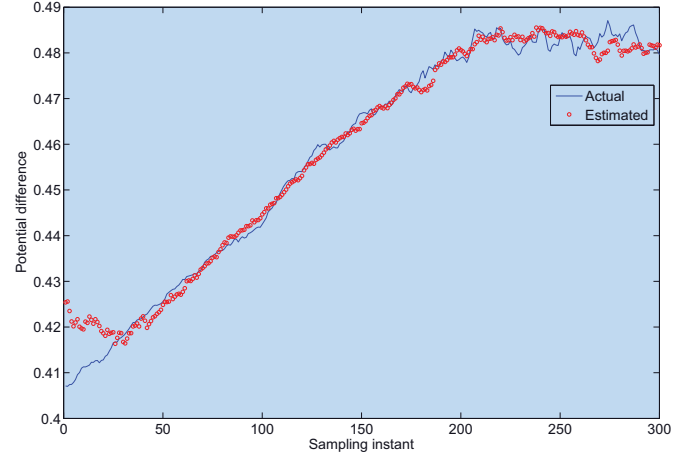Fig. 3. UKF estimates of mole fraction for case study

Fig. 1. EKF estimates of mole fraction for case study

The same differential algebraic system is considered and the UKF approach proposed in this paper is tested. The main advantage of UKF lies in the fact that it does not require linearization to compute covariance matrices. The UKF estimator gives very good estimates of mole fraction and potential difference as shown in Figure 3 and Figure
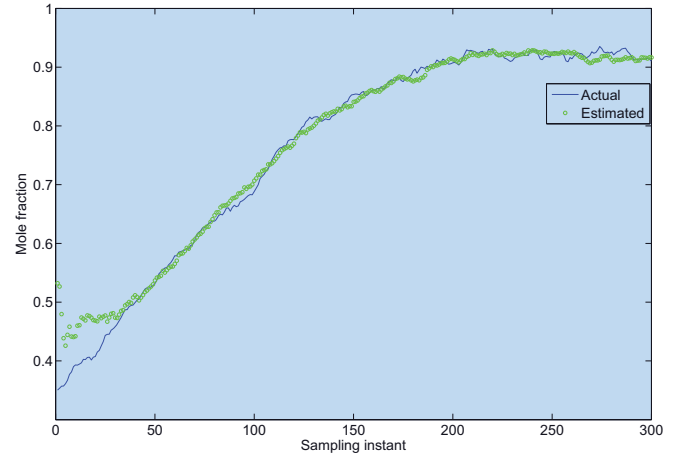
7. CONCLUSIONS

In this paper, EKF and UKF formulations for nonlinear DAEs were proposed. The proposed EKF approach handles the case where the measurement functions are a function of both the differential and algebraic states. While UKF for ODE systems are well studied, there is very little work on the application of the UKF approach to DAE
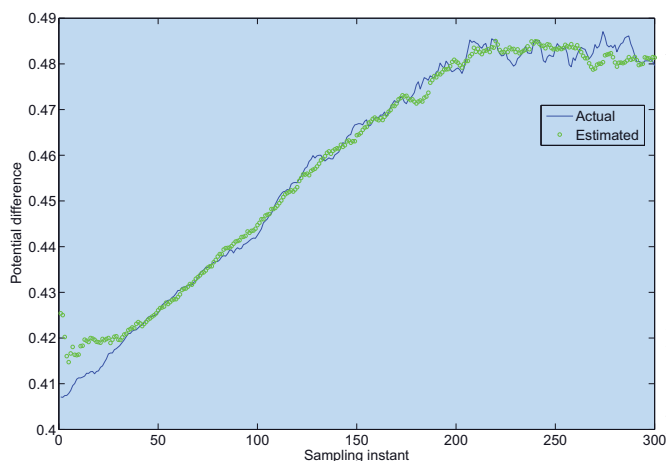
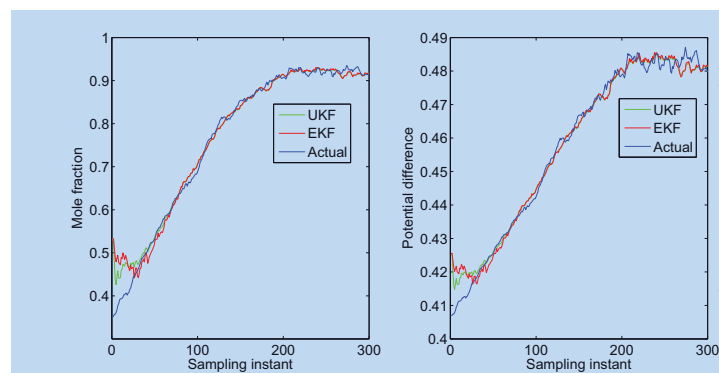Fig. 4. UKF estimates of potential difference for case study

Fig. 5. Comparison of UKF and EKF estimates

systems. One possible approach to use unscented transformation in the estimation of DAE systems is proposed in this work. A case study is presented to demonstrate both the approaches. In this case study, the algebraic state is directly measured. It is shown that while both the proposed approaches provide satisfactory estimation, the UKF approach outperforms the EKF approach.

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