Chemical Engineering Science 65 (2010) 4548–4556

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Recursive state estimation techniques for nonlinear differential algebraic systems

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ARTICLE INFO

Article history:
Received 9 October 2009
Received in revised form
10 April 2010
Accepted 16 April 2010
Available online 7 May 2010

Keywords:
Differential algebraic systems
State estimation
Recursive nonlinear dynamic data reconciliation (RNDDR)

ABSTRACT

Kalman filter and its variants have been used for state estimation of systems described by ordinary differential equation (ODE) models. While state and parameter estimation of ODE systems has been studied extensively, differential algebraic equation (DAE) systems have received much less attention. However, most realistic chemical engineering processes are modelled as DAE systems and hence state and parameter estimation of DAE systems is a significant problem. Becerra et al. (2001) proposed an extension of the extended kalman filter (EKF) for estimating the states of a system described by nonlinear differential-algebraic equations (DAE). One limitation of this approach is that it only utilizes measurements of the differential states, and is therefore not applicable to processes in which algebraic states are measured. In this paper, we address the state estimation of constrained nonlinear DAE systems. The novel aspects of this work are: (i) development of a modified EKF approach that can utilize measurements of both algebraic and differential states, (ii) development of a recursive approach for the inclusion of constraints, and (iii) development of approaches that utilize unscented sampling in state and parameter estimation of nonlinear DAE systems; this has not been attempted before. The utility of these estimators is demonstrated using electrochemical and reactive distillation processes.

1. Introduction

Nonlinear differential algebraic equation (DAE) models can be naturally used to describe the behaviour of several chemical and physical systems. These models arise when some fast rate processes are modelled using a quasi-steady-state approximation, especially involving reaction and separation processes. Algebraic equations in dynamic models also occur when they are used to describe vapor–liquid equilibrium relationships. Other areas where DAE models arise are mechanical systems, electrical systems and biological systems. A DAE model is characterized by its index (Petzold, 1988). 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. In this paper, the focus is on state estimation for nonlinear index one DAE systems that are common in chemical engineering.

State estimation techniques have been well developed for dynamic processes described by ordinary differential equations. The Kalman filter (KF) is an optimal estimator for linear dynamical systems in the presence of state and measurement uncertainties (Gelb, 1988; Sorenson, 1985). For estimating the states of systems described by nonlinear ordinary differential equations (ODEs), the extended Kalman filter (EKF) has been developed. Simultaneous state and parameter estimation is achieved in KF and EKF by augmenting the states (Jazwinski, 1970). Other estimators that have been developed for nonlinear ODE systems are the unscented Kalman filter (UKF) (Julier et al., 2000), ensemble Kalman filter (EnKF) (Houtekamer and Mitchell, 1998), and particle filter (Arulampalam et al., 2002). In order to ensure that the estimates satisfy constraints, extensions of the EKF—such as the recursive nonlinear dynamic data reconciliation (RNDDR) (Vachhani et al., 2005; Teixeira et al., 2009)—have also been developed. All the estimators discussed above are recursive, which makes them efficient for online deployment (Muske and Edgar, 1997).

An alternative estimator using an explicit optimization based approach for state and parameter estimation of nonlinear dynamic processes (ODE systems) is the moving horizon estimator (MHE) (Robertson et al., 1996). MHE solves an optimization problem at every time step. This makes it easy to handle constraints and bounds on the state variables. The standard MHE formulation includes an arrival cost term that summarizes the accumulated uncertainties in state estimates till the current window of interest. The arrival cost cannot be calculated analytically for general nonlinear constrained state estimation

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doi:10.1016/j.ces.2010.04.020

problems even with ODE models. Moreover, the calculation of arrival cost for DAE systems has not been discussed in the literature. For linear unconstrained ODE systems, the standard Kalman filter update formula can be used to express the arrival cost. For constrained linear ODE systems, the arrival cost is approximated by the one for the unconstrained problem (Qu and Hahn, 2009). For nonlinear systems, the arrival cost is estimated by approximating a constrained nonlinear ODE system as an unconstrained linear time-varying system (Tenny and Rawlings, 2002). Albuquerque and Biegler (1995) solve the state and parameter estimation problem in ODE systems using a data reconciliation framework. This approach differs from the traditional state estimation approaches (such as EKF, MHE) in that the terms related to the state uncertainties are not included in the objective function. Hence, the idea of arrival cost is not relevant to this approach. Albuquerque and Biegler (1997) extended the approach discussed in Albuquerque and Biegler (1995) to DAE systems. Computational complexity is an important concern in the application of MHE to large-scale processes that are modelled as DAE systems.

The KF has been used by several researchers for state estimation of systems described by linear DAE models (Nikoukhah et al., 1992; Chisci and Zappa, 1992). For processes modelled using nonlinear DAEs, Becerra et al. (1999, 2001) proposed a modification of EKF for state estimation and demonstrated its application on an experimental setup. They also explored the use of square root formulation of the EKF which has better numerical stability than the standard EKF (Park and Kailath, 1995). A limitation of their approach is that it can only handle measurements which are functions of the differential states. In particular, measurements of the algebraic states cannot be utilized in their approach. This becomes a serious limitation especially for processes such as distillation, where only measurements of algebraic states such as temperatures are available online. 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 also show how this method can be modified to include unscented sampling for better covariance approximation. Finally, we demonstrate how this approach can be modified to include constraints as in the recursive nonlinear dynamic data reconciliation (RNDDR) approach. The utility of these methods is demonstrated on electrochemical and reactive distillation processes.

The paper is organized as follows. Section 2 provides an introduction to DAE systems. EKF, UKF and RNDDR algorithms for DAE systems are discussed in Sections 3, 4 and 5, respectively. Simulation results with discussions are presented in Section 6 followed by conclusions in Section 7.

2. Differential algebraic systems

We consider a continuous nonlinear semi-explicit DAE system with discrete measurements sampled uniformly at a rate Δt, which is described by the following model:

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

$$g(x(t),z(t)) = 0, \quad k\Delta t \le t \le (k+1)\Delta t \tag{2}$$

$$y_{k+1} = h(x_{k+1},z_{k+1}) + v_{k+1} \tag{3}$$

where x_{k+1} are the differential states, z_{k+1} are the algebraic states at time $t=(k+1)\Delta t$, 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}. In the above model, for simplicity no manipulated inputs have been considered, although they can be also included. The index of a DAE system is defined as the number of differentiations required to convert the DAE into an ODE. While there are DAE systems of orders higher than 1 in chemical engineering, index 1 DAE systems are more common, and are considered in this work.

3. Modified EKF for DAE systems

For state and parameter estimation of nonlinear ODE systems, the extended Kalman filter (EKF) has been well studied. However, modifications required in EKF for application to DAE systems have not been thoroughly explored. At first sight it may seem appropriate to convert the DAE system to an ODE system and apply EKF to the resulting ODE system. However, there are three problems with this simplistic approach. Firstly, even for simulating a DAE system it has been shown that converting it to an ODE system and using an ODE solver can introduce significant numerical errors. This implies that the use of EKF can give rise to significant errors in the predicted estimates, if an ODE solver is used on the converted ODE model. Secondly, the updated estimates obtained using an EKF will not necessarily satisfy the algebraic constraints, leading to inconsistent initialization for the next time step. It is therefore necessary to appropriately modify EKF for it to be used for a DAE system. Thirdly, if the DAE model is reduced to ODE model consisting of only the differential states (reduced order), measurements which are functions of algebraic states cannot be utilized for the state estimation. Becerra et al. (2001) developed a modified EKF estimation approach for nonlinear index-1 DAEs, which solves some of the problems described above. We describe this approach first.

Let $\hat{x}_{k|k}$ and $\hat{z}_{k|k}$ be the updated estimates of the differential and algebraic states, respectively, at time instant k, and let $P_{k|k}$ be the covariance matrix of errors in the updated differential state estimates. It is also assumed that the state estimates are consistent, that is, they satisfy the algebraic constraints:

$$g(\hat{x}_{k|k},\hat{z}_{k|k}) = 0 \tag{4}$$

Starting with these estimates a DAE solver is used to solve the following differential-algebraic system:

$$\hat{x}_{k+1} = \hat{x}_k + \int_{(k)\Delta t}^{(k+1)\Delta t} f(x(t),z(t))\,dt + w_{k+1} \tag{5}$$

$$g(x(t),z(t)) = 0, \quad k\Delta t \le t \le (k+1)\Delta t \tag{6}$$

The solution of the above DAE at time $t=(k+1)\Delta t$ gives the predicted estimates $\hat{x}_{k+1|k}$ and $\hat{z}_{k+1|k}$. In the method proposed by Becerra et al. (1999), only the covariance matrix of errors in the differential states is computed. This computation is performed using a reduced linearized system model obtained by eliminating the algebraic states. The reduced linearized system is given by

$$\dot{x} = Ax \tag{7}$$

where

$$A = (J_1 - J_2 J_4^{-1} J_3) \tag{8}$$

$$\begin{bmatrix} J1 & J2 \\ J3 & J4 \end{bmatrix} = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial z} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial z} \end{bmatrix} \tag{9}$$

The covariance matrix of errors in the differential states can now be computed as in EKF

$$P_{k+1|k} = \overline{A}_k P_{k|k} \overline{A}_k^T + Q_{k+1} \tag{10}$$

where $\overline{A} = \exp(A\Delta t)$.

The updated estimates of the differential states are obtained by linearizing the measurement model and using the Kalman filter update equation, similar to the EKF. First, the Kalman gain is computed using

$$K_{k+1} = P_{k+1|k}H_{k+1}^T(H_{k+1}P_{k+1|k}H_{k+1}^T + R_{k+1})^{-1} \tag{11}$$

where $H_{k+1} = \partial h/\partial x$ is the linearized measurement model evaluated at $\hat{x}_{k+1|k}$. It may be noted that the above computation implicitly assumes that the measurements are functions of differential states only. The updated estimates of the differential estimates are obtained using the Kalman update equation given by

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K_{k+1}(y_{k+1} - h(\hat{x}_{k+1|k})) \tag{12}$$

The covariance matrix of errors in the updated differential state estimates is also computed using the standard EKF procedure and is given by

$$P_{k+1|k+1} = (I - K_{k+1}H_{k+1})P_{k+1|k} \tag{13}$$

Finally, the updated estimates of the algebraic states are computed such that they satisfy the nonlinear algebraic equations, that is a nonlinear equation solver is used to solve the following equations:

$$g(\hat{x}_{k+1|k+1}, \hat{z}_{k+1|k+1}) = 0 \tag{14}$$

It may be noted that the algebraic state estimates $\hat{z}_{k+1|k+1}$ are computed using only the updated differential state estimates $\hat{x}_{k+1|k+1}$ and neither directly utilize the prior algebraic state estimates, nor do they utilize information that may be available through measurements of the algebraic states. In the following section, we propose an approximate EKF procedure which eliminates all these disadvantages.

4. Proposed approach: Extended Kalman Filter (EKF) 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 is derived. This linearized ODE model is used for the covariance propagation of augmented state. The propagation of states is the same as in Becerra et al. (2001) approach. The gain matrix is calculated from 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 using the augmented Kalman gain matrix. Only the differential states are retained from the augmented corrected states. The corrected algebraic states are recalculated from the nonlinear algebraic equations. Notice that the estimator can still be setup using only the differential states. However, as mentioned before, we would like to use the algebraic states directly in the estimator.

The nonlinear DAE system given by Eqs. (1)–(3) is considered with discrete measurements sampled at regular intervals with sampling period Δt. In the proposed method, states are augmented and the estimated state and error covariance at time k are defined by $X_{k|k}^{aug}$ and $P_{k|k}^{aug}$, respectively. The basic idea behind the covariance propagation is explained next before the complete estimation algorithm is described.

For the purpose of obtaining the error covariance matrix in the augmented state estimates, a linearized approximation of the DAE system is obtained:

$$\dot{x} = Ax + Bz$$

$$0 = Cx + Dz \tag{15}$$

where

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial z} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial z} \end{bmatrix} \tag{16}$$

Differentiating the linearized algebraic equation once, we get

$$0 = C\dot{x} + D\dot{z} \tag{17}$$

Then

$$\dot{z} = -D^{-1}C\dot{x} \tag{18}$$

$$\dot{z} = -D^{-1}CAx - D^{-1}CBz \tag{19}$$

Writing in matrix form

$$\begin{bmatrix} \dot{x} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} A & B \\ -D^{-1}CA & -D^{-1}CB \end{bmatrix} \begin{bmatrix} x \\ z \end{bmatrix} \tag{20}$$

The augmented form is

$$\dot{x}^{aug} = A^{aug}x^{aug} \tag{21}$$

The transition matrix is evaluated as

$$\phi = \exp(A^{aug}\Delta t) \tag{22}$$

4.1. Estimation algorithm

- 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

$$P_{k+1|k}^{aug} = \phi P_{k|k}^{aug}\phi^T + \Gamma Q_{k+1}\Gamma^T \tag{23}$$

where

$$\Gamma = \begin{bmatrix} I \\ -D^{-1}C \end{bmatrix} \tag{24}$$

- The augmented Kalman gain is computed as

$$K_{k+1}^{aug} = P_{k+1|k}^{aug}H_{k+1}^{augT}(H_{k+1}^{aug}P_{k+1|k}^{aug}H_{k+1}^{augT} + R_{k+1})^{-1} \tag{25}$$

where H_{k+1}^{aug} is the linearized measurement model evaluated at $\hat{x}_{k+1|k}^{aug}$.

- The updated state estimate is given by

$$\hat{x}_{k+1|k+1}^{aug} = \hat{x}_{k+1|k}^{aug} + K_{k+1}^{aug}(y_{k+1} - h(\hat{x}_{k+1|k}^{aug})) \tag{26}$$

Of these only the differential states $x_{k+1/k+1}$ are retained.

- Given $\hat{x}_{k+1|k+1}$, calculate estimates of the algebraic states $z_{k+1|k+1}$ using

$$g(\hat{x}_{k+1|k+1}, \hat{z}_{k+1|k+1}) = 0 \tag{27}$$

- The updated covariance matrix is calculated as

$$P_{k+1|k+1}^{aug} = (I - K_{k+1}^{aug}H_{k+1}^{aug})P_{k+1|k}^{aug} \tag{28}$$

It should be noted that as in EKF, Eq. (28) is an approximate method used to estimate the error covariance matrix of the updated state estimates. While the updated state estimates of the algebraic states have been computed using the algebraic constraints and not through the Kalman update equation, Eq. (28) does not take this into account while estimating the error covariance matrix of the updated estimates. Another approximation that is possible is to compute the error covariance matrix of

the updated algebraic state estimates (and its cross correlation with the differential state estimates) based on linearization of the algebraic equations. This will result in a singular augmented covariance matrix.

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 equals 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. The estimates obtained using this approach are more accurate as compared to those based on a linearized model (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; der Merwe et al., 2000; Julier, 2002; Vachhani et al., 2006; 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 using a DAE solver. The covariance matrix of errors for the propagated states is calculated using the propagated states and the covariance matrix of the process noise. Unscented samples for the differential and algebraic states are generated again 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. The UKF algorithm for DAE systems is explained below.

- At the kth instant, $\hat{x}_{k|k}$ is the filtered estimate of differential states and $P_{k|k}$ is the associated covariance matrix. $2n+1$ 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:

$$\hat{X}_{k|k,0} = \hat{x}_{k|k}, \quad W_0 = \frac{\kappa}{(n+\kappa)} \tag{29}$$

$$\hat{X}_{k|k,i} = \hat{x}_{k|k} + (\sqrt{(n+\kappa)P_{k|k}})_i, \quad W_i = \frac{1}{2(n+\kappa)} \tag{30}$$

$$\hat{X}_{k|k,i+n} = \hat{x}_{k|k} - (\sqrt{(n+\kappa)P_{k|k}})_i, \quad W_{i+n} = \frac{1}{2(n+\kappa)} \tag{31}$$

  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 $\hat{X}_{k|k,i}$ is same as $\hat{x}_{k|k}$. The weighted covariance matrix of the sample is equal to $P_{k|k}$.
- Calculate $\hat{Z}_{k|k,i}$ from $g(\hat{X}_{k|k,i}, \hat{Z}_{k|k,i}) = 0$. This ensures that the sigma points are consistent.
- Propagate $\hat{X}_{k|k,i}$ and $\hat{Z}_{k|k,i}$ using DAE solver 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

$$\hat{x}_{k+1|k} = \sum_{i=0}^{2n} W_i \hat{X}_{k+1|k,i} \tag{32}$$

- Calculate $P^{xx}_{k+1|k}$

$$P^{xx}_{k+1|k} = \sum_{i=0}^{2n} W_i (\hat{X}_{k+1|k,i} - \hat{x}_{k+1|k})(\hat{X}_{k+1|k,i} - \hat{x}_{k+1|k})^T + Q_{k+1} \tag{33}$$

- Perform unscented sampling with $\hat{x}_{k+1|k}$ as mean and $P^{xx}_{k+1|k}$ as covariance matrix to obtain new $\hat{X}_{k+1|k,i}$.
- Recalculate $\hat{Z}_{k+1|k,i}$ from $g(\hat{X}_{k+1|k,i}, \hat{Z}_{k+1|k,i}) = 0$.
- Form $\hat{X}^{aug}_{k+1|k,i}$ by augmenting $\hat{X}_{k+1|k,i}$ with $\hat{Z}_{k+1|k,i}$.
- Calculate $\hat{x}^{aug}_{k+1|k}$

$$\hat{x}^{aug}_{k+1|k} = \sum_{i=0}^{2n} W_i \hat{X}^{aug}_{k+1|k,i} \tag{34}$$

- Calculate

$$Y_{k+1,i} = h(\hat{X}^{aug}_{k+1|k,i}) \tag{35}$$

- Compute the Kalman gain matrix

$$K_{k+1} = P_{xv,k+1}(P_{vv,k+1})^{-1} \tag{36}$$

  where

$$P_{vv,k+1} = \sum_{i=0}^{2n} W_i (Y_{k+1,i} - \hat{y}_{k+1})(Y_{k+1,i} - \hat{y}_{k+1})^T + R_{k+1} \tag{37}$$

$$P_{xv,k+1} = \sum_{i=0}^{2n} W_i (\hat{X}^{aug}_{k+1,i} - \hat{x}^{aug}_{k+1|k})(Y_{k+1,i} - \hat{y}_{k+1})^T \tag{38}$$

$$\hat{y}_{k+1} = \sum_{i=0}^{2n} W_i Y_{k+1,i} \tag{39}$$

- The Kalman gain corresponding to differential states is K^{diff}_{k+1}, which is a matrix with just the first n (number of differential states) rows of K_{k+1}.
- Compute estimates for corrected differential states

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K^{diff}_{k+1}(y_{k+1} - \hat{y}_{k+1}) \tag{40}$$

- Given the corrected differential states, $\hat{x}_{k+1|k+1}$, compute $\hat{z}_{k+1|k+1}$ from $g(\hat{x}_{k+1|k+1}, \hat{z}_{k+1|k+1}) = 0$.
- Compute covariance matrix of error in the updated differential estimates using

$$P_{k+1|k+1} = P_{k+1|k} - K^{diff}_{k+1} P_{vv,k+1} K^{diff^T}_{k+1} \tag{41}$$

It may be noted that in the above approach, only the covariance matrix of the error in the estimates of the differential states needs to be computed.

6. RNDDR approach for DAE systems

In the previous sections EKF and UKF approaches were discussed for state estimation in nonlinear DAE systems. However, bounds on either the differential or the algebraic states were not considered in the DAE model. Bounds on states have to be enforced in many realistic chemical engineering problems. The EKF and the UKF approaches discussed in this paper need to be modified with ad hoc clipping strategies to enforce such bounds. However, we had previously developed recursive nonlinear dynamic data reconciliation (RNDDR) to address the issue of constraints and bounds in an EKF framework for ODE systems. This approach can be easily extended to semi-explicit index-1 DAE systems that is of interest in this paper. The RNDDR

algorithm is explained below. It can be noted that in the absence of algebraic variables, the RNDDR approach for DAE systems reduces to the RNDDR approach for ODE systems. The nonlinear DAE system equations (1)–(3) is considered with discrete measurements sampled at regular intervals with sampling period Δt.

The proposed RNDDR algorithm consists of following steps:

- The prediction step of the RNDDR approach is the same as in the proposed EKF approach for DAE systems (the approach discussed in Section 4.1).
- The updated differential state estimates $\hat{x}_{k+1|k+1}$ and algebraic state estimates are obtained through a solution to the following optimization problem:

$$\min_{x^{aug}_{k+1}} (x^{aug}_{k+1}-\hat{x}^{aug}_{k+1|k})^T (P^{aug}_{k+1|k})^{-1} (x^{aug}_{k+1}-\hat{x}^{aug}_{k+1|k}) + (y_{k+1}-h(x^{aug}_{k+1}))^T R^{-1}_{k+1} (y_{k+1}-h(x^{aug}_{k+1})) \quad (42)$$

subject to the following constraints

$$g(X^{aug}_{k+1}) = 0 \quad (43)$$

Additional constraints and bounds on the algebraic and differential states can be added to the constraints.

- The updated error covariance matrix is calculated as in the proposed EKF approach (Section 4.1, Eq. (28)).

In setting up the objective function defined by (42), it is assumed that the augmented error covariance matrix is non-singular. However, if the computed augmented error covariance matrix becomes singular, then the first term of Eq. (42) can be written only for the differential states.

7. Simulation studies

7.1. Case study 1

The utility of the proposed EKF and UKF approaches is tested on an electrochemical case study. The case study considers a galvanostatic charge process of a thin film nickel hydroxide electrode (Celik et al., 2002). The operation can be charging, open-circuit or discharging depending on the value of i_{app} (positive, zero or negative). The rate of change of the mole fraction of nickel hydroxide (y_1) is given by

$$\frac{\rho V}{W}\frac{dy_1}{dt} = \frac{j_1}{F} \quad (44)$$

$$j_1 + j_2 - i_{app} = 0 \quad (45)$$

where

$$j_1 = i_{01}\left[2(1-y_1)\exp\left(\frac{0.5F}{RT}(y_2-\phi_{eq,1})\right) - 2y_1 \times \exp\left(\frac{-0.5F}{RT}(y_2-\phi_{eq,1})\right)\right] \quad (46)$$

$$j_2 = i_{02}\left[\exp\left(\frac{F}{RT}(y_2-\phi_{eq,2})\right) - \exp\left(\frac{-F}{RT}(y_2-\phi_{eq,2})\right)\right] \quad (47)$$

and y_2 is the potential difference between the solid and liquid interface. Eq. (44) is the species balance equation, and Eq. (45) 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 Faraday's constant $F = 96487\,\mathrm{C/mol}$, ideal gas constant $R = 8.314\,\mathrm{J/mol\,K}$, temperature $T = 298.15\,\mathrm{K}$, equilibrium potential of nickel reaction $\phi_{eq,1} = 0.420\,\mathrm{V}$, equilibrium potential of oxygen reaction $\phi_{eq,2} = 0.303\,\mathrm{V}$, density of nickel active material $\rho = 3.4\,\mathrm{g/cm^3}$, molecular weight $W = 92.7\,\mathrm{g/mol}$, effective length $V = 1 \times 10^{-5}\,\mathrm{cm}$, applied current density on the nickel electrode $i_{app} = 1 \times 10^{-5}\,\mathrm{A/cm^2}$, exchange current density of the nickel reaction $i_{01} = 1 \times 10^{-04}\,\mathrm{A/cm^2}$, exchange current density of the oxygen reaction $i_{02} = 1 \times 10^{-08}\,\mathrm{A/cm^2}$. The initial guess to the estimator is $[y_1, y_2] = [0.5322, 0.4254]$ and the actual initial state used in the simulation study is [0.35024, 0.4071]. It can be easily verified that both the initial state and initial guess are consistent. The tuning parameters used in EKF are

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

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 algebraic state. Since in this process, only the algebraic state is measured, the method of Becerra et al. (2001) cannot be used, and the proposed modified EKF approach is necessary. Figs. 1 and 2 show the estimates for the mole fraction and potential difference.

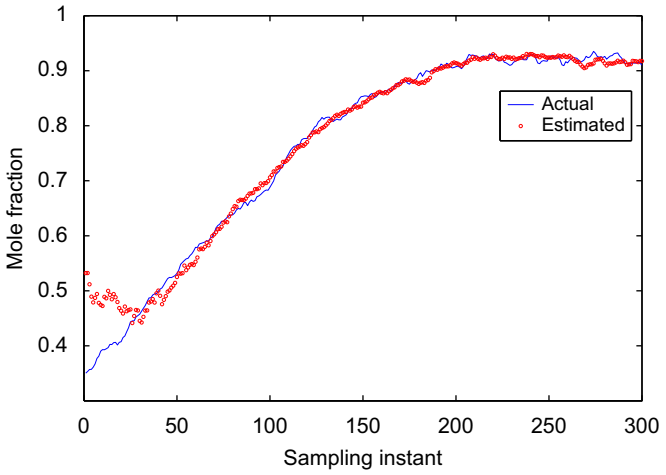

Fig. 1. EKF estimates of mole fraction for case study.

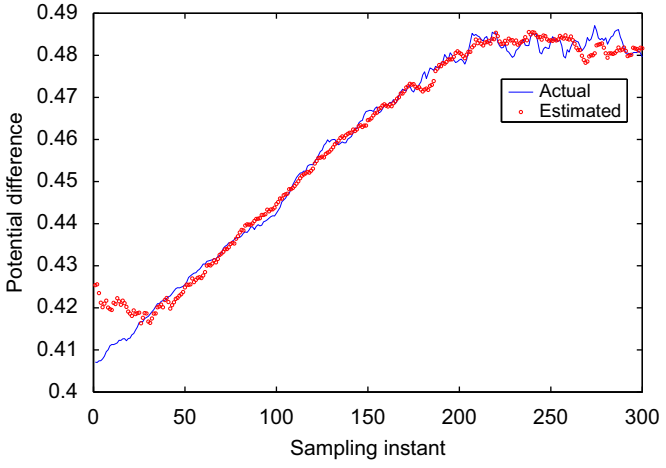

Fig. 2. EKF estimates of potential difference for case study.

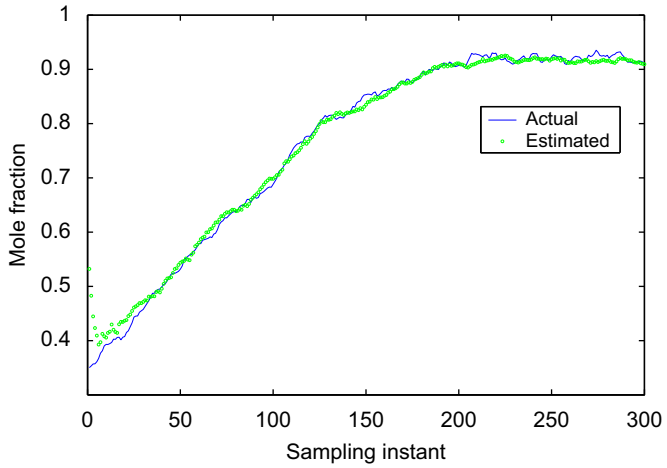

Fig. 3. UKF estimates of mole fraction for case study.

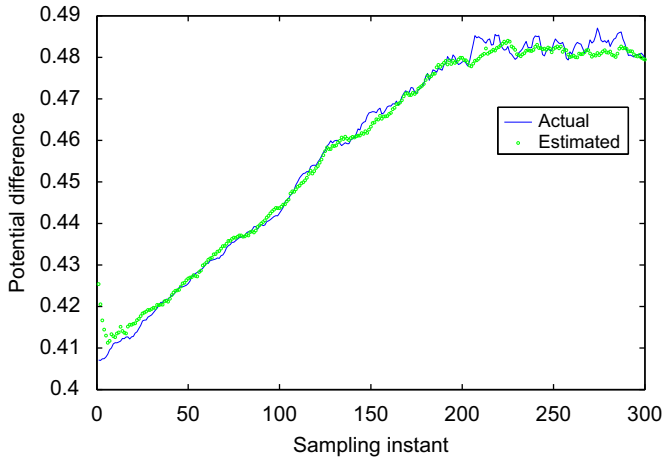

Fig. 4. UKF estimates of potential difference for case study.

Table 1
RMSE values of EKF and UKF.

Method	RMSE y_1	RMSE y_2
EKF	0.0246	0.0029
UKF	0.0178	0.0024

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 Figs. 3 and 4. The tuning parameters for the UKF are same as used in EKF implementation. Table 1 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. This performance improvement is due to better approximation of the covariance propagation.

7.2. Case study 2: metathesis of 2-pentene

The second case study is a reactive distillation process involving the metathesis of 2-pentene (Chen et al., 2000). Metathesis of 2-pentene involves dissociation of 2-pentene (B) to form 2-butene (A) and 3-hexene (C) and it is an equimolar and reversible reaction as shown in

$$2C_5H_{10} \Leftrightarrow C_4H_8 + C_6H_{12} \tag{48}$$

Following assumptions are made while formulating the model of the reactive distillation process

- The condenser is a total condenser.
- Adiabatic column.
- The molar heat of vaporization is constant.
- Reaction proceeds only in the liquid phase and it is kinetically controlled.
- Vapor hold up is negligible.
- Vapor and liquid leaving each stage are in equilibrium.
- Each stage is a perfectly mixed CSTR.
- Liquid hold up is constant.

The mass balance for component i on any stage j is written in unsteady form as

$$\frac{dx_{j,i}}{d\tau} = \frac{H_T}{F}\frac{1}{H_j}(F_j z_{j,i} + L_{j-1}x_{j-1,i} + V_{j+1}y_{j+1,i} - V_j y_{j,i} - L_j x_{j,i}) + \frac{H_T}{H_T^R}\frac{Da}{k_{f,ref}}\delta_j \sum_{r=1}^{R}(v_{r,i}\varepsilon_{j,r}) \tag{49}$$

where $d\tau = (F/H_T)\,dt$, $H_T = \sum_{j=0}^{N} H_j$, $H_T^R = \sum_{j=0}^{N}(\delta_j H_j)$. δ_j is a parameter used to calculate the total reactive liquid hold up within a reactive column. δ_j is equal to one if reaction occurs on stage j, otherwise $\delta_j = 0$. The Damköhler number, $Da = (H_T^R/F)/(1/k_{f,ref})$, is a dimensionless ratio of a characteristic liquid residence time (H_T^R/F) to the characteristic reaction time $(1/k_{f,ref})$. $k_{f,ref}$ is a forward rate constant evaluated at a reference temperature which is the boiling point of the lowest boiling pure component in the system.

The total number of moles generated at any stage j is given by

$$R_j = \delta_j H_j \sum_{r=1}^{R}(v_{T,r}\varepsilon_{j,r}) \tag{50}$$

$$\varepsilon_{j,r} = k_{f,r}\left(\prod_{i=1}^{C} a_{j,i}^{(|v_{r,i}|-v_{r,i})/2} - \frac{1}{K_r}\prod_{i=1}^{C} a_{j,i}^{(|v_{r,i}|+v_{r,i})/2}\right) \tag{51}$$

$$v_{T,r} = v_{r,1} + v_{r,2} + \cdots + v_{r,3} \tag{52}$$

$j = 0,1,\ldots,N$; $i = 1,2\ldots,C$; $r = 1,2,\ldots,R$, where N is the total number of stages, C is the number of components and R is the number of reactions.

The reaction equilibrium and reaction rate is expressed as

$$K_r = A_r \exp\left(\frac{B_r}{T} + C_r \ln(T)\right) \tag{53}$$

$$k_{f,r} = a_r \exp\left(\frac{b_r}{T}\right) \tag{54}$$

The rate model is

$$r = k_f\left(a_{C_5H_{10}}^2 - \frac{a_{C_4H_8}a_{C_6H_{12}}}{K_{eq}}\right) \tag{55}$$

The reaction equilibrium constants and rate constant for metathesis of 2-pentene are shown in Eqs. (56) and (59):

$$K_{eq} = 0.25 \tag{56}$$

$$k_f = 1.0661 \times 10^5 \exp(-3321.2/T)\,\mathrm{h}^{-1}, \quad T(K) \tag{57}$$

The summation of mole fractions of all components in vapor phase is equal to one in any stage. These equations form the algebraic part of DAE system. The algebraic equations for the DAE

system are

$$\sum_{i=1}^{C} y_{j,i} = 1 \tag{58}$$

where

$$y_{j,i} = \frac{psat_i x_{j,i}}{P} \tag{59}$$

The normal boiling point of C_5H_{10} is chosen as reference and the value of $k_{f,ref}$ is 2.328 h^{-1}. $psat_i$ is the saturation pressure of the ith component. The system has ideal vapor–liquid equilibrium and a negligible heat of reaction at atmospheric pressure. The specifications of the simulation are taken from Okasinski and Doherty (1998). The reactive distillation system chosen has 14 stages including total condenser and reboiler.

The resultant system of equations from mass balances and formulations is a DAE system of index 1. The equations are of the form

$$\frac{dx}{dt} = f(x,T,u) \tag{60}$$

$$0 = g(x,T,u) \tag{61}$$

where x is the mole fraction, T is the temperature and u is the input to the system. If relative volatility is assumed to be constant, then the temperature can be obtained explicitly in terms of the liquid mole fractions, and the process can be modelled as ODE system. In this case study, Raoult's law is used and consequently, the process model is a DAE system.

The DAE system in this case study consists of liquid mole fractions as differential states and temperature as algebraic states. The mass balances of components on different stages in unsteady form are differential equations, and the summation of vapor mole fractions of all components on different stages are algebraic equations. The estimation problem defined here is to estimate the states that are the mole fractions of the components namely, 2-pentene, 2-butene and 3-hexene, from the available measurements which are temperatures of the trays. The number of measurements available is 14 temperature measurements and they are corrupted with Gaussian noise. The differential states in this problem are 28 in number which are the mole fractions of 2-butene and 2-pentene in all the stages and the 14 algebraic variables are the temperatures of the trays. The mole fractions of 3-hexene on all the trays are obtained once the mole fractions of 2-butene and 2-pentene on all trays are computed. For this process, it is also necessary to ensure that the state estimates of the two mole fractions at each stage are bounded between 0 and 1. Thus, for state estimation, the proposed modified RNDDR approach for DAE systems has to be used.

The initial guess of the estimator $\hat{x}_{0/0}$ is chosen to be considerably different from the actual initial state. The tuning parameters used in this case study are

$$\Delta t = 0.05\,\text{h}, \quad P_0 = 0.1 * (\text{diag}(\hat{x}_{0/0}(1:42)^2))$$

$$Q = 10^{-6}(\text{diag}(\hat{x}_{0/0}(1:28)^2)), \quad R = 0.225 * 10^{-5}(\text{diag}(\hat{x}_{0/0}(29:42)^2))$$

The actual dynamics are obtained by changing the reflux ratio from 4.0 to 6.0. The above specified problem is a nonlinear estimation of DAE system with inequality constraints and bounds. The estimates of mole fractions of component A on the top and bottom stages are seen in Figs. 5 and 6, respectively. It is clear from both the figures that the estimator is able to track the dynamics in the first few time instants. Figs. 7 and 8 show the estimates of mole fractions of component B on top and bottom stages, respectively. The estimate of mole fraction of component C on the bottom stage is also shown in Fig. 9. The filtering of measurements (temperature) is also evident from Figs. 10 and 11. Figs. 10 and 11 show the temperature estimates of bottom stage and 6th stage, respectively. An important point to note is that the estimates satisfy algebraic constraints and also the additional

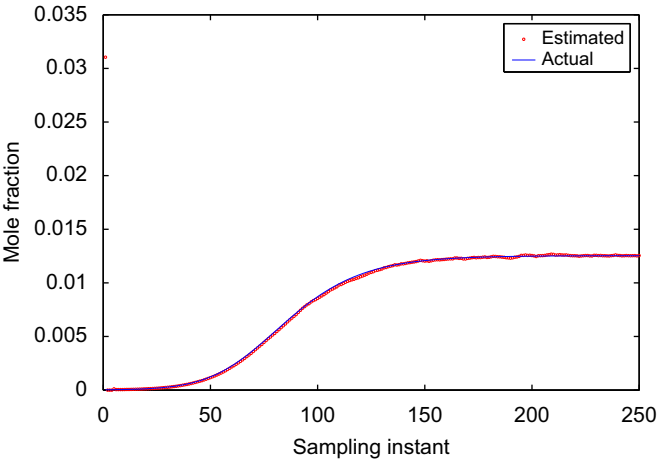

Fig. 6. Estimated mole fraction of component A on bottom stage.

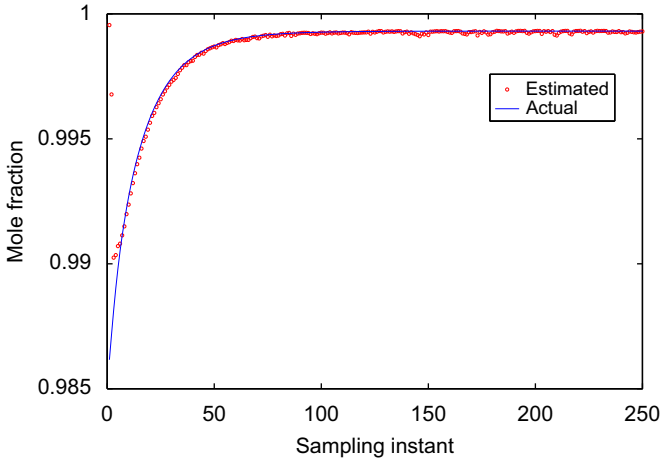

Fig. 5. Estimated mole fraction of component A on top stage.

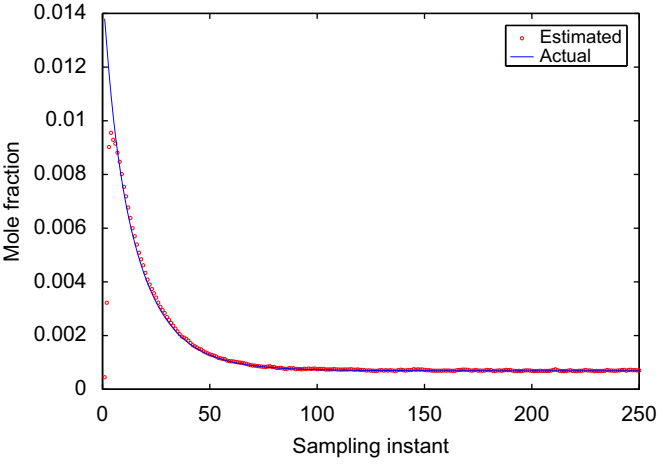

Fig. 7. Estimated mole fraction of component B on top stage.

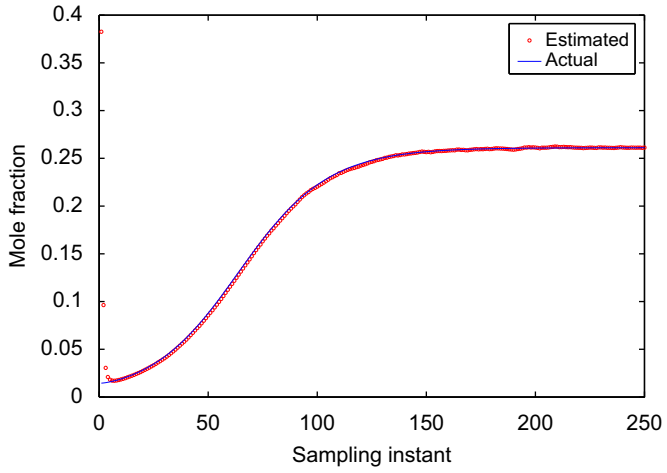

Fig. 8. Estimated mole fraction of component B on bottom stage.

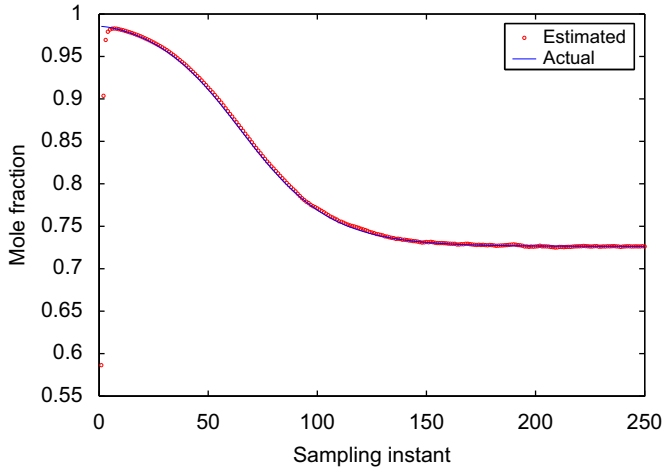

Fig. 9. Estimated mole fraction of component C on bottom stage.

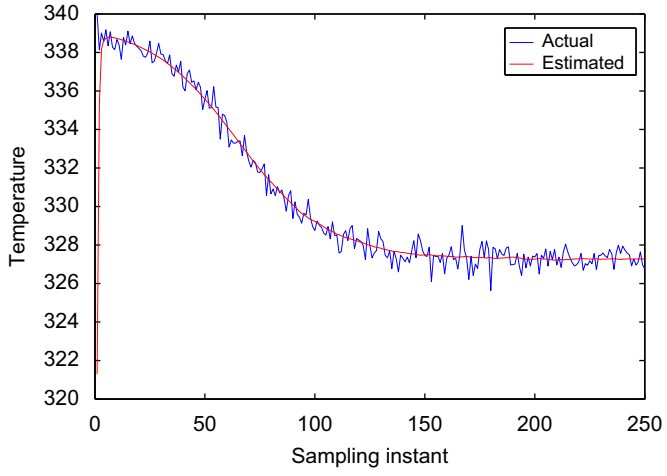

Fig. 10. Temperature estimates for bottom stage.

constraints which are the summation of mole fractions of components on any stage should equal one and the mole fraction of the components should be between 0 and 1. This case study demonstrates the use of the RNDDR approach for nonlinear DAE systems where the measurements are functions of algebraic states with additional state constraints.

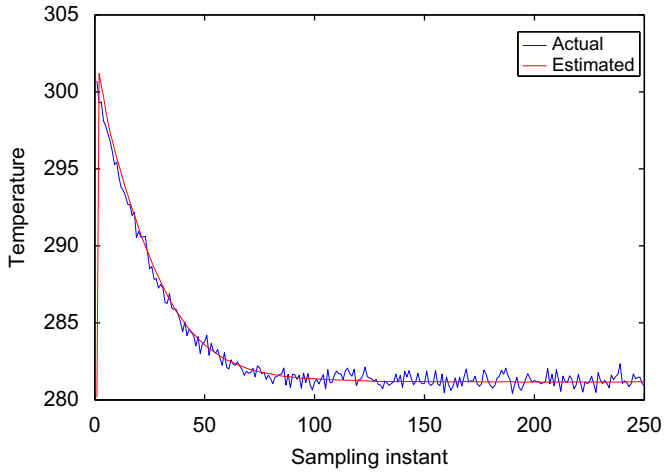

Fig. 11. Temperature estimates for 6th stage.

8. Conclusions

In this paper, the problem of state estimation in nonlinear DAE systems was addressed. This is a significant problem as many chemical processes can be modelled as DAE systems. EKF and UKF formulations for state estimation of nonlinear DAEs were proposed. The proposed EKF approach handles the case where the measurements are functions of both differential and algebraic states. While UKF for ODE systems is well studied, there is very little work on the application of UKF to DAE systems. One possible approach to include unscented transformation in the estimation of DAE systems is proposed in this work. The use of unscented transformation for nonlinear DAE systems has not been discussed before in literature. An electrochemical case study is used to study the performance of the EKF and UKF approaches. The algebraic state is directly measured in this electrochemical case study. It is shown that while both the approaches provide satisfactory estimation, the UKF approach outperforms the EKF approach. RNDDR formulation for DAE systems is also presented in this work. The RNDDR approach enables us to include additional constraints that need to be satisfied. The performance of the RNDDR approach is studied using a reactive distillation case study. In this case study, mole fractions are the differential states and tray temperatures are the algebraic states. The goal of this case study is to perform constrained estimation of the mole fractions given tray temperature measurements. It is shown that the RNDDR approach provides reliable estimates for the mole fractions and could be an attractive method for constrained estimation in nonlinear DAE systems.

Acknowledgements

The authors thank the National Science Foundation for partial support through the Grant CTS-0341608.

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