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Development of iterative extended Kalman filter for DAE System

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Abstract: Extended Kalman filtering (EKF) is widely used for estimating states of systems modelled as ordinary differential equations (ODEs). The performance of this approach may deteriorate if the initial estimate is poor i.e. far from true state. Iterative version of EKF developed by Wishner et al. (1969) for systems modelled as ODEs can alleviate this difficulty with negligible additional computational efforts as it involves smoothing of the prior estimate. There are many systems that involve different time scales and are described by Differential-Algebraic equations (DAEs). Extension of Bayesian state estimation approach such as EKF for handling nonlinear DAEs is relatively recent development (Beccera et al. (2001) and Mandela et al. (2010)). In this work, taking motivation from Wishner et al. (1969) , an iterative EKF (IEKF) scheme is proposed for systems modelled as DAEs . The efficacy of the proposed DAE-IEKF is evaluated using simulation studies of Nickel-Hydrogen electrode system and divided wall distillation column system. Analysis of the simulation results reveals that the proposed approach results in a reasonable improvement in the estimation performance when compared with performance of the conventional DAE-EKF.

Keywords: Extended Kalman Filter (EKF), Differential - Algebraic Equation Systems (DAEs), Nonlinear State Estimation.

INTRODUCTION

Differential-algebraic equations (DAEs) describe system that involve different time scales, which are very common in chemical engineering systems. Extended Kalman filter (EKF) for DAEs was proposed by Becerra et al. (2001) and it was later modified by Mandela et al (2010) in order to accommodate measurements of both differential and algebraic variables. The performance of DAE-EKF deteriorates (Purohit et al. (2015)) when initial estimate is poor and measurements of estimated states are unavailable. In order to improve the performance of EKF estimator, either initial estimate should be closed to true state or measurement of estimated state should be available. However, measurement of some variables such as concentration, involves large time delay whereas temperature measurement is very fast. Thus, the improvement in state estimates may require the development of multirate state estimation scheme (Purohit et al. (2013)). The measurement of quality variables such as concentration is expensive. The performance of other approaches such as UKF (Mandela et al (2010), Purohit et al. (2015)) and En-KF (Yash et al. (2012)) is superior over EKF for DAE systems but they are computationally more expensive.

Iterative EKF approaches (Jazwinski (1970), Wishner et al. (1969)) have reported improved performance over conventional EKF for systems described by differential equations (ODEs). While this approach is computationally inexpensive, an added advantage of this approach over other Bayesian estimators like UKF or EnKF is that it simultaneously smooths the prior estimates while estimating the current state. This feature can help improving the estimation performance particularly for nonlinear systems. Thus, in this work, an iterative EKF (IEKF) for DAE system is proposed and simulation results are presented for two case studies: NHE electrode involving two states, a differential and an algebraic state, and a large dimensional divided wall distillation column (i.e. Petlyuk column)

This paper is organized in four sections. The model used for simulation and state estimation is presented in Section 1. Details of the DAE-EKF algorithm and Iterative DAE-EKF are presented in Section 2. Brief description of example case studies and simulations results are presented in Section 3. Finally, conclusions reached through the study are summarized in Section 4.

1. MODEL FOR PLANT SIMULATION AND STATE ESTIMATION

The DAE system under consideration can be represented in abstract form as

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}\left[\mathbf{x}(t), \mathbf{z}(\mathbf{t}), \mathbf{m}(t), \mathbf{d}\left(t\right)\right]$$
$$\overline{0} = \mathbf{G}\left[\mathbf{x}(t), \mathbf{z}(t)\right]$$
$$\mathbf{y}(t) = \mathbf{h}\left(\mathbf{x}, \mathbf{z}\right)$$

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where, $\mathbf{x} \in R^{nd}$ represents the differential state variables, $\mathbf{z} \in R^{na}$ represents the algebraic state variables, $\mathbf{m} \in R^m$ represents the input variables, $\mathbf{d} \in R^d$ represent the unmeasured disturbance variables. The output variables are denoted as $\mathbf{y}$. $\mathbf{f}$, $\mathbf{G}$ and $\mathbf{h}$ are nonlinear functions. The state estimation and predictions using this model are carried out under the following simplifying assumptions (Purohit J. L. (2014)):

1) The measurements, $\mathbf{y}_k$, are obtained at a regular interval, Δt, and the measurement equation at k^{th} sampling instant is given as follows

$$\mathbf{y}_k = \mathbf{h}\left(\mathbf{x}_k, \mathbf{z}_k\right) + \mathbf{v}_k \tag{1}$$

The measurement noise, $\mathbf{v}_k$, is considered as a zero mean white noise process with Gaussian distribution, i.e. $\mathbf{v}_k \sim \mathcal{N}(\overline{\mathbf{0}}, \mathbf{R})$, where $\mathbf{R}$ represents the covariance matrix.

2) The inputs are piecewise constant over the interval i.e.

$$\mathbf{m}(t) = \mathbf{m}_k \quad \text{for} \quad t_k \le t < t_{k+1} = t_k + \Delta t$$

Further, the true value of the inputs ($\mathbf{m}$) is related to the known. Thus value of the inputs ($\mathbf{u}$) as follows

$$\mathbf{m}_k = \mathbf{u}_k + \mathbf{w}_{u,k} \tag{2}$$

where $\mathbf{w}_{u,k} \in \mathbb{R}^m$ denotes an unknown disturbance in the inputs such that $\mathbf{w}_{u,k} \sim \mathcal{N}(\overline{\mathbf{0}}, \mathbf{Q}_u)$.

3) The sampling interval is small enough so that the variation of the unmeasured disturbances can be adequately approximated using the piecewise constant functions of the form

$$\mathbf{d}_k = \overline{\mathbf{d}} + \mathbf{w}_{d,k} \quad \text{for} \quad t_k \le t < t_{k+1} = t_k + h$$

$\mathbf{w}_{d,k} \in \mathbb{R}^{d_u}$ denotes a disturbance in the unmeasured disturbance such that $\mathbf{w}_{d,k} \sim \mathcal{N}(\overline{\mathbf{0}}, \mathbf{Q}_d)$ and $\overline{\mathbf{d}}$ represents the mean or the steady state value of the unmeasured disturbance at some desired operating point.

Thus, the plant is simulated by solving the following set of DAEs

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \int_{kh}^{(k+1)h} \mathbf{f}\left[\mathbf{x}(\tau), \mathbf{z}(\tau), \mathbf{m}_k, \mathbf{d}_k\right] d\tau \tag{3}$$

$$\overline{0} = \mathbf{G}\left[\mathbf{x}(\tau), \mathbf{z}(\tau)\right] \tag{4}$$

using a suitable DAE solver. For the sake of convenience, the following notation is adopted to represent the DAE represented by (3-4) in discrete form

$$\mathbf{x}_k = \mathbf{F}\left[\mathbf{x}_{k-1}, \mathbf{z}_{k-1}, \mathbf{u}_{k-1}, \mathbf{w}_{k-1}\right] \tag{5}$$

$$\overline{0} = \mathbf{G}\left[\mathbf{x}_k, \mathbf{z}_k\right] \tag{6}$$

where $\mathbf{w}_k \in R^{n_w}$ represents augmented state noise vector, i.e.

$$\mathbf{w}_k = \left[\, \mathbf{w}_{u,k}^T \;\; \mathbf{w}_{d,k}^T \,\right]^T$$

with covariance matrices $\mathbf{Q} = \mathbf{diag}\left[\, \mathbf{Q}_u \;\; \mathbf{Q}_d \,\right]$.

2. STATE ESTIMATION APPROACHES

2.1 DAE-EKF (Mandela et al (2010))

For the purpose of state estimation in DAE system, differential and algebraic states are augmented. An augmented state vector is defined as,

$$\mathcal{X}_k, = \left[\, \mathbf{x}_k^T \;\; \mathbf{z}_k^T \,\right]^T \tag{7}$$

and Jacobian matrices $(\mathcal{A}_{k-1}, \mathcal{B}_{w,k-1})$ are defined as

$$\mathcal{A}_{k-1} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \tag{8}$$

$$\mathcal{B}_{w,k-1} = \begin{bmatrix} \left[\dfrac{\partial \mathbf{f}}{\partial \mathbf{w}}\right] \\ -\left[\dfrac{\partial \mathbf{G}}{\partial \mathbf{z}}\right]^{-1}\left[\dfrac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]\left[\dfrac{\partial \mathbf{f}}{\partial \mathbf{w}}\right] \end{bmatrix}$$

where

$$A_{11} = \left[\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]$$

$$A_{12} = \left[\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right]$$

$$A_{21} = -\left[\frac{\partial \mathbf{G}}{\partial \mathbf{z}}\right]^{-1}\left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]\left[\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]$$

$$A_{22} = -\left[\frac{\partial \mathbf{G}}{\partial \mathbf{z}}\right]^{-1}\left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]\left[\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right]$$

The Jacobian matrices are evaluated at

$$(\widehat{\mathbf{x}}_{k-1|k-1}, \widehat{\mathbf{z}}_{k-1|k-1}, \mathbf{u}_{k-1}, \overline{\mathbf{0}})$$

The state transition matrix is obtained as

$$\mathbf{\Phi}_k = \exp\left[\mathcal{A}_k \Delta t\right]$$

Given estimates $(\widehat{\mathbf{x}}_{k-1|k-1}, \widehat{\mathbf{z}}_{k-1|k-1})$, the prediction step is carried out using a suitable DAE solver

$$\widehat{\mathbf{x}}_{k|k-1} = \mathbf{F}[\widehat{\mathbf{x}}_{k-1|k-1}, \widehat{\mathbf{z}}_{k-1|k-1}, \mathbf{u}_{k-1}, \overline{\mathbf{0}}] \tag{9}$$

$$\overline{0} = \mathbf{G}\left[\widehat{\mathbf{x}}_{k|k-1}, \widehat{\mathbf{z}}_{k|k-1}\right] \tag{10}$$

The update of the predicted covariance matrix, $\mathbf{P}_{k|k-1}^{aug}$,of the augmented state estimates, $\widehat{\mathcal{X}}_{k|k-1}$,is carried out as follows

$$\mathbf{P}_{k|k-1}^{aug} = \mathbf{\Phi}_{k-1}\mathbf{P}_{k-1|k-1}^{aug}\mathbf{\Phi}_{k-1}^T + \mathbf{\Gamma}_{w,k-1}\mathbf{Q}_w\mathbf{\Gamma}_{w,k-1}^T$$

$$\mathbf{\Gamma}_{w,k} = \int_0^{\Delta t} \exp\left[\mathcal{A}_k \tau\right] \mathcal{B}_{w,k} d\tau$$

The augmented Kalman gain is computed as

$$\mathbf{L}_k^{aug} = \mathbf{P}_{k|k-1}^{aug}\mathbf{H}_k^{aug^T}\left[\mathbf{V}_k\right]^{-1}$$

$$\mathbf{V}_k = \mathbf{H}_k^{aug}\mathbf{P}_{k|k-1}^{aug}\mathbf{H}_k^{aug^T} + \mathbf{R}$$

where augmented output measurement matrix is defined as $\mathbf{H}_k^{aug} = \left[\, \dfrac{\partial \mathbf{h}}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\widehat{\mathbf{x}}_{k|k}} \;\; \dfrac{\partial \mathbf{h}}{\partial \mathbf{Z}}\Big|_{\mathbf{z}=\widehat{\mathbf{z}}_{k|k}} \,\right]$ and $\mathbf{L}_k^{aug} = \left[\, \mathbf{L}_{x,k} \;\; \mathbf{L}_{z,k} \,\right]^T$, The state estimate is updated as

$$\begin{bmatrix} \widehat{\mathbf{x}}_{k|k} \\ \widehat{\mathbf{z}}_{k|k} \end{bmatrix} = \begin{bmatrix} \widehat{\mathbf{x}}_{k|k-1} \\ \widehat{\mathbf{z}}_{k|k-1} \end{bmatrix} + \mathbf{L}_k^{aug}\mathbf{e}_k \tag{11}$$

$$\mathbf{e}_k = \mathbf{y}_{m,k} - \mathbf{H}_k^{aug}\widehat{\mathcal{X}}_{k|k-1} \tag{12}$$

The updated differential, $\widehat{\mathbf{x}}_{k|k}$ and algebraic states $\widetilde{\mathbf{z}}_{k|k}$ together may not satisfy the algebraic equations, the algebraic states, $\widehat{\mathbf{z}}_{k|k}$, are recomputed using the differential states $\widehat{\mathbf{x}}_{k|k}$ by solving for

$$\overline{0} = \mathbf{G}\left[\widehat{\mathbf{x}}_{k|k}, \widehat{\mathbf{z}}_{k|k}\right] \tag{13}$$

The augmented state error covariance matrix is updated as

$$\mathbf{P}^{aug}_{k|k} = \left[\mathbf{I} - \mathbf{L}^{aug}_{k}\mathbf{H}^{aug}_{k}\right]\mathbf{P}^{aug}_{k|k-1} \tag{14}$$

2.2 Iterative EKF (Wishner et al. (1969))

In EKF, local linearized model about some estimate is used to transform the statistical properties of the system. The performance of EKF thus, depends upon the quality of estimate about which linearization is carried out. The poor approximation of nonlinear system due to bad initial estimate that is used as a point of linearization lead to degradation of state estimate (Purohit et al. (2015)). The performance of EKF can be improved by iterative schemes (Jazwinski (1970), Wishner et al. (1969)) for systems represented by ODEs. The method of Jazwinski (1970) is useful when measurement function is nonlinear, whereas the method of Wishner et al. (1969) addresses both nonlinearity, in measurement function and system function. In the method of Wishner et al. (1969), the conditional mean calculation is closely related with estimation of x_k. In other words, this technique is mainly deal with maximization of the posteriori probability density. The iterative EKF (Wishner et al. (1969)) for ODEs is presented below.

$$\widehat{\mathbf{x}}^{(i+1)}_{k|k} = \widehat{\mathbf{x}}^{(i)}_{k|k-1} + L^{(i)}_{k}\left[\mathbf{y}_k - \mathbf{h}\left(\widehat{\mathbf{x}}^{(i)}_{k|k}\right)\right] \tag{15}$$

$$-L^{(i)}_{k}\mathbf{H}^{(i)}_{k}\left(\widehat{\mathbf{x}}^{(i)}_{k|k-1} - \widehat{\mathbf{x}}^{(i)}_{k|k}\right) \tag{16}$$

$$\mathbf{H}^{(i)}_{k} = \frac{\partial \mathbf{h}}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\widehat{\mathbf{x}}^{(i)}_{k|k}} \tag{17}$$

$$\mathbf{L}^{(i)}_{k} = \mathbf{P}^{(i)}_{k|k-1}\mathbf{H}^{(i)^T}_{k}\mathbf{V}^{-1}_{k} \tag{18}$$

$$\mathbf{V}_k = \left[\mathbf{H}^{(i)}_{k}\mathbf{P}^{(i)}_{k|k-1}\mathbf{H}^{(i)^T}_{k} + \mathbf{R}\right] \tag{19}$$

$$\widehat{\mathbf{x}}^{(i)}_{k|k-1} = \widehat{\mathbf{x}}^{(i)}_{k|k} + \mathbf{\Phi}^{(i)}_{k|k-1}\left(\widehat{\mathbf{x}}_{k-1|k-1} - \widehat{\mathbf{x}}^{(i)}_{k-1|k}\right) \tag{20}$$

$$\widehat{\mathbf{x}}^{(i+1)}_{k-1|k} = \widehat{\mathbf{x}}_{k-1|k-1} + S^{(i)}_{k}\left(\widehat{\mathbf{x}}^{(i+1)}_{k|k} - \widehat{\mathbf{x}}^{(i)}_{k|k-1}\right) \tag{21}$$

$$\widehat{\mathbf{x}}^{(i)}_{k|k} = \mathbf{F}\left(\widehat{\mathbf{x}}^{(i)}_{k-1|k}\right) \tag{22}$$

$$S^{(i)}_{k} = \mathbf{P}_{k-1|k-1}\mathbf{\Phi}^{(i)T}_{k|k-1}\mathbf{P}^{(i)^{-1}}_{k|k-1} \tag{23}$$

$$\mathbf{P}^{(i)}_{k|k-1} = \mathbf{\Phi}^{(i)}_{k|k-1}\mathbf{P}_{k-1|k-1}\mathbf{\Phi}^{(i)^T}_{k|k-1} + \mathbf{Q} \tag{24}$$

$$\mathbf{P}_{k|k} = \left[\mathbf{I} - \mathbf{L}^{(n)}_{k}\mathbf{H}^{(n)^T}_{k}\right]\mathbf{P}^{(n)}_{k|k-1} \tag{25}$$

where, $\mathbf{\Phi}^{(i)}_{k|k-1}$ is to be evaluated at $\widehat{\mathbf{x}}^{(i)}_{k-1|k}$, and $i = 0, 1, 2, 3, ...n$ iterations. In order to improve the initial estimate at each sampling instant, $\widehat{\mathbf{x}}_{k-1|k-1}$, is updated during $t_k + \Delta t$ by eq. 21 iteratively. This updated estimate $\widehat{\mathbf{x}}^{(i)}_{k-1|k}$ is then used to update the propagated state $\widehat{\mathbf{x}}^{(i)}_{k|k-1}$ by eq. 20. The filtered state $\widehat{\mathbf{x}}^{(i)}_{k|k}$ is then updated by eq. 15. This iterations are initialized by setting $\widehat{\mathbf{x}}^{(0)}_{k|k} = \widehat{\mathbf{x}}_{k|k-1}$; $\widehat{\mathbf{x}}^{(0)}_{k|k-1} = \widehat{\mathbf{x}}_{k|k-1}$; and $\widehat{\mathbf{x}}^{(0)}_{k-1|k} = \widehat{\mathbf{x}}_{k-1|k-1}$and continued till difference between the iterated filtered states is insignificant.

Iterative EKF (IEKF) for DAEs: The proposed IEKF for DAE system is presented below. The differential and algebraic states are augmented as given by eq. 7.

$$\begin{bmatrix}\widehat{\mathbf{x}}^{(i+1)}_{k|k}\\ \widehat{\mathbf{z}}^{(i+1)}_{k|k}\end{bmatrix} = \begin{bmatrix}\widehat{\mathbf{x}}^{(i)}_{k|k-1}\\ \widehat{\mathbf{z}}^{(i)}_{k|k-1}\end{bmatrix} + \mathbf{L}^{aug^{(i)}}_{k}\left(\mathbf{y}_k - \mathbf{h}\begin{bmatrix}\widehat{\mathbf{x}}^{(i)}_{k|k}\\ \widehat{\mathbf{z}}^{(i)}_{k|k}\end{bmatrix}\right) \tag{26}$$

$$-\mathbf{L}^{aug^{(i)}}_{k}\mathbf{H}^{aug^{(i)}}_{k}\left(\begin{bmatrix}\widehat{\mathbf{x}}^{(i)}_{k|k-1}\\ \widehat{\mathbf{z}}^{(i)}_{k|k-1}\end{bmatrix} - \begin{bmatrix}\widehat{\mathbf{x}}^{(i)}_{k|k}\\ \widehat{\mathbf{z}}^{(i)}_{k|k}\end{bmatrix}\right) \tag{27}$$

$$\begin{bmatrix}\widehat{\mathbf{x}}^{(i)}_{k|k-1}\\ \widehat{\mathbf{z}}^{(i)}_{k|k-1}\end{bmatrix} = \begin{bmatrix}\widehat{\mathbf{x}}^{(i)}_{k|k}\\ \widehat{\mathbf{z}}^{(i)}_{k|k}\end{bmatrix} + \mathbf{\Phi}^{(i)}_{k|k-1}\left(\begin{bmatrix}\widehat{\mathbf{x}}_{k-1|k-1}\\ \widehat{\mathbf{z}}_{k-1|k-1}\end{bmatrix} - \begin{bmatrix}\widehat{\mathbf{x}}^{(i)}_{k-1|k}\\ \widehat{\mathbf{z}}^{(i)}_{k-1|k}\end{bmatrix}\right) \tag{28}$$

$$\widehat{\mathbf{x}}^{(i)}_{k|k} = \mathbf{F}\left(\widehat{\mathbf{x}}^{(i)}_{k-1|k}\right) \tag{29}$$

$$\overline{0} = \mathbf{G}\left[\widehat{\mathbf{x}}^{(i)}_{k|k}, \widehat{\mathbf{z}}^{(i)}_{k|k}\right] \tag{30}$$

$$\begin{bmatrix}\widehat{\mathbf{x}}^{(i+1)}_{k-1|k}\\ \widehat{\mathbf{z}}^{(i+1)}_{k-1|k}\end{bmatrix} = \begin{bmatrix}\widehat{\mathbf{x}}_{k-1|k-1}\\ \widehat{\mathbf{z}}_{k-1|k-1}\end{bmatrix} \tag{31}$$

$$+S^{(i)}_{k}\left(\begin{bmatrix}\widehat{\mathbf{x}}^{(i+1)}_{k|k}\\ \widehat{\mathbf{z}}^{(i+1)}_{k|k}\end{bmatrix} - \begin{bmatrix}\widehat{\mathbf{x}}^{(i)}_{k|k-1}\\ \widehat{\mathbf{z}}^{(i)}_{k|k-1}\end{bmatrix}\right) \tag{32}$$

$$\mathbf{L}^{aug^{(i)}}_{k} = \mathbf{P}^{aug^{(i)}}_{k|k-1}\mathbf{H}^{aug^{(i)^T}}_{k} \tag{33}$$

$$\left(\mathbf{H}^{aug^{(i)}}_{k}\mathbf{P}^{aug^{(i)}}_{k|k-1}\mathbf{H}^{aug^{(i)^T}}_{k} + \mathbf{R}\right)^{-1} \tag{34}$$

$$S^{(i)}_{k} = \mathbf{P}^{aug}_{k-1|k-1}\mathbf{\Phi}^{(i)^T}_{k|k-1}\mathbf{P}^{aug^{(i)^{-1}}}_{k|k-1} \tag{35}$$

$$\mathbf{P}^{aug^{(i)}}_{k|k-1} = \mathbf{\Phi}^{(i)}_{k|k-1}\mathbf{P}^{aug}_{k-1|k-1}\mathbf{\Phi}^{(i)^T}_{k|k-1} \tag{36}$$

$$+\mathbf{\Gamma}_{w,k-1}\mathbf{Q}_w\mathbf{\Gamma}^T_{w,k-1} \tag{37}$$

$$\mathbf{P}^{aug}_{k|k} = \left[\mathbf{I} - \mathbf{L}^{aug^{(n)}}_{k}\mathbf{H}^{aug^{(n)^T}}_{k}\right]\mathbf{P}^{aug^{(n)}}_{k|k-1} \tag{38}$$

The iterations are to be initialized in a similar fashion as mentioned by Wishner et al. (1969).

3. RESULTS AND DISCUSSIONS

The EKF-DAE of Mandela et al (2010) and proposed IEKF-DAE in the present work were applied for the purpose of estimations of differential and algebraic states in two DAE systems, viz. 1) Nickel-Hydroxide electrode system and 2) Divided wall distillation column and their performances were compared. The performances of EKF and IEKF were compared based on sum of square of estimation errors ($SSEE$) defined as

$$SSEE_i = \sum_{i=1}^{N}\left(\mathbf{x}_{i,k} - \widehat{\mathbf{x}}_{i,k|k}\right)^2 \tag{39}$$

where, $\mathbf{x}_{i,k}$ represents i^{th} element of the true state vector at instant k, $\widehat{\mathbf{x}}_{i,k|k}$ represents i^{th} element of the corre-

Table 1. Parameter values for NHE System

Faraday's constant F	96487 C/mol
Ideal gas constant R	8.314 J/mol K
Temperature T	298.15 K
Equilibrium potential of nickel reaction $\Phi_{eq,1}$	0.420 V
Equilibrium potential of oxygen reaction $\Phi_{eq,2}$	0.303 V
Density of nickel active material ρ	3.4 g/cm^3
Molecular weight W	92.7 g/mol
Effective length V	1×10^{-5} cm
Applied current density on the nickel electrode i_{app}	1×10^{-5} A/cm^2
Exchange current density of the nickel reaction i_{01}	1×10^{-04}A/cm^2
Exchange current density of the oxygen reaction i_{02}	1×10^{-08} A/cm^2

sponding estimated state vector and N represents number of data points in a simulation experiment. In both case studies, the number of iterations in IEKF were kept fixed at 3, however, the iterations can be terminated based on suitable convergence criteria. It should be noted that IEKF reduces to EKF for one iteration.

DAE example systems considered in the present work are briefly described below.

3.1 Nickel Hydroxide Electrode System

A thin film nickel hydroxide electrode (Celik et al. (2002)) system involves a galvanostatic charge process. There are three modes of operations in this system namely, charging, open-circuit or discharging, depending on the value of i_{app} (positive, zero or negative), respectively. The DAE model involving the dynamic mole balance for the mole fraction of nickel hydroxide (y_1) is given by

$$\frac{\rho V}{W}\frac{dy_1}{dt} = \frac{j_1}{F} \tag{40}$$

$$j_1 + j_2 - i_{app} = 0 \tag{41}$$

$$j_1 = i_{o1}\left[2\left(1-y_1\right)\exp\left(\frac{0.5F}{RT}\left(y_2-\Phi_{eq,1}\right)\right) - 2y_1\exp\left(-\frac{0.5F}{RT}\left(y_2-\Phi_{eq,1}\right)\right)\right]$$

$$j_2 = i_{o2}\left[\exp\left(\frac{F}{RT}\left(y_2-\Phi_{eq,2}\right)\right) - \exp\left(-\frac{F}{RT}\left(y_2-\Phi_{eq,2}\right)\right)\right]$$

where, y_2 is the potential difference at the solid-liquid interface. Species balance is described by differential equation 40 and charge balance is described by algebraic equation 41 and j_1 and j_2 are derived from Butler-Volmer kinetics. The identical parameter values and initialization as used by Mandela et al (2010) and Yash et al. (2012) were used in the present work and presented in Table 1. Consistent initial condition that satisfy algebraic constraints is one of the basic problems while solving DAE. Estimators, EKF and IEKF were initialized by taking $[\,y_1\ y_2\,] = [\,0.5322\ 0.4254\,]$ and the actual initial state used in the simulation study was $[\,0.35024\ 0.4074\,]$. The

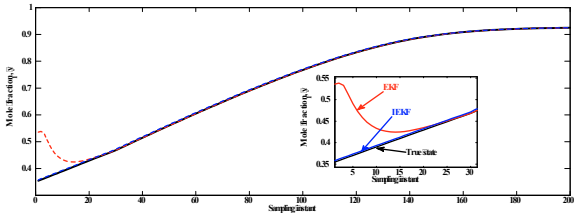

Fig. 1. Estimation of differential state y_1 : NHE system

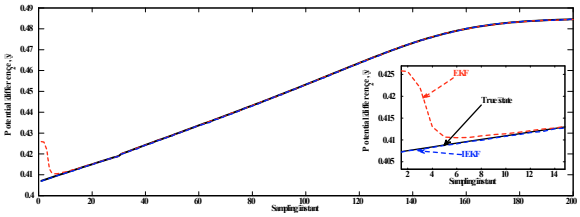

Fig. 2. Estimation of algebraic state, y_2 : NHE system

Table 2. SSEE and RMSE values for Iterative EKF and EKF: NHE System

Estimated states⟶	Differential state	Algebraic state
	SSEE values	
IEKF	0.0015	6.12e-008
EKF	0.1594	9.11e-004
	RMSE values	
IEKF (present work)	0.0022	0.00015
UKF Mandela et al (2010)	0.0178	0.0024
EnKF Yash et al. (2012)	0.0101	0.003

consistent initial conditions used in the present work are obtanined from Mandela et al (2010) and Yash et al. (2012). The tuning parameters (eqs. 42-43) used in EKF and iterative EKF are

$$\Delta t = 15 \text{ sec}, P_0 = \begin{bmatrix} 0.005 & 0 \\ 0 & 0.005 \end{bmatrix} \tag{42}$$

$$Q_{k+1} = 0.00001, R_{k+1} = 0.0001 \tag{43}$$

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. Only the differential state is assumed to be corrupted with process noise.

The $SSEE$ values for Nickel-Hydroxide electrode system are shown in Table 2. $SSEE$ value for differential and algebraic states are significantly smaller in case of IEKF. The improvement in initial estimate is evident from Figures 1 and 2. The root mean square error ($RMSE$) obtained for IEKF in the present work were also compared with UKF (Mandela et al (2010)) and En-KF (Yash et al. (2012)) for Nickel-Hydroxide electrode system in Table 2 which shows that proposed IEKF-DAE performs reasonably better than UKF and EnKF for DAE.

3.2 Divided Wall Distillation Column

Energy integration in thermally coupled distillation systems such as dividing-wall columns provide significant

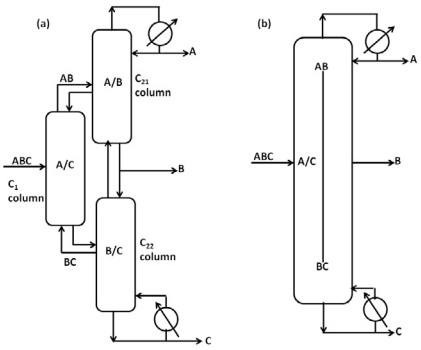

Fig. 3. Three product Petluyk Column: a) Simulation model b) Dividing Wall Petluyk Column

Table 3. Nominal steady state conditions: Petlyuk Column (Fig. 1 (a)

Relative volatility $[A\ B\ C]$	$[4.2\ 2.1\ 1]$
No of stages in C_1 column	20+20
No of stages in C_{21} column	20+20
No of stages in C_{22} column	20+20
Feed rate, F	1 kmol/min
Feed composition $[A\ B\ C]$	$[33.3\ 33.3\ 33.3]$ mol %
Reflux rate, L	1.0033 kmol/min
Vapor boilup rate, V	1.3381 kmol/min
Distillate, D	0.3348 kmol/min
Bottoms, B	0.3333 kmol/min
Side product, S	0.3318 kmol/min
Liquid split, R_L	0.3465
Vapor split, R_V	0.5982
Distillate purity	99.5 mol%
Bottoms purity	99.5 mol%
Side product purity	99.45 mol%

energy savings, typically up to 30% for three product (Petlyuk) column and 40% for four-product (Kaibal) columns and capital savings when compared with energy intensive conventional distillation arrangements (Dwiwedi et al. (2013)). The dynamics and control of Petlyuk column has been the focus of research in recent years by using multivariable PI control (Dwiwedi et al. (2013), Kiss and van Diggelen (2010), Hernandez et al. (2005)) as well as advanced controllers such as LQG/LQR (Kiss and van Diggelen (2010)) and Model Predictive Control (Rohit and Kiss (2012)). Kiss and van Diggelen (2010) compared multiloop PID control with advanced controller such as *Linear Quadratic Gaussian control* (LQG)/*Linear Quadratic Regulation (*LQR), H^∞ controller and μ-synthesis. They (Kiss and van Diggelen (2010)) have used Kalman filter in LQG approach. Rohit and Kiss (2012) used MPC as tool for dynamic optimization of a ternary system in DWC. An experimental implementation of MPC on DWC was investigated by Christina et al. (2011).

In distillation systems, typically temperatures are measured online whereas online measurements of concentrations are unavailable due either large capital investment or large measurement delay as compared to temperature measurements. Thus, in order to estimate concentrations from temperature measurements and for the further development of observer based advanced controller such as MPC/NMPC, a suitable state estimator is required. The dynamic mathematical model of distillation systems is

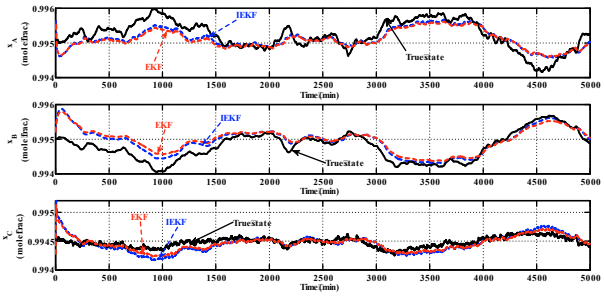

Fig. 4. Estimation of three product compositions: Petluyk Column

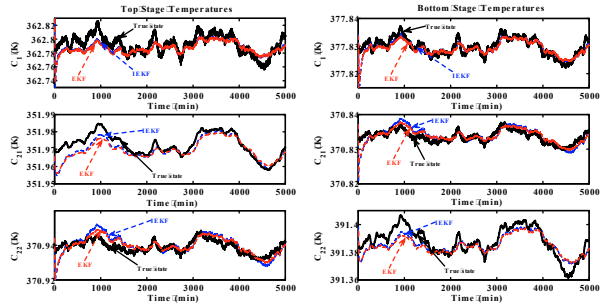

Fig. 5. Estimation of Algebraic States: Petluyk Column

a typical example of DAE systems. It involves algebraic equations for vapor-liquid equilibrium relations and differential equations for mole balances of liquid compositions over each stage. The problems associated with state and parameter estimation in DWC has not been addressed in literature. Kiss and van Diggelen (2010) have used Kalman filter in LQG control of Petlyuk column. In this work, the Petlyuk DWC (Dwiwedi et al. (2013)) was considered for state estimation of differential and algebraic states using DAE-EKF and iterative DAE-EKF. There are 366 differential states and 120 algebraic states in Petlyuk column (Fig.3), which is an example of a relatively large dimension DAE system. The steady state conditions are presented in Table 3. For more details on Petlyuk column case study, Dwiwedi et al. (2013) may be referred. For state estimation, temperatures from C_1, C_{21} and C_{22} columns (ref. Fig. 3 (a)) were considered as measurements. Out of total 120 algebraic states (temperatures), 44 temperatures were assumed to be measured. Each temperature measurement was assumed to be corrupted with zero-mean, normally distributed white noise sequence with a standard deviation of 0.1 K. In simulation studies for Petlyuk column, it was assumed that true values of the inputs ($\mathbf{m}$) are related to the known values of the inputs ($\mathbf{u}$) as given by equation (2). The standard deviations (σ) for simulating the unmeasured disturbances were chosen to be 0.5 % of the inputs ($\mathbf{u}$). Thus, the covariance of the initial states is chosen as follows,

$$\mathbf{Q}_u = diag\left[\,(0.2517e-004)^2\ \ (0.4476e-004)^2\,\right] \qquad (44)$$

$$\mathbf{P}(0|0) = \mathbf{\Gamma}_u(0)\mathbf{Q}_u\mathbf{\Gamma}_u^T(0) \qquad (45)$$

The state covariance matrix was initialized by using eq. 45. It may be noted that only the disturbance free component of the known inputs is used in for state estimation.

Table 4. SSEE values in Petluyk Column: Iterative DAE-EKF

Estimator	IEKF			
Estimated States	Differential (mol fraction)			Algebraic (K)
	x_A	x_B	x_C	T
C_1 (Top)	**0.0014**	**0.0014**	**3.1e-006**	**0.5646**
C_1 Bottom	2.5e-006	2.8e-005	**3.1e-005**	**0.0168**
C_{21} Top	**2.9e-004**	**2.9e-004**	**2.3e-022**	**0.0806**
C_{21} Bottom	7.9e-007	5.0e-005	4.4e-005	0.0122
C_{22} Top	8.0e-007	2.8e-004	2.6e-004	0.0777
C_{22} Bottom	3.6e-022	**2.7e-004**	**2.7e-004**	**0.1642**

Table 5. SSEE values in Petluyk Column: DAE-EKF

Estimator	EKF			
Estimated States	Differential (mol fraction)			Algebraic (K)
	x_A	x_B	x_C	T
C_1 (Top)	0.0016	0.0015	3.4e-006	0.635
C_1 Bottom	2.1e-006	2.7e-005	3.4e-005	0.0192
C_{21} Top	3.9e-004	3.9e-004	2.9e-022	0.1056
C_{21} Bottom	6.7e-007	3.2e-005	3.0e-005	0.0089
C_{22} Top	6.7e-007	1.8e-004	1.7e-004	0.0527
C_{22} Bottom	3.7e-022	3.4e-004	3.4e-004	0.2056

The present work investigated the performances of EKF and IEKF for Petlyuk column. Figures 4 and 5 shows estimated differential and algebraic states compared with true states, respectively. The *SSEE* values of differential and algebraic states for Petlyuk column are reported in Tables 4 and 5. The NHE case study indicated that improvements in the estimator performance arises from smoothing of the initial state. To examine relative merits of DAE-EKF and the proposed DAE-IEKF post the initial convergence, simulations were carried out under the scenario when the initial estimation error was negligible. The performances of EKF and IEKF are reported in 4 and 5. The improvements in state estimation performance obtained using IEKF in some of the states are indicated by bold numbers in Table 4 when compared with their counterparts in Table 5. These results indicate that smoothing step in IEKF contributes to improving estimator performance.

4. CONCLUSIONS

The performance of EKF depends on availability of good initial estimate and accuracy of linearized model. In absence of good initial estimate, performance of EKF degrades and it may lead to large bias in estimated states. However, EKF is more attractive option, particularly for online implementation on large dimension system as it is computationally more efficient than other nonlinear observers such as UKF and En-KF. In this work, an iterative EKF approach, was proposed for DAE system and its performance is evaluated for two case studies, Nickel-Hydroxide electrode system and Petlyuk DWC system. In case of Nickel-Hydroxide electrode system, superior performance of iterative EKF was obtained compared to EKF, UKF (Mandela et al (2010)) and EnKF (Yash et al. (2012)). The simulation study using Petlyuk DWC, which is an example of a large dimensional system, indicated that smoothing step in the proposed IEKF contributes to estimator performance improvement. Further investigations are being carried out using this large dimensional system to evaluate relative performances of DAE-EKF, DAE-UKF and the prosed DAE-IEKF.

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