Modified Extended Kalman Filtering for Nonlinear Stochastic Differential Algebraic Systems

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Abstract: The extended Kalman filter (EKF) is one of the most widely used nonlinear filtering technique for a system of differential algebraic equations (DAEs). In this work we propose an alternate EKF approach for state estimation of nonlinear DAE systems that addresses shortcomings of the EKF approaches available in literature (Becerra et al., 2001; Mandela et al., 2010). The proposed approach is based on the idea that since the algebraic equations are assumed to be exact, the error covariance matrix of only the differential states needs to be directly propagated during the prediction step. The error covariance matrix for algebraic states and cross covariance matrix between the errors in differential and algebraic states, which are required to incorporate effect of prior algebraic state estimates on the update step, can be computed from the differential state error covariance matrix alone using the linearized algebraic equations. The update step of the proposed work also follows a similar philosophy and ensures that the covariance update is not approximate. The efficacy of the proposed EKF approach is evaluated using benchmark case studies of a Galvanostatic charge process and a drum boiler.

1. INTRODUCTION

Modeling of various physical and chemical processes often gives rise to nonlinear differential algebraic equations (DAEs). For a process involving different time scales, the fast rate phenomena are usually modeled using quasi-steady state approximation to yield algebraic equations that are coupled with differential equations.

State estimation of DAEs has received relatively less attention compared to the estimation of systems described by ordinary differential equations (ODEs). For system with linear DAE models, Nikoukhah et al. (1992) applied Kalman filter (KF) approach for state estimation. In case of nonlinear DAE systems, Becerra et al. (2001) presented an EKF approach in square-root form. In their approach, an implicit stochastic differential equation (SDE) model is derived from the linearization of DAEs to propagate the error covariance matrix of differential states. However, they assumed that only the differential states are measured and hence their method cannot incorporate the information available via measurements of algebraic states during the EKF update step. To address this issue, Mandela et al. (2010) developed an alternate EKF approach that can incorporate measurements of both differential and algebraic states. In their work, an augmented state vector consisting of both differential and algebraic state variables is considered. The corresponding error covariance matrix of the augmented state is propagated using an implicit SDE model which is derived from the linearization of DAEs. Their approach enabled incorporation of algebraic states since the augmented prior covariance matrix was considered during the update step. However, the update step uses an approximate method to update the augmented covariance matrix to avoid singular augmented covariance matrix. Some other approaches have been reported for estimation of a DAE system, such as unscented Kalman filter (Mandela et al., 2010), ensemble Kalman filter (Puranik et al., 2012), particle filter (Haßkerl et al., 2016) and iterative EKF (Purohit and Patwardhan, 2018). Although these approaches provide improved performance, they are computationally more complex than the existing EKF approaches.

In the current work, we propose an alternate EKF approach which avoids the drawbacks of approaches available in literature. In particular, our approach can incorporate measurements of both differential and algebraic states as well as does not use an approximate method to obtain error-covariance matrix during the update step. The approach is based on the key idea that since the differential equations are assumed to be stochastic while the algebraic equations are considered to be exact, it is more appropriate to propagate the error covariance matrix of only the differential states during the prediction step. The error covariance matrix of algebraic states and the cross-covariances of differential and algebraic state errors can be computed from the error covariance matrix of the differential states since the algebraic and differential states are related through the deterministic algebraic equations. Thus, the error-covariance matrix of the augmented state vector, which is required in the update step, is computed from the error covariance matrix of the differential states alone. A similar philosophy of directly updating only the differential state error covariance matrix during the measurement update step is followed. The effectiveness of proposed EKF approach is demonstrated on two benchmark case studies.

The rest of the paper is organized as follows. Section 2 introduces the problem at hand and summarizes the relevant EKF approach from literature. Section 3 presents the proposed EKF approach for state estimation of nonlinear DAE systems. Section 4 applies the proposed EKF approach on two benchmark case studies. The paper is concluded in Section 5.

2. PROBLEM FORMULATION AND RELEVANT EKF APPROACH

2.1 Problem formulation

Consider a process described by a set of index one semi-explicit nonlinear differential algebraic equations

$$\frac{d\mathrm{x}^{\mathrm{d}}}{dt} = f\left(\mathrm{x}^{\mathrm{d}}(t),\, \mathrm{x}^{\mathrm{a}}(t)\right) + w(t) \tag{1a}$$

$$0 = g\left(\mathrm{x}^{\mathrm{d}}(t), \mathrm{x}^{\mathrm{a}}(t)\right) \tag{1b}$$

$$\mathrm{y}_t = h\left(\mathrm{x}^{\mathrm{d}}(t), \mathrm{x}^{\mathrm{a}}(t)\right) \tag{1c}$$

where $\mathrm{x}^{\mathrm{d}} \in \mathbb{R}^{n_d}$ and $\mathrm{x}^{\mathrm{a}} \in \mathbb{R}^{n_a}$ represent the differential and algebraic state variables respectively; $\mathrm{y}_t \in \mathbb{R}^{n_m}$ represents the true measured variables. The continuous-time white Gaussian process noise is denoted by $w(t)$. The known nonlinear differential, algebraic and measurement functions are represented by f, g and h respectively. With the assumption that measurements are available regularly at the sampling interval T_s and are corrupted with white Gaussian noise v_k, above DAE model equations (1a)-(1c) can be represented in discrete-time form as,

$$\mathrm{x}^{\mathrm{d}}_k = \mathrm{x}^{\mathrm{d}}_{k-1} + \int_{(k-1)T_s}^{kT_s} f\left(\mathrm{x}^{\mathrm{d}}(t),\, \mathrm{x}^{\mathrm{a}}(t)\right) dt + w_{k-1} \tag{2a}$$

$$0 = g\left(\mathrm{x}^{\mathrm{d}}_k,\, \mathrm{x}^{\mathrm{a}}_k\right) \tag{2b}$$

$$\mathrm{y}_k = h\left(\mathrm{x}^{\mathrm{d}}_k,\, \mathrm{x}^{\mathrm{a}}_k\right) + \mathrm{v}_k \tag{2c}$$

$$w_{k-1} \sim \mathcal{N}(0, \mathrm{Q}_{k-1}),\ \mathrm{v}_k \sim \mathcal{N}(0, \mathrm{R}_k),\ \mathrm{x}^{\mathrm{d}}_0 \sim \mathcal{N}(\bar{\mathrm{x}}_0, \mathrm{P}^{\mathrm{d}}_0) \tag{2d}$$

Here at time $t_k = kT_s$, the discretized process noise w_{k-1}, measurement noise v_k and initial conditions $\mathrm{x}^{\mathrm{d}}_0$ for the differential states are assumed to be mutually independent Gaussian random variables. The corresponding initial conditions $\mathrm{x}^{\mathrm{a}}_0$ for the algebraic states are assumed to be consistent with the differential states initial conditions, i.e. (2b) is satisfied. The differential equation (2a) and measurement model (2c) are assumed to involve stochastic uncertainties, while the algebraic relationship (2b) is assumed to be exact.

The estimation problem is to estimate the states $\mathrm{x}^{\mathrm{d}}_k$ and $\mathrm{x}^{\mathrm{a}}_k$ at k^{th} time instant using process model (2a)-(2b) and measurements y_k (2c) available till the k^{th} time instant.

2.2 Relevant EKF approach (Mandela et al., 2010)

State augmentation has been used in Mandela et al. (2010) to apply EKF on a nonlinear DAE system (2a)-(2c). In their work, the error covariance matrix of an augmented state vector $\mathrm{x}^{\mathrm{aug}} = \left[(\mathrm{x}^{\mathrm{d}})^T\ (\mathrm{x}^{\mathrm{a}})^T\right]^T$ is propagated during the prediction step to get an augmented error covariance matrix containing the auto and cross-covariance terms of differential and algebraic states.

Let at time $t_{k-1} = (k-1)T_s$, $\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}$ be the differential and algebraic state estimates respectively. Let $\mathrm{P}^{\mathrm{aug}}_{k-1|k-1}$ be the error covariance matrix of the augmented state vector. The algorithm is summarized for one complete cycle from time instant t_{k-1} to t_k.

Prediction step: With the initial conditions $\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}$, the following set of coupled equations are numerically integrated from time instant t_{k-1} to t_k to obtain predicted state estimates $\hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1}$:

$$\frac{d\hat{\mathrm{x}}^{\mathrm{d}}}{dt} = f\left(\hat{\mathrm{x}}^{\mathrm{d}}(t), \hat{\mathrm{x}}^{\mathrm{a}}(t)\right);\ 0 = g\left(\hat{\mathrm{x}}^{\mathrm{d}}(t), \hat{\mathrm{x}}^{\mathrm{a}}(t)\right) \tag{3}$$

To propagate the augmented error covariance matrix, an implicit linearized stochastic differential equation (SDE) model is derived by first linearizing DAE process model (1a)-(1b) around updated state estimates ($\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}$) and then differentiating the linearized algebraic equation to give an augmented system

$$\begin{bmatrix}\dot{\mathrm{x}}^{\mathrm{d}}\\ \dot{\mathrm{x}}^{\mathrm{a}}\end{bmatrix} = \begin{bmatrix}\mathrm{F}^{\mathrm{d}} & \mathrm{F}^{\mathrm{a}}\\ -(\mathrm{G}^{\mathrm{a}})^{-1}\mathrm{G}^{\mathrm{d}}\mathrm{F}^{\mathrm{d}} & -(\mathrm{G}^{\mathrm{a}})^{-1}\mathrm{G}^{\mathrm{d}}\mathrm{F}^{\mathrm{a}}\end{bmatrix}\begin{bmatrix}\mathrm{x}^{\mathrm{d}}\\ \mathrm{x}^{\mathrm{a}}\end{bmatrix} = \mathrm{J}^{\mathrm{aug}}\ \mathrm{x}^{\mathrm{aug}} \tag{4}$$

with the linearization matrices defined as ,

$$\begin{bmatrix}\mathrm{F}^{\mathrm{d}} & \mathrm{F}^{\mathrm{a}}\\ \mathrm{G}^{\mathrm{d}} & \mathrm{G}^{\mathrm{a}}\end{bmatrix} = \begin{bmatrix}\dfrac{df}{d\mathrm{x}^{\mathrm{d}}} & \dfrac{df}{d\mathrm{x}^{\mathrm{a}}}\\[2ex] \dfrac{dg}{d\mathrm{x}^{\mathrm{d}}} & \dfrac{dg}{d\mathrm{x}^{\mathrm{a}}}\end{bmatrix}_{\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1},\ \hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}} \tag{5}$$

The state transition matrix $\Phi_k = \exp(\mathrm{J}^{\mathrm{aug}}\, T_s)$ is used to compute augmented predicted error covariance matrix by

$$\mathrm{P}^{\mathrm{aug}}_{k|k-1} = \Phi_k\, \mathrm{P}^{\mathrm{aug}}_{k-1|k-1}\, \Phi_k^T + \Gamma\, \mathrm{Q}_{k-1}\, \Gamma^T \tag{6}$$

$$\text{where,}\qquad \Gamma = \begin{bmatrix}\mathrm{I}\\ \mathrm{G}^{\mathrm{a}})^{-1}\mathrm{G}^{\mathrm{d}}\end{bmatrix} \tag{7}$$

It should be noted that the full covariance matrix of the entire augmented state vector is directly propagated through the SDE model even though the algebraic and differential states are related through the deterministic algebraic equations (2b).

Update step: Let $\mathrm{H}^{\mathrm{aug}}_k$ be the linearized measurement model evaluated around the augmented state estimate $(\hat{\mathrm{x}}^{\mathrm{aug}}_{k|k-1})^T = \left[(\hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1})^T\ (\hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1})^T\right]$. Then, the augmented Kalman gain matrix is computed as

$$\mathrm{L}_k = \mathrm{P}^{\mathrm{aug}}_{k|k-1}(\mathrm{H}^{\mathrm{aug}}_k)^T\left[\mathrm{H}^{\mathrm{aug}}_k\, \mathrm{P}^{\mathrm{aug}}_{k|k-1}\, (\mathrm{H}^{\mathrm{aug}}_k)^T + \mathrm{R}_k\right]^{-1} \tag{8}$$

The updated differential state estimate is given by,

$$\hat{\mathrm{x}}^{\mathrm{d}}_{k|k} = \hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1} + \mathrm{L}^{\mathrm{d}}_k\left[\mathrm{y}_k - h(\hat{\mathrm{x}}^{\mathrm{aug}}_{k|k-1})\right] \tag{9}$$

where $\mathrm{L}^{\mathrm{d}}_k$ is the Kalman gain corresponding to the differential states which is a matrix with first n_d rows of L_k.

The updated algebraic state estimate is determined from the differential state estimate $\hat{\mathrm{x}}^{\mathrm{d}}_{k|k}$ using $g\left(\hat{\mathrm{x}}^{\mathrm{d}}_{k|k}, \hat{\mathrm{x}}^{\mathrm{a}}_{k|k}\right) = 0$. The augmented error covariance matrix is updated as:

$$\mathrm{P}^{aug}_{k|k} = [\mathrm{I} - \mathrm{L}_k \mathrm{H}^{\mathrm{aug}}_k]\, \mathrm{P}^{\mathrm{aug}}_{k|k-1} \tag{10}$$

It can be noted that the covariance update (10) in the above approach is approximate. Although the updated algebraic estimates are determined from the algebraic equations and not through Kalman update (9), the covariance update (10) does not take this into consideration while estimating the error covariance matrix of updated estimates. In particular, the error covariance matrix of algebraic states and its cross-covariance terms in the augmented error covariance matrix do not represent the uncertainty associated with the updated algebraic state estimates. The approximate value of augmented error covariance matrix may adversely affect the state estimates at subsequent time instants. One possible remedy suggested in Mandela et al. (2010) is to compute error covariance of algebraic states and error cross-covariances using linearization of algebraic equations. However, this will produce a singular augmented error covariance matrix which will have to be propagated through the process model in the prediction step and this has not been pursued in their work.

3. PROPOSED EKF APPROACH

In this work, we present a modified EKF approach for state estimation of nonlinear DAE systems that ensures better approximation of error covariance matrix during both prediction and update steps. The proposed approach is based on the observation that since the algebraic equations are assumed to be exact, the algebraic and differential states are not independent. In particular, the algebraic states can be computed from the differential states so as to satisfy the algebraic equations. Thus, the uncertainties associated with the algebraic states can be computed from the uncertainties in the differential states. Therefore, in the present work, we propose the following ideas for covariance matrix computations:

(1) Prediction step: In this step we propose to directly propagate the error covariance matrix of only the differential states. Towards this end, the linearized algebraic equations are used to express the algebraic states in terms of differential states. Subsequent substitution of the resulting expressions in the differential equations, leads to a stochastic differential equation involving the differential states alone. This equation is then used to propagate the error covariance matrix of the differential states. The error covariance matrix of the algebraic state, and the cross-covariance matrices of errors in algebraic and differential states at the end of the prediction step are obtained using the linearized algebraic equations (evaluated around the predicted state estimates).
(2) Update step: Similar to the philosophy in the prediction step, only the error covariance matrix of the differential states is directly updated upon availability of the measurements. The error covariance matrix of the updated algebraic states is not needed in the subsequent prediction step and is thus directly not computed. However, if needed it can be computed using the linearized algebraic model (evaluated around the updated state estimates).

Details of these steps are discussed next.

3.1 Prediction Step

To propagate the error covariance of differential states, the process model (1a)-(1b) is linearized around the state estimates $\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}$ as

$$\dot{\mathrm{x}}^{\mathrm{d}} - \dot{\hat{\mathrm{x}}}^{\mathrm{d}}_{k-1|k-1} = \mathrm{F}^{\mathrm{d}}(\mathrm{x}^{\mathrm{d}} - \hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}) + \mathrm{F}^{\mathrm{a}}(\mathrm{x}^{\mathrm{a}} - \hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}) + w(t) \tag{11a}$$

$$0 = \mathrm{G}^{\mathrm{d}}(\mathrm{x}^{\mathrm{d}} - \hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}) + \mathrm{G}^{\mathrm{a}}(\mathrm{x}^{\mathrm{a}} - \hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}) \tag{11b}$$

where $\dot{\hat{\mathrm{x}}}^{\mathrm{d}}_{k-1|k-1} = f\left(\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}, \hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}\right)$ and the linearization matrices are evaluated similar to (5). An implicit SDE model involving differential states is derived by eliminating the perturbed algebraic state variable $\left(\mathrm{x}^{\mathrm{a}} - \hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}\right)$ in (11a) using its value obtained from (11b) as,

$$\dot{\mathrm{x}}^{\mathrm{d}} - \dot{\hat{\mathrm{x}}}^{\mathrm{d}}_{k-1|k-1} = \mathrm{J}^{\mathrm{d}}\left(\mathrm{x}^{\mathrm{d}} - \hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}\right) + w(t) \tag{12}$$

$$\text{where,} \qquad \mathrm{J}^{\mathrm{d}} = \left[\mathrm{F}^{\mathrm{d}} - \mathrm{F}^{\mathrm{a}}\left(\mathrm{G}^{\mathrm{a}}\right)^{-1}\mathrm{G}^{\mathrm{d}}\right] \tag{13}$$

Let $\mathrm{P}^{\mathrm{d}}_{k-1|k-1}$ be the error covariance of the differential states at time t_{k-1}. The predicted error covariance of differential states at time t_k can now be obtained from discretization of (12) as,

$$\mathrm{P}^{\mathrm{d}}_{k|k-1} = \Phi_k\, \mathrm{P}^{\mathrm{d}}_{k-1|k-1}\, \Phi^T_k + \mathrm{Q}_{k-1} \tag{14}$$

where $\Phi_k = \exp(\mathrm{J}^{\mathrm{d}}\, T_s)$ is the state transition matrix. It should be noted that the implicit SDE model (12), and differential state error covariance matrix (14) are similar to the work of Becerra et al. (2001). But in their work, the predicted algebraic state estimate or the uncertainties associated with it are not employed in the correction step and thus the effect of predicted algebraic estimates is completely ignored. In the proposed work, we account for this effect by computing an augmented error covariance matrix incorporating auto and cross error covariance terms of differential and algebraic states. The error covariance of algebraic states and the error covariances between differential and algebraic states are determined using linearized algebraic model (11b) as:

$$\mathrm{P}^{\mathrm{a}}_{k|k-1} = \left[(\mathrm{G}^{\mathrm{a}}_{k|k-1})^{-1}\mathrm{G}^{\mathrm{d}}_{k|k-1}\right]\mathrm{P}^{\mathrm{d}}_{k|k-1}\left[(\mathrm{G}^{\mathrm{a}}_{k|k-1})^{-1}\mathrm{G}^{\mathrm{d}}_{k|k-1}\right]^T \tag{15a}$$

$$\mathrm{P}^{\mathrm{da}}_{k|k-1} = -\mathrm{P}^{\mathrm{d}}_{k|k-1}\left[(\mathrm{G}^{\mathrm{a}}_{k|k-1})^{-1}\mathrm{G}^{\mathrm{d}}_{k|k-1}\right]^T, \mathrm{P}^{\mathrm{ad}}_{k|k-1} = \left[\mathrm{P}^{\mathrm{da}}_{k|k-1}\right]^T \tag{15b}$$

where $\mathrm{G}^{\mathrm{d}}_{k|k-1}$, $\mathrm{G}^{\mathrm{a}}_{k|k-1}$ are the linearization matrices of the algebraic equations as mentioned in (5) evaluated around $\hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1}$, $\hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1}$. Further, let $\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}$ be the estimated states at time t_{k-1}. The predicted estimates of the states at time t_k, i.e. $\hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1}$ are obtained by numerically integrating the following coupled equations from time instant t_{k-1} to t_k:

$$\frac{d\hat{\mathrm{x}}^{\mathrm{d}}}{dt} = f\left(\hat{\mathrm{x}}^{\mathrm{d}}(t), \hat{\mathrm{x}}^{\mathrm{a}}(t)\right);\ 0 = g\left(\hat{\mathrm{x}}^{\mathrm{d}}(t), \hat{\mathrm{x}}^{\mathrm{a}}(t)\right) \tag{16}$$

with the initial conditions $\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}$. Thus, at the end of the prediction step, the predicted state estimates and the predicted error covariance matrix are available as

$$\hat{\mathrm{x}}^{\mathrm{aug}}_{k|k-1} = \begin{bmatrix} \hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1} \\ \hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1} \end{bmatrix}, \quad \mathrm{P}^{\mathrm{aug}}_{k|k-1} = \begin{bmatrix} \mathrm{P}^{\mathrm{d}}_{k|k-1} & \mathrm{P}^{\mathrm{da}}_{k|k-1} \\ \mathrm{P}^{\mathrm{ad}}_{k|k-1} & \mathrm{P}^{\mathrm{a}}_{k|k-1} \end{bmatrix} \tag{17}$$

3.2 Update step:

The predicted state estimates $\hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1}$ are propagated through the measurement model (2c) to provide the predicted measurement $\hat{\mathrm{y}}_{k|k-1}$:

$$\hat{\mathrm{y}}_{k|k-1} = h\left(\hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1}, \hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1}\right) \tag{18}$$

The linearized measurement model is

$$\mathrm{y}_k - \hat{\mathrm{y}}_{k|k-1} = \mathrm{H}^{\mathrm{d}}_k\,(\mathrm{x}^{\mathrm{d}}_k - \hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1}) + \mathrm{H}^{\mathrm{a}}_k\,(\mathrm{x}^{\mathrm{a}}_k - \hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1}) + \mathrm{v}_k \tag{19}$$

where $\mathrm{H}^{\mathrm{d}}_k = \dfrac{dh}{d\mathrm{x}^{\mathrm{d}}}$, $\mathrm{H}^{\mathrm{a}}_k = \dfrac{dh}{d\mathrm{x}^{\mathrm{a}}}$ are the linearization matrices evaluated around the predicted state estimate $\hat{\mathrm{x}}^{\mathrm{aug}}_{k|k-1}$. Defining $\mathrm{H}^{\mathrm{aug}}_k = \begin{bmatrix} \mathrm{H}^{\mathrm{d}}_k & \mathrm{H}^{\mathrm{a}}_k \end{bmatrix}$ and $\mathbf{E}$ as the expectation operator, the augmented Kalman gain is computed from (17) and (19) as follows,

$$\mathrm{L}_k = \mathrm{P}_{\varepsilon e}\;[\mathrm{P}_{ee}]^{-1} \tag{20}$$

$$\text{where,}\quad \mathrm{P}_{\varepsilon e} = \mathbf{E}\left[\left(\begin{bmatrix} \mathrm{x}^{\mathrm{d}}_k - \hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1} \\ \mathrm{x}^{\mathrm{a}}_k - \hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1} \end{bmatrix}\right)\left(\mathrm{y}_k - \hat{\mathrm{y}}_{k|k-1}\right)^T\right]$$

$$= \mathrm{P}^{\mathrm{aug}}_{k|k-1}(\mathrm{H}^{\mathrm{aug}}_k)^T \tag{21}$$

$$\mathrm{P}_{ee} = \mathbf{E}\left[\left(\mathrm{y}_k - \hat{\mathrm{y}}_{k|k-1}\right)\left(\mathrm{y}_k - \hat{\mathrm{y}}_{k|k-1}\right)^T\right]$$

$$= \mathrm{H}^{\mathrm{aug}}_k\,\mathrm{P}^{\mathrm{aug}}_{k|k-1}\,(\mathrm{H}^{\mathrm{aug}}_k)^T + \mathrm{R}_k \tag{22}$$

The updated differential state estimate is given by,

$$\hat{\mathrm{x}}^{\mathrm{d}}_{\mathrm{k|k}} = \hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1} + \mathrm{L}^{\mathrm{d}}_k\left[\mathrm{y}_k - \hat{\mathrm{y}}_{k|k-1}\right] \tag{23}$$

where $\mathrm{L}^{\mathrm{d}}_k$ defines the Kalman gain corresponding to differential states which is a matrix with first n_d rows of L_k. The updated algebraic state estimate is determined from the updated differential state estimate using

$$g\left(\hat{\mathrm{x}}^{\mathrm{d}}_{k|k}, \hat{\mathrm{x}}^{\mathrm{a}}_{k|k}\right) = 0 \tag{24}$$

Since the algebraic state estimate is dependent on the estimate of the differential states, the covariance update is performed only for the differential states. To derive this covariance update expression, consider the estimation error in differential states which is simplified using (23) as:

$$\varepsilon^{\mathrm{d}}_{k|k} = \mathrm{x}^{\mathrm{d}}_k - \hat{\mathrm{x}}^{\mathrm{d}}_{k|k} = \mathrm{x}^{\mathrm{d}}_k - \hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1} - \mathrm{L}^{\mathrm{d}}_k\left[\mathrm{y}_k - \hat{\mathrm{y}}_{k|k-1}\right] \tag{25}$$

Defining prediction errors as $\varepsilon^{\mathrm{d}}_{k|k-1} = \mathrm{x}^{\mathrm{d}}_k - \hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1}$ and $\varepsilon_{k|k-1} = \mathrm{x}^{\mathrm{aug}}_k - \hat{\mathrm{x}}^{\mathrm{aug}}_{k|k-1}$, the estimation error (25) is expressed using the linearized measurement model (19) as,

$$\begin{aligned} \varepsilon^{\mathrm{d}}_{k|k} &= \varepsilon^{\mathrm{d}}_{k|k-1} - \mathrm{L}^{\mathrm{d}}_k\left[\mathrm{H}^{\mathrm{aug}}_k\,\mathrm{x}^{\mathrm{aug}}_k + \mathrm{v}_k - \mathrm{H}^{\mathrm{aug}}_k\,\hat{\mathrm{x}}^{\mathrm{aug}}_{k|k-1}\right] \\ &= \left[\mathrm{I}_{nd\times nd}\;\; 0_{nd\times na}\right]\varepsilon_{k|k-1} - \mathrm{L}^{\mathrm{d}}_k\,\mathrm{H}^{\mathrm{aug}}_k\,\varepsilon_{k|k-1} - \mathrm{L}^{\mathrm{d}}_k\,\mathrm{v}_k \\ &= [\tilde{\mathrm{I}} - \mathrm{L}^{\mathrm{d}}_k\,\mathrm{H}^{\mathrm{aug}}_k]\varepsilon_{k|k-1} - \mathrm{L}^{\mathrm{d}}_k\,\mathrm{v}_k \end{aligned} \tag{26}$$

$$\text{where } \tilde{\mathrm{I}} = \left[\mathrm{I}_{nd\times nd}\;\; 0_{nd\times na}\right]$$

Using estimation error expression (26), the updated error covariance matrix of the differential states is obtained as,

$$\mathrm{P}^{\mathrm{d}}_{k|k} = \mathbf{E}\left[\varepsilon^{\mathrm{d}}_{k|k}(\varepsilon^{\mathrm{d}}_{k|k})^T\right]$$

$$= \left[\tilde{\mathrm{I}} - \mathrm{L}^{\mathrm{d}}_k\mathrm{H}^{\mathrm{aug}}_k\right]\mathrm{P}^{\mathrm{aug}}_{k|k-1}\left[\tilde{\mathrm{I}} - \mathrm{L}^{\mathrm{d}}_k\mathrm{H}^{\mathrm{aug}}_k\right]^T + \mathrm{L}^{\mathrm{d}}_k\,\mathrm{R}_k\,[\mathrm{L}^{\mathrm{d}}_k]^T \tag{27}$$

The error covariance matrix of the algebraic states is not needed for prediction step at next time instant, but if required, can be computed similar to (15a) but with linearization performed around the updated state estimates $\hat{\mathrm{x}}^{\mathrm{d}}_{k|k}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k|k}$.

3.3 Summary of proposed EKF for online implementation

A brief summary of online implementation (one cycle) of the proposed EKF approach is presented next.
Given: Consistent estimates $\hat{\mathrm{x}}^{\mathrm{d}}_{k-1|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k-1|k-1}$ and error covariance of differential states $\mathrm{P}^{\mathrm{d}}_{k-1|k-1}$.
Step 1: Integrate the coupled equations (16) numerically to get the predicted state estimates $\hat{\mathrm{x}}^{\mathrm{d}}_{k|k-1}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k|k-1}$.
Step 2: Propagate the error covariance of differential states using (14). Using (15a)-(15b), obtain the prediction error covariance in augmented form $\mathrm{P}^{\mathrm{aug}}_{k|k-1}$ (17).
Step 3: Compute the augmented Kalman gain (20). Use it in (23)-(24) to obtain the updated state estimates $\hat{\mathrm{x}}^{\mathrm{d}}_{k|k}$ and $\hat{\mathrm{x}}^{\mathrm{a}}_{k|k}$.
Step 4: Update the error covariance of differential states $\mathrm{P}^{\mathrm{d}}_{k|k}$ from (27).
One cycle is now completed. Go to Step 1 for the next cycle with $k = k + 1$.

4. RESULTS AND DISCUSSION

The proposed modified EKF approach is applied for state estimation of two DAE case studies: 1) Galvanostatic charge process and 2) Drum boiler. To obtain reliable results, the estimation is performed for multiple Monte-Carlo simulation runs and the performance is compared with the existing EKF approach (Mandela et al., 2010) based on the following metrics:
(1) Average Root Mean Squared Error (ARMSE):

$$\mathrm{ARMSE}_i = \frac{1}{M}\sum_{j=1}^{M}\sqrt{\frac{1}{N}\sum_{k=1}^{N}\left(\mathrm{x}^{\mathrm{aug}(j)}_{k,i} - \hat{\mathrm{x}}^{\mathrm{aug}(j)}_{k|k.i}\right)^2} \tag{28}$$

where, $\mathrm{x}^{\mathrm{aug}(j)}_{k,i}$ and $\hat{\mathrm{x}}^{\mathrm{aug}(j)}_{k|k,i}$ denote the augmented true and estimated i^{th} state at k^{th} time instant for the j^{th} simulation run. N is number of sampling instants while M is number of Monte-Carlo simulation runs.
(2) Non-credibility Index (NCI) (Kottakki et al., 2016): Varies with time instant and provides a relative evaluation of the estimation error using updated error covariance matrix. NCI ≈ 0 denotes balanced performance implying that the filter uncertainty associated with state estimate is commensurate with the actual uncertainty.

All the computations are performed in MATLAB® version 9.7 running on Ubuntu 18.04 operating system on a computer with Intel Octa Core i7 processor and 8 GB RAM. The state prediction equations (16) are numerically integrated using 4^{th} order Runge-Kutta method.

4.1 Galvanostatic charge process

A two state DAE model of a Galvanostatic charge process is available in Mandela et al. (2010). x_1 and x_2 are the differential and algebraic states, respectively with x_2

Table 1. Results: Galvanostatic charge process

Method	ARMSE: diff. state x_1	ARMSE: alg. state x_2	Avg. CPU time (sec)
EKF-existing	0.0264	0.0032	0.0028
EKF-proposed	0.0206	0.0027	0.0029

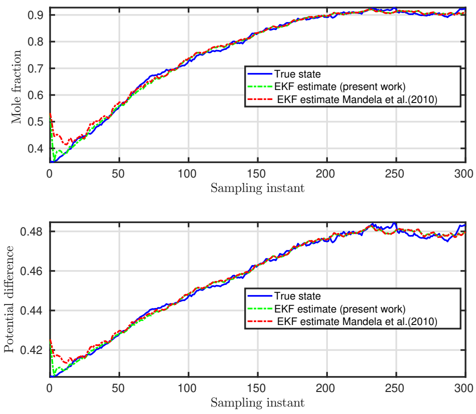

Fig. 1. State estimates: Galvanostatic charge process

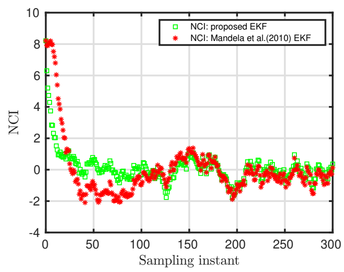

Fig. 2. NCI: Galvanostatic charge process

measured. Initial estimate for both EKF estimators is $\hat{\mathrm{x}}^{\mathrm{aug}}_{0|0} = [0.5322\ 0.4254]^T$. In the Monte Carlo simulations performed in this work, the initial true state $\mathrm{x}^{\mathrm{aug}}_0$ for each simulation run was different and was obtained by adding Gaussian noise with zero mean and process noise covariance Q to the steady state $[0.35024\ 0.4071]^T$. The relevant filter parameters are $T_s = 15$ sec, $\mathrm{Q} = 1e^{-5}$, $\mathrm{R} = 1e^{-4}$, $\mathrm{P}^{\mathrm{aug}}_0 = 0.005\,\mathrm{I}_{2\times2}$. Note that the proposed EKF uses the initial guess only for the differential state error covariance. The ARMSE values ($M = 100$) and average computational times are reported in Table 1. It can be noted that the proposed EKF outperforms the existing EKF (Mandela et al., 2010) and results in 22% and 15.6% reduction in ARMSE values respectively for the two states relative to the existing EKF with similar computational effort. The improvement is also evident from the estimation results for a typical simulation run (Fig. 1) with the proposed EKF tracking the true states very quickly when compared with the existing EKF. The NCI values (Fig. 2) with proposed EKF (stays close to zero throughout) show balanced performance when compared to existing EKF (transits to negative between 40-90 instants).

4.2 Drum boiler

A DAE model of the drum boiler system (Astrom and Bell, 2000) is summarized in (29a)-(29c) with 4 differential and

Table 2. Operational data: Drum boiler

Parameter	Value
Drum volume V_{d}	40 m^3
Riser volume V_{r}	37 m^3
Downcomer volume V_{dc}	11 m^3
Drum area A_{d}	20 m^2
Total mass of metal tubes and drum m_{t}	300,000 kg
Total riser mass m_{r}	160,000 kg
Friction coefficient k	25
Residence time of steam in drum $\mathrm{T_d}$	12 sec
Parameter β in empirical equation	0.3
steam volume under the drum level at no condensation V°_{sd}	7.793 m^3
Total rate of steam condensation q_{ct}	11 kg/sec
Metal specific heat C_p	0.5 kJ/kg K
Downcomer area A_{dc}	0.38 m^2
mass of drum m_{d}	10,000 kg

2 algebraic states. The differential states are drum pressure (P), total water volume (V_{wt}), steam-mass fraction (α_{r}) and steam volume in the drum (V_{sd}). The algebraic state variables are downcomer flow rate (q_{dc}) and water volume in steam drum (V_{wd}).

$$\begin{bmatrix} e_{11} & e_{12} & 0 & 0 \\ e_{21} & e_{22} & 0 & 0 \\ e_{31} & 0 & e_{33} & 0 \\ e_{41} & 0 & e_{43} & e_{44} \end{bmatrix} \begin{bmatrix} \frac{dP}{dt} \\ \frac{dV_{\mathrm{wt}}}{dt} \\ \frac{d\alpha_{\mathrm{r}}}{dt} \\ \frac{dV_{\mathrm{sd}}}{dt} \end{bmatrix} = \begin{bmatrix} q_{\mathrm{f}} - q_{\mathrm{s}} \\ Q_{\mathrm{u}} + q_{\mathrm{f}} h_{\mathrm{f}} - q_{\mathrm{s}} h_{\mathrm{s}} \\ Q_{\mathrm{u}} - \alpha_{\mathrm{r}} h_c\, q_{\mathrm{dc}} \\ \frac{\rho_{\mathrm{s}}}{\mathrm{T_d}}(V^{\circ}_{\mathrm{sd}} - V_{\mathrm{sd}}) + \frac{h_{\mathrm{f}} - h_{\mathrm{w}}}{h_c} q_{\mathrm{f}} \end{bmatrix} \tag{29a}$$

$$\frac{1}{2}\, k\, q^2_{\mathrm{dc}} - \rho_{\mathrm{w}}\, A_{\mathrm{dc}}\, (\rho_{\mathrm{w}} - \rho_{\mathrm{s}})\, g\, \bar{\alpha}_{\mathrm{v}}\, V_{\mathrm{r}} = 0 \tag{29b}$$

$$V_{\mathrm{wt}} - V_{\mathrm{dc}} - V_{\mathrm{wd}} - (1 - \bar{\alpha}_{\mathrm{v}}) V_{\mathrm{r}} = 0 \tag{29c}$$

where, $h_c = h_{\mathrm{s}} - h_{\mathrm{w}}$. The terms e_{ij} in coefficient matrix in (29a) are functions of the state variables (Astrom and Bell, 2000). Notation is q: mass flow rate, h: enthalpy, ρ: density, A: Area, V: volume, m: mass, $\mathtt{t}$: temperature, $\bar{\alpha}_v$: steam volume fraction, Q_{u}: heat input to the risers and g: gravitational acceleration with consistent SI units. The subscripts s, w, f, d, r, dc used are for steam, water, feedwater, drum, riser and downcomer respectively. The measurements available from the drum boiler system are the drum pressure (P) and the drum level $l = \dfrac{V_{\mathrm{sd}} + V_{\mathrm{wd}}}{A_{\mathrm{d}}}$. Drum boiler is simulated using the operational data listed in Table 2 (Astrom and Bell, 2000; Emara-Shabaik et al., 2009). For evaluating variables h_{s}, h_{w}, ρ_{s}, ρ_{w}, $\mathtt{t}_{\mathrm{s}}$ and their partial derivatives at pressure P, quadratic approximations of the steam table obtained using simple linear regression technique over the range $P = 6 - 15$ MPa, are employed (Parikh, 2008):

$$h_{\mathrm{s}} = -0.9337P^2 + 0.9375P + 2812.1 \tag{30a}$$

$$h_{\mathrm{w}} = -0.8903P^2 + 62.21P + 875.21 \tag{30b}$$

$$\rho_{\mathrm{s}} = 0.2309P^2 + 2.3688P + 8.6275 \tag{30c}$$

$$\rho_{\mathrm{w}} = 0.0524P^2 - 18.145P + 864.52 \tag{30d}$$

$$\mathtt{t}_{\mathrm{s}} = -0.2908P^2 + 13.378P + 206.32 \tag{30e}$$

In our work, the response of drum boiler system to step change (10% increase) in steam mass flow rate (q_{f}) is simulated with a sampling interval (T_s) of 1 sec. The nominal values of input are: $u_0 = [q_{\mathrm{f}}\ Q\ q_{\mathrm{s}}]_0 = [49.9$ kg/s 8604.8 kJ/sec 49.9 kg/s$]$. The true initial states for the Monte-Carlo simulations were generated in a manner similar to the case study in Section 4.1. The initial

Table 3. Drum boiler: Results (ARMSE (e))

Algorithm	$e_1 \times 10^2$	$e_2 \times 10^2$	$e_3 \times 10^4$	$e_4 \times 10^2$	e_5	$e_6 \times 10^2$
EKF-existing	0.76136	4.8057	2.3540	4.4334	1.8775	6.8223
EKF-proposed	0.76135	2.9632	0.9473	1.9455	0.7710	3.2134

guess to EKF estimators $\hat{\mathrm{x}}_{0|0}^{\mathrm{aug}}$ and steady state values are: $\hat{\mathrm{x}}_{0|0}^{\mathrm{aug}} = [8.6\ 57.1\ 0.0520\ 4.9884\ 1192.6\ 19.1596]^T$, $\mathrm{x}_s^{\mathrm{aug}} = [8.5\ 57.0\ 0.0510\ 4.8884\ 1194.5\ 19.0316]^T$. The relevant filter parameters used in EKF estimators are:

$$\mathrm{P}_0^{\mathrm{aug}} = \mathrm{diag}(0.01, 0.01, 1.0358 \times 10^{-6}, 0.01, 3.567, 0.01638),$$
$$\mathrm{Q} = 10^{-5} \times \mathrm{diag}(4, 4, 10^{-4}, 4),\ \ \mathrm{R} = 10^{-5} \times \mathrm{diag}(4, 4)$$

Table 3 lists the results and shows superior performance of the proposed EKF. In particular, the reduction in ARMSE values obtained with the proposed EKF relative to the existing EKF are 38%, 59.7%, 56%, 58% and 53% respectively for states $2-6$. Avg. computational times are similar (existing- 0.0275 sec, proposed- 0.0281 sec). The tracking performance for a typical simulation run (Fig. 3) also shows that the existing EKF approach takes more time to track actual states than the proposed EKF approach. The NCI values (Fig. 4) with the proposed EKF approach quickly converge near zero and remain there indicating balanced performance. In case of existing EKF approach, the NCI values transit from large positive peak to negative at the beginning and remain there implying pessimistic performance.

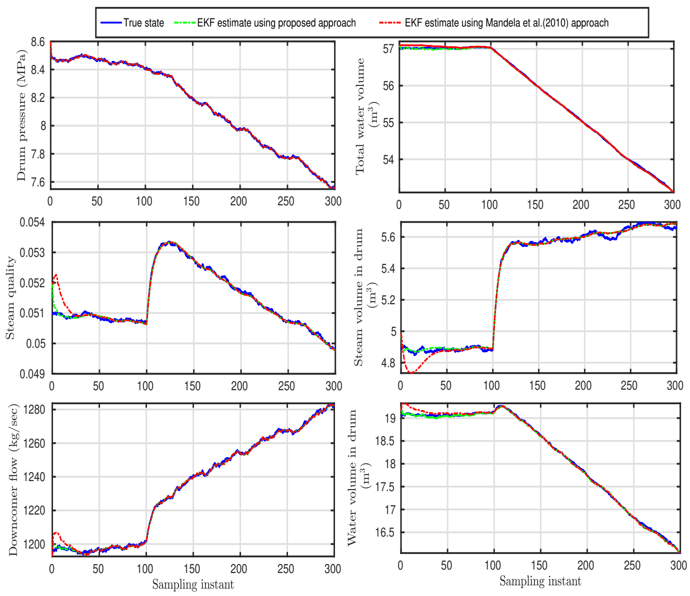

Fig. 3. State estimates: Drum boiler

5. CONCLUSION

In this work, we have presented a modified EKF approach for state estimation of nonlinear DAE systems where the differential equation is stochastic while the algebraic equation is deterministic. The proposed approach exploits the deterministic nature of the algebraic equation by directly computing the error covariance matrix of only the differential states during the estimation cycle since the algebraic and differential states are related through the deterministic algebraic equations. The error covariance matrix of the algebraic states and its cross error covariances with the differential states are obtained from the error covariance matrix of the differential states using the linearized algebraic equations. This in turn enables incorporation of measurements of both differential and algebraic states in the update step of the presented approach. Application of the proposed approach for state estimation of two benchmark case studies reveals its superior performance over existing EKF approach in literature.

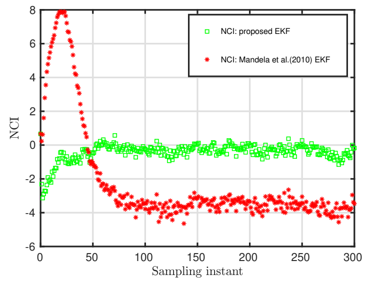

Fig. 4. NCI: Drum boiler

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