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An Ensemble Kalman Filter for Systems Governed by Differential Algebraic Equations (DAEs)

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Abstract: Many process systems can be realistically described by a set of nonlinear differential algebraic equations (DAEs). To carry out state estimation of these systems, the conventional sequential Bayesian estimation schemes have to be modified to accommodate nonlinear algebraic constraints. In this work, we present a modified formulation of the Ensemble Kalman Filter for state estimation of systems described by DAEs. The proposed formulation can utilize measurements obtained either from, the differential or algebraic states. The efficacy of the proposed EnKF formulation is demonstrated by simulating two benchmark examples from the literature. The simulation results indicate that the proposed EnKF algorithm can efficiently track both the differential and the algebraic states with reasonable accuracy.

Keywords: differential algebraic systems, nonlinear state estimation, ensemble Kalman filter

1. INTRODUCTION

The problem of state estimation for processes described by differential equations has received a lot of attention in the literature. However, many process systems can be realistically described by a set of nonlinear differential algebraic equations. Such situations arise when different phenomena occur at different time scales. The fast phenomena are often modelled by a quasi steady state approximation, which yields an algebraic equation. For example, algebraic equations arise while modelling thermodynamic equilibrium associated with chemical species simultaneously present in vapour and liquid phases of a chemical process. DAE systems also arise in mechanical and electrical systems.

To achieve effective monitoring and tight control of DAE systems, it becomes necessary to develop schemes for accurately estimating internal states of the system. The Kalman filter has been developed for linear DAE systems by Nikoukhah et al. (1992) and Chisci and Zappa (1992). The extension of the Kalman Filter for non linear DAE systems has been explored previously by Becerra et al. (2001), through successful demonstrations on an experimental setup. In their proposed approach, the model equations are linearized at every time instant. The algebraic states are computed using the linearized algebraic equations, under the assumption that the linearized matrix associated with the algebraic equations is invertible. The algebraic states, thus obtained, are substituted back into the differential equations to yield a system consisting of only differential equations. As a consequence, this state estimator can accommodate measurements obtained only from the differential states.

The requirement that measurements obtained can only be from differential states, can be a serious limitation for systems such as distillation columns, where the measurement available most readily is the temperature, which is obtained from the algebraic vapour liquid equilibrium equations (Mandela et al., 2010). To overcome this limitation, Mandela et al. (2010) have come up with a formulation that extends the work of Becerra et al. (2001) that eliminates the need of measurements being obtained only from differential states. In their proposed approach, the measurements can be obtained either from the differential or algebraic states, or both. The states are propagated using a DAE solver. For the purpose of error covariance update, the system of differential and algebraic equations is linearized around the updated state estimates at the given sampling instant. The resulting linearized algebraic equations are differentiated to yield a differential equation system for the algebraic states as well. Thus, the differential algebraic equation system is transformed to a set of ordinary differential equations, so that the error covariance can be updated similar to the EKF formulation. However, a limitation in the proposed approach is that the re-computation of the algebraic states to satisfy the algebraic equations is ignored. Another disadvantage of the proposed EKF is that the state and measurement equations are linearized around at every sampling instant. This simplification can lead to relatively larger errors in the estimates of the states.

Mandela et al. (2010) have also proposed an unscented Kalman filter (UKF) formulation for systems described

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by DAEs. The main advantage of the UKF is that it circumvents the problems caused by linearization in the EKF. In the UKF algorithm, the statistical properties of the states, such as the mean and estimation error covariances are obtained as sample statistics using deterministically sampled points, known as 'sigma points'. In the UKF algorithm for DAEs, the prediction and correction steps are carried out initially for the differential states. To make all the sigma points consistent, the algebraic states are recomputed from the algebraic equations using the propagated or corrected differential states. The covariance matrix for errors in states is computed using the regular covariance propagation equation of the UKF. However, similar to the EKF, the UKF algorithm too assumes that the conditional densities of the states can be adequately approximated as a Gaussian distribution.

The Ensemble Kalman Filter (EnKF) belongs to a class of particle filters that are being increasingly used for nonlinear state estimation (Evensen, 2007; Prakash et al., 2010). The EnKF can accommodate non-Gaussian distributions of the states and disturbances, as there are no assumptions made about the conditional densities of the states and the unmeasured disturbances and noise. This filter works on the basic premise that the observed states can be sufficiently described by their first two moments, i.e. the mean and covariance, which are computed as sample statistics.

In this work, we present a constrained-EnKF formulation for systems described by DAEs. The key factor that characterizes a DAE is its index. Loosely, the index of a DAE is defined as the number of differentiations that would be needed to convert it to a purely explicit ordinary differential system (Petzold, 1988). An advantage of the proposed EnKF formulation is that the algorithm is independent of the index of the DAE, and hence can be conveniently employed for higher index DAE systems. Also, the proposed method can be employed irrespective of whether the measurement is from differential states or algebraic states or both. The effectiveness of the proposed approach is demonstrated by simulation on two benchmark case studies. We also compare the performance of the proposed EnKF with that of the EKF and UKF formulations proposed by Mandela et al. (2010).

The remainder of the paper is organized as follows. Section 2 describes the process model employed for simulation and state estimation. The proposed constrained-EnKF formulation for DAE systems is described in detail in Section 3. The results obtained using the proposed state estimator, on two benchmark simulation case studies are presented Section 4. A short description of the EKF and UKF formulations of Mandela et al. (2010) are given in Appendix A and Appendix B respectively.

2. MODEL FOR STATE ESTIMATION

The process model employed to describe the DAE system under consideration is detailed in this section. The first principles model for a continuous, nonlinear DAE process can be described by the following equations

$$\begin{aligned} \dot{\mathbf{x}}(t) &= \mathbf{f}(\mathbf{x}, \mathbf{z}, \mathbf{u}) \\ \mathbf{g}(\mathbf{x}, \mathbf{z}, \mathbf{u}) &= \bar{\mathbf{0}} \\ \mathbf{y}(t) &= \mathbf{h}(\mathbf{x}, \mathbf{z}) \end{aligned} \tag{1}$$

$\mathbf{x} \in \mathbb{R}^{nd}$ are the differential states of the process, $\mathbf{z} \in \mathbb{R}^{na}$ are the algebraic states of the process, $\mathbf{u} \in \mathbb{R}^{u}$ are the manipulated inputs, $\mathbf{y} \in \mathbb{R}^{r}$ represents the true measured outputs.

For simulation of the process and modelling for state estimation, the following assumptions are made

(1) The measurements are available at regular intervals, with sampling time T.

(2) The measurement noise can be modelled as a zero-mean white noise with a known distribution

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

where $\mathbf{v} \in \mathbb{R}^{r}$ denotes the measurement noise

(3) The manipulated inputs are piece-wise constant over the sampling interval

$$\mathbf{u}(t) = \mathbf{u}_k \quad \text{for } t_k \leq t < t_k + T$$

(4) The choice of the sampling time, T, is small enough so that the variation of unmeasured disturbances can be adequately approximated as piecewise constant functions. The unmeasured disturbances are assumed to evolve as a zero mean white noise sequence with a known distribution, whose source is unknown. They are modelled as additive signals in the state dynamics.

Under Assumptions 1-3, a discrete time representation of the true dynamics can be obtained as follows

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k + \int_{kT}^{(k+1)T} \mathbf{f}\left(\mathbf{x}(\tau), \mathbf{z}(\tau), \mathbf{u}_k\right) d\tau + \mathbf{w}_k \qquad (2) \\ &= \mathbf{F}\left(\mathbf{x}_k, \mathbf{z}_k, \mathbf{u}_k\right) + \mathbf{w}_k \\ \mathbf{g}\left(\mathbf{x}(\tau), \mathbf{z}(\tau), \mathbf{u}\right) &= \bar{\mathbf{0}} \qquad (3) \\ \mathbf{y}_k &= \mathbf{h}(\mathbf{x}_k, \mathbf{z}_k) + \mathbf{v}_k \qquad (4) \end{aligned}$$

Since the disturbances are a stationary stochastic process, $\mathbf{w}_k \in \mathbb{R}^{nd}$ denotes a zero-mean white noise sequence with a known distribution. It is assumed that $\mathbf{w}_k$ and $\mathbf{v}_k$ are mutually uncorrelated, independent random variables. It is assumed that the distribution of initial state $\mathbf{x}_0$ is known.

3. ENSEMBLE KALMAN FILTER FOR DAE: FORMULATION

Since we are working with nonlinear equations, and since the algebraic constraints effectively dictate that we are allowed only a reduced solution space, generating a computationally tractable suboptimal Bayesian problem is necessitated. This is achieved through the EnKF formulation as stated below. At the initial time $t = 0$ $(k = 0)$, N_p particles of the differential states, $\hat{\mathbf{x}}_0^{(i)}; (i = 1, 2, \ldots, N_p)$, are drawn from its known distribution, with mean $\hat{\mathbf{x}}_0$. The corresponding algebraic states, $\hat{\mathbf{z}}_0^{(i)}$, are obtained such that they satisfy the algebraic equation, given the ensemble of the differential states. At every sampling instant, N_p random samples of the process noise, $\mathbf{w}_k$, and measurement noise, $\mathbf{v}_k$ $\left(\mathbf{w}_k^{(i)}, \mathbf{v}_k^{(i)};\ i = 1, 2, \ldots, N_p\right)$, are drawn from their respective known distributions. Each particle is then propagated through the nonlinear DAEs as follows

$$\begin{aligned}\boldsymbol{\chi}_{k+1|k}^{(i)} &= \mathbf{F}\left(\hat{\mathbf{x}}_{k|k}^{(i)}, \hat{\mathbf{z}}_{k|k}^{(i)}, \mathbf{u}_k\right)\\ \mathbf{g}\left(\boldsymbol{\chi}_{k+1|k}^{(i)}, \hat{\boldsymbol{\zeta}}_{k+1|k}^{(i)}, \mathbf{u}_k\right) &= \bar{\mathbf{0}}\end{aligned} \tag{5}$$

The unknown process disturbances are modelled as

$$\hat{\mathbf{x}}_{k+1|k}^{(i)} = \boldsymbol{\chi}_{k+1|k}^{(i)} + \mathbf{w}_{d,k}^{(i)} \tag{6}$$

The algebraic states $\hat{\mathbf{z}}_{k+1|k}^{(i)}$ are computed from $\mathbf{g}\left(\hat{\mathbf{x}}_{k+1|k}^{(i)}, \hat{\mathbf{z}}_{k+1|k}^{(i)}, \mathbf{u}_k\right) = \bar{\mathbf{0}}$ to ensure that all the ensemble particles are consistent with respect to the algebraic equations. The prediction of the measurement is then obtained as follows

$$\hat{\mathbf{y}}_{k+1|k}^{(i)} = \mathbf{h}\left(\hat{\mathbf{x}}_{k+1|k}^{(i)}, \hat{\mathbf{z}}_{k+1|k}^{(i)}\right) + \mathbf{v}_{k+1}^{(i)} \tag{7}$$

The mean of the differential and algebraic states and the predicted measurement are obtained as follows

$$\bar{\mathbf{x}}_{k+1|k} = \frac{1}{N_p}\sum_{i=1}^{N_p} \hat{\mathbf{x}}_{k+1|k}^{(i)} \tag{8}$$

$$\bar{\mathbf{z}}_{k+1|k} = \frac{1}{N_p}\sum_{i=1}^{N_p} \hat{\mathbf{z}}_{k+1|k}^{(i)} \tag{9}$$

$$\bar{\mathbf{y}}_{k+1|k} = \frac{1}{N_p}\sum_{i=1}^{N_p} \hat{\mathbf{y}}_{k+1|k}^{(i)} \tag{10}$$

A constrained optimisation problem is formulated to compute the measurement update of the particles. The covariance of the prediction error of the states is obtained as

$$\boldsymbol{\varepsilon}_{k+1|k}^{(i)} = \begin{bmatrix}\hat{\mathbf{x}}_{k+1|k}^{(i)}\\ \hat{\mathbf{z}}_{k+1|k}^{(i)}\end{bmatrix} - \begin{bmatrix}\bar{\mathbf{x}}_{k+1|k}\\ \bar{\mathbf{z}}_{k+1|k}\end{bmatrix} \tag{11}$$

$$\mathbf{P}_{k+1|k} = \frac{1}{N_p - 1}\sum_{i=1}^{N_p}\left(\boldsymbol{\varepsilon}_{k+1|k}^{(i)}\right)\left(\boldsymbol{\varepsilon}_{k+1|k}^{(i)}\right)^T \tag{12}$$

The constrained optimisation problem is solved for every particle of the ensemble of the differential and algebraic states and is formulated as follows

$$\begin{aligned}\left(\hat{\mathbf{x}}_{k+1|k+1}^{(i)}, \hat{\mathbf{z}}_{k+1|k+1}^{(i)}\right) = \min_{\mathbf{x}_{k+1}^{(i)}, \mathbf{z}_{k+1}^{(i)}} &\left(\boldsymbol{\epsilon}_{k+1}^{(i)}\right)^T \mathbf{P}_{k+1|k}^{-1}\left(\boldsymbol{\epsilon}_{k+1}^{(i)}\right)\\ &+ \left(\mathbf{e}_{k+1}^{(i)}\right)^T \mathbf{R}^{-1}\left(\mathbf{e}_{k+1}^{(i)}\right)\end{aligned}$$

Subject to

$$\begin{aligned}\mathbf{g}\left(\mathbf{x}_{k+1}^{(i)}, \mathbf{z}_{k+1}^{(i)}, \mathbf{u}_k\right) &= \bar{\mathbf{0}}\\ \mathbf{x}_L \le \mathbf{x}_{k+1}^{(i)} &\le \mathbf{x}_H\\ \mathbf{z}_L \le \mathbf{z}_{k+1}^{(i)} &\le \mathbf{z}_H\end{aligned} \tag{13}$$

where,

$$\boldsymbol{\epsilon}_{k+1}^{(i)} = \begin{bmatrix}\mathbf{x}_{k+1}^{(i)}\\ \mathbf{z}_{k+1}^{(i)}\end{bmatrix} - \begin{bmatrix}\hat{\mathbf{x}}_{k+1|k}^{(i)}\\ \hat{\mathbf{z}}_{k+1|k}^{(i)}\end{bmatrix} \tag{14}$$

$$\mathbf{e}_{k+1}^{(i)} = \mathbf{y}_{k+1} - \hat{\mathbf{y}}_{k+1|k}^{(i)} \tag{15}$$

Since the initial distribution of the states is assumed to be known, we can expect to have a good initial guess at every time step for the optimization problem, and a solution can be obtained quickly through any standard solver using local search methods. The mean of the ensemble of the differential states is computed as follows

$$\bar{\mathbf{x}}_{k+1|k+1} = \frac{1}{N_p}\sum_{i=1}^{N_p} \hat{\mathbf{x}}_{k+1|k+1}^{(i)} \tag{16}$$

If $\mathbf{g}(\cdot)$ is nonlinear, the mean of the ensemble of algebraic states may not be consistent with the updated estimate of the differential state. Thus to get an estimate of the updated algebraic state, $\bar{\mathbf{z}}_{k+1|k+1}$, the algebraic equation is solved using $\bar{\mathbf{x}}_{k+1|k+1}$. Thus, $\bar{\mathbf{z}}_{k+1|k+1}$ is obtained as a solution of

$$\mathbf{g}\left(\bar{\mathbf{x}}_{k+1|k+1}, \bar{\mathbf{z}}_{k+1|k+1}, \mathbf{u}_k\right) = \bar{\mathbf{0}} \tag{17}$$

From the above formulation it can be seen that the proposed algorithm can accommodate measurements obtained from either differential or algebraic states or both.

In contrast to the EKF formulation of Mandela et al. (2010), the EnKF algorithm does not require augmentation of the differential and algebraic state equations to propagate the estimation error covariance. The update of the estimation error in the EKF covariance is done in the conventional way. However this may not be accurate because the algebraic states are being recomputed after the update step. Further, the EKF algorithm cannot be used when we have a non Gaussian process or measurement noise, while the proposed EnKF formulation has no such limitation.

4. SIMULATION CASE STUDIES

We test the efficacy of the proposed EnKF algorithm by testing it on two benchmark case studies– the Nickel Hydroxide electrode and the pH balancing system. The performance of the proposed EnKF is compared with the EKF and UKF for DAE systems, proposed by Mandela et al. (2010). All the simulations are carried out in MATLAB using a DASSL interface as a DAE solver.

4.1 Nickel Hydroxide Electrode

The system presented here models the galvanostatic charge process of a thin film nickel hydroxide electrode (Celik et al., 2002). The rate of change of the mole fraction of nickel hydroxide is (y_1) given by

$$\frac{\rho V}{W}\frac{dy_1}{dt} = \frac{j_1}{F} \tag{18}$$

$$j_1 + j_2 - i_{app} = 0 \tag{19}$$

where

$$\begin{aligned}j_1 = i_{o1}\Big[2(1-y_1)\exp\Big(\frac{0.5F}{RT}(y_2 - \Phi_{eq,1})\Big)\\ -2y_1\exp\Big(\frac{-0.5F}{RT}(y_2 - \Phi_{eq,1})\Big)\Big]\end{aligned} \tag{20}$$

$$j_2 = i_{o2}\left[\exp\Big(\frac{F}{RT}(y_2 - \Phi_{eq,2})\Big) - \exp\Big(\frac{-F}{RT}(y_2 - \Phi_{eq,2})\Big)\right] \tag{21}$$

where y_2 is the potential difference at the solid liquid interface. (18) is the species balance while (19) denotes the charge balance. j_1 and j_2 are derived from Butler-Volmer kinetics. Only the differential state is assumed to be corrupted with process noise. The parameters and initial condition values are summarized in table I. The measured variable is y_2, which is obtained from the algebraic

Table 1. Ni-H electrode problem: Parameters and Initial Conditions

Parameter	Value
Faraday's Constant F	96487 C/mol
Ideal Gas Constant R	8.314 J/molK
Temperature T	298.15 K
equilibrium potential for nickel reaction $\Phi_{eq,1}$	0.420 V
equilibrium potential for oxygen reaction $\Phi_{eq,2}$	0.303 V
Density of nickel ρ	$3.4 g/cm^3$
Molecular Weight W	92.7 g/mol
effective length V	1×10^{-5} cm
applied current density on nickel electrode i_{app}	$1 \times 10^{-5} A/cm^2$
exchange current density of nickel reaction i_{o1}	$1 \times 10^{-4} A/cm^2$
exchange current density of oxygen reaction i_{o2}	$1 \times 10^{-8} A/cm^2$
Variable	**Initial Value**
y_1	0.35024
y_2	0.4074
$\hat{y}_1$	0.5322
$\hat{y}_2$	0.4254

equation (21). Conditions identical with Mandela et al. (2010) have been used for the simulation of the process. Thus, to simulate the process, we choose a sampling time T of 15 sec. The process noise and the measurement noise are assumed to be zero mean Gaussian with covariance, $\mathbf{Q}$, is 0.00001 and $\mathbf{R}$, is 0.0001 respectively. An efficient algorithm for generating samples for a Gaussian distribution is described by Evensen (2007). The initial estimation error covariance in the differential state is assumed to be $\mathbf{P}_0 = 0.005$. The EnKF was implemented with number of particles, $N_p = 20$. The results of the state tracking are shown in Fig. 1. It can be seen from the figures that the EnKF algorithm tracks the two states satisfactorily, despite mismatch in the initial states and also during change in process conditions. To compare the EKF, UKF and the EnKF algorithms, the EKF and UKF algorithm were implemented under identical conditions. Also, the process simulations were carried out using identical realizations of the state and the measurement noise. To make the results independent of specific noise realizations, ten stochastic simulations were carried out under identical conditions for each of the algorithms. The performance of the three state estimators was compared using the root mean square error(RMSE) of the state estimate. The mean values, μ, of RMSE and its standard deviation, σ, are tabulated in Table 3. From the table it can be seen that the proposed EnKF formulation has a far better performance, compared to the EKF and a comparable performance with respect to the UKF.

Now, consider the case where the measurement noise has the following multimodal distribution

$$\mathbf{R}(\mathbf{v}) = 0.5\frac{1}{\sigma_1\sqrt{2\pi}}e^{-\frac{\mathbf{v}-\mu_1}{2\sigma_1^2}} + 0.5\frac{1}{\sigma_1\sqrt{2\pi}}e^{-\frac{\mathbf{v}-\mu_2}{2\sigma_2^2}} \quad (22)$$

The parameters are $\sigma_1^2 = \sigma_2^2 = 0.0001, \mu_1 = 0.005$, and $\mu_2 = -0.005$. The EKF and the UKF formulations can only be used when the process and measurement noise have a Gaussian distribution. However, the EnKF formulation can effectively accommodate non-Gaussian distributions of the noise. The results of the state tracking are shown in Fig. 2. From the figure it can be seen that the EnKF is able to satisfactorily track the two states, even in the presence of noise with a multi-modal distribution.

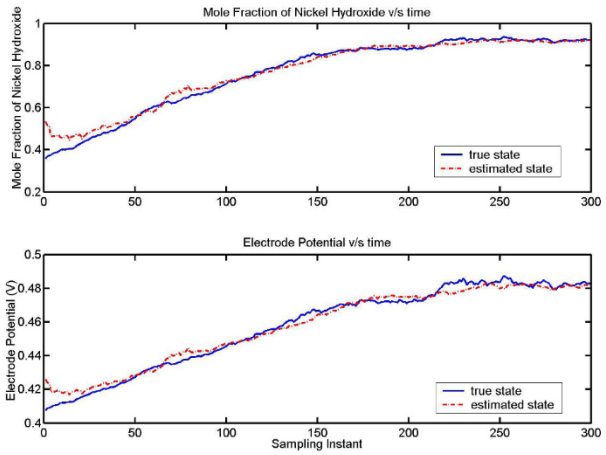

Fig. 1. Ni-H electrode: Estimates of the states obtained with EnKF

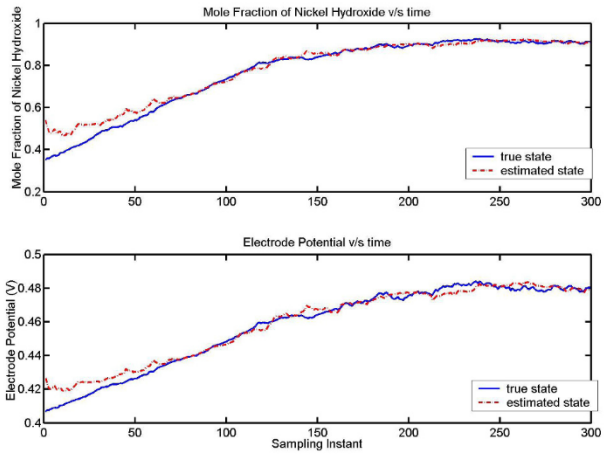

Fig. 2. Ni-H electrode: Estimates of the states obtained with EnKF in presence of multi-modal measurement noise

4.2 pH system

The second problem where we apply the EnKF formulation is a pH balancing problem (Parrish and Brosilow, 1988).The process is a continuously stirred tank reactor, where a feed with unknown pH is flowing into the reactor. We add a basic solution, with known molarity, to the reactor maintain the pH at a desired level. The flow-rate of the basic solution is the manipulated variable. The process is modelled using the following set of DAEs:-

$$V\frac{dN^+}{dt} = mCr - (F+m)N^+ \quad (23)$$

$$(H^+)^3 + (K_a + N^+)(H^+)^2 + (N^+K_a - K_w - K_aU)H^+ - K_aK_w = 0 \quad (24)$$

where N^+, the differential state, is the concentration of the cation of the base in the CSTR, while hydrogen ion concentration, (H^+), is the algebraic state. The parameters and initial conditions are summarized in Table 2. The measurement equation, in this case, is the pH, which is

$$\mathbf{y}_k = -log_{10}[H^+] + \mathbf{v}_k \tag{25}$$

Table 2. pH Balance Problem: Parameters and Initial Conditions

Parameter	Value
Equilibrium constant for water K_w	10^{-14}
Relative strength of acid mixture in the CSTR K_a	0.001
Feed rate to the tank F	13 L/min
Flow rate of the base m	15 L/min
Concentration of the base solution Cr	1 equiv/L
Concentration of the acid and its salts U	0.13 mol/L
Volume of tank V	90 L
Variable	**Initial Value**
N^+	0.005
H^+	0.086
$\hat{N}^+$	0.01
$\hat{H}^+$	0.0068

A step change of -25% is given in the base flow (F). To simulate the effect of process noise, a zero-mean Gaussian white noise with covariance $\mathbf{Q} = 0.00001$ was added to the differential state; while the measurement noise is simulated by adding a zero-mean Gaussian white noise, with covariance $\mathbf{R} = 0.0001$ to the measurement. The sampling time, T, is 0.1 min. The process is initialized with $\mathbf{x}_0 = [0.005 \quad 0.086]$. The effect of uncertainty in the initial state is simulated by initializing the estimator with $\hat{\mathbf{x}}_0 = [0.01 \quad 0.0068]$ and the initial error covariance in the differential state is assumed to be $\mathbf{P}_0 = 0.00025$.

The performance of the three state estimators– EKF, UKF and EnKF is ascertained by running ten stochastic simulation runs and comparing the RMSE values of the state estimates. The estimates of the state are plotted in Fig. 3. From the figure, it can be seen that the state estimator can track the states with reasonable accuracy. The RMSE values obtained are given in Table 3. It can be seen from the table, that the performance of the proposed EnKF algorithm is superior by an order of magnitude, compared to the EKF and is comparable to the performance of the UKF.

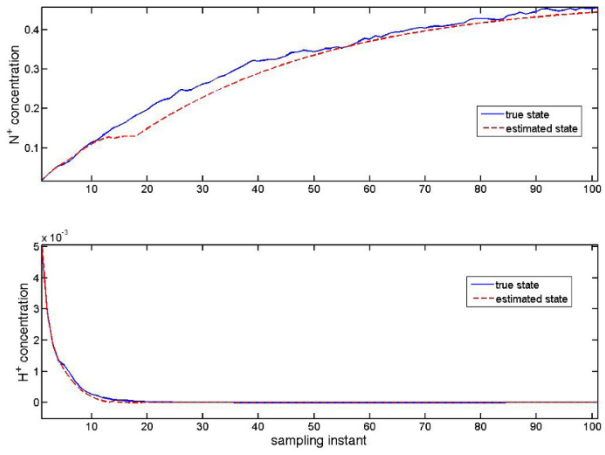

Fig. 3. pH balance system: Estimates for the algebraic state with EKF

Table 3. Comparison of the RMSE values of the states

State estimator	differential state		algebraic state	
	$\mu \times 10^{-2}$	$\sigma \times 10^{-3}$	$\mu \times 10^{-2}$	$\sigma \times 10^{-3}$
Nickel-Hydrogen Electrode				
EKF	1.804	0.992	15.914	1.274
UKF	1.193	3.184	8.094	1.847
EnKF	1.014	2.605	8.463	2.307
pH system				
	$\mu \times 10^{-2}$	$\sigma \times 10^{-4}$	$\mu \times 10^{-5}$	$\sigma \times 10^{-5}$
EKF	1.564	34.033	11.681	4.804
UKF	1.090	1.619	6.695	1.345
EnKF	1.134	2.407	5.891	1.206

5. CONCLUSIONS

In this work, we have presented a constrained-EnKF formulation that can be applied for state estimation of processes described by DAEs. A key feature of the proposed algorithm is that it is independent of the index of the DAE. Moreover, it can handle measurements of either the differential or algebraic states. In the proposed formulation, random particles are drawn only for the differential states, while the ensemble of the algebraic states is computed using the particles of the differential states and the algebraic equation. The measurement update step in the proposed EnKF is formulated as a constrained optmization problem, so that the filtered estimates of the differential and algebraic states satisfy the algebraic equation and their respective physical bounds. The effectiveness of the proposed algorithm was demonstrated on two benchmark simulation case studies. The simulation studies show that the proposed EnKF for DAEs can track the differential and algebraic states of the system with reasonable accuracy, even in the presence of non-Gaussian disturbances. The results obtained indicate that the proposed algorithm has a superior performance compared to the EKF and its performance is slightly better than the UKF.

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Appendix A. EKF FORMULATION FOR DAE

The steps involved in the algorithm proposed by Mandela et al. (2010) are as follows:

(1) The differential and algebraic states are propagated in time from t_k to t_{k+1} using a DAE solver.

(2) The prediction of the estimation error covariance matrix is obtained from

$$P^{aug}_{k+1|k} = \phi_k P^{aug}_{k|k} \phi_k^T + \Gamma_k Q_{k+1} \Gamma_k^T \tag{A.1}$$

where

$$\phi_k = \exp(A^{aug}_k \Delta t) \tag{A.2}$$

$$\Gamma_k = \begin{bmatrix} I \\ -D_k^{-1} C_k \end{bmatrix} \tag{A.3}$$

A^{aug}_k is defined as follows

$$A^{aug}_k = \begin{bmatrix} A_k & B_k \\ -D_k^{-1} C_k A_k & -D_k^{-1} C_k B_k \end{bmatrix} \tag{A.4}$$

$$\begin{bmatrix} A_k & B_k \\ C_k & D_k \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f}{\partial x} & \dfrac{\partial f}{\partial z} \\ \dfrac{\partial g}{\partial x} & \dfrac{\partial g}{\partial z} \end{bmatrix} \tag{A.5}$$

where the partial derivatives on the RHS of (A.5) are evaluated at $(\hat{\mathbf{x}}_{k|k}, \hat{\mathbf{z}}_{k,k}, \mathbf{u}_k)$

(3) Thus the system has now been defined in an augmented form, $x^{aug} = [x \quad z]^T$. The augmented Kalman gain is now calculated

$$K^{aug}_{k+1} = P^{aug}_{k+1|k} H^{augT}_{k+1} (H^{aug}_{k+1} P^{aug}_{k+1|k} H^{augT}_{k+1} + R_{k+1})^{-1} \tag{A.6}$$

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

(4) The updated estimate is computed as

$$\hat{\mathbf{x}}^{aug}_{k+1|k+1} = \hat{\mathbf{x}}^{aug}_{k+1|k} + K^{aug}_{k+1} (\mathbf{y}_{k+1} - h(\hat{\mathbf{x}}^{aug}_{k+1|k})) \tag{A.7}$$

(5) To ensure consistency with the algebraic equations, the algebraic states are recomputed from

$$g(\hat{\mathbf{x}}_{k+1|k+1}, \hat{\mathbf{z}}_{k+1|k+1}) = 0 \tag{A.8}$$

(6) The covariance of the state estimation error is computed from

$$P^{aug}_{k+1|k+1} = (I - K^{aug}_{k+1} H^{aug}_{k+1}) P^{aug}_{k+1|k} \tag{A.9}$$

Appendix B. UKF FORMULATION FOR DAE

The salient points of the UKF algorithm for DAEs are as follows

(1) At the k^{th} sampling instant, let $\hat{\mathbf{x}}_{k|k}$ be the estimate of the differential states, with covariance $\mathbf{P}_{k|k}$. The sigma points of the differential states and their weights (w_i) are chosen according to the standard UKF algorithm for ODE systems.

(2) The sigma points of the algebraic states, $\hat{\mathbf{z}}_{k|k,i}$, are now computed from the algebraic equations

$$\mathbf{g}\left(\hat{\mathbf{x}}_{k|k,i}, \hat{\mathbf{z}}_{k|k,i}, \mathbf{u}\right) = \bar{\mathbf{0}} \tag{B.1}$$

(3) The sigma points are now propagated through the DAE solver to obtain $\hat{\mathbf{x}}_{k+1|k,i}$ and $\hat{\mathbf{z}}_{k+1|k,i}$.

(4) The mean and covariance of the predicted differential state are obtained as

$$\hat{\mathcal{X}}_{k+1|k} = \sum_{i=0}^{2nd} w_i \hat{\mathbf{x}}_{k+1|k,i} \tag{B.2}$$

$$\mathbf{P}_{k+1|k} = \sum_{i=0}^{2nd} w_i \boldsymbol{\varepsilon}_{k+1|k,i} \boldsymbol{\varepsilon}^T_{k+1|k,i} + \mathbf{Q} \tag{B.3}$$

$$\boldsymbol{\varepsilon}_{k+1|k,i} = \left(\hat{\mathbf{x}}_{k+1|k,i} - \hat{\mathcal{X}}_{k+1|k}\right)$$

(5) Define an augmented state vector $\hat{\mathbf{x}}^{aug}_{k+1|k,i} = \left[\hat{\mathbf{x}}_{k+1|k,i} \quad \hat{\mathbf{z}}_{k+1|k,i}\right]$ and obtain its mean as

$$\hat{\mathcal{X}}^{aug}_{k+1|k} = \sum_{i=0}^{2nd} w_i \hat{\mathbf{x}}^{aug}_{k+1|k,i} \tag{B.4}$$

The prediction of the measurement is obtained as

$$\mathbf{Y}_{k+1|k,i} = \mathbf{h}\left(\mathbf{x}^{aug}_{k+1|k,i}\right) \tag{B.5}$$

(6) The Kalman gain is computed as

$$\mathbf{K}_{k+1} = \mathbf{P}_{xv,k+1|k} \mathbf{P}^{-1}_{vv,k+1|k} \tag{B.6}$$

where

$$\mathbf{P}_{vv,k+1|k} = \sum_{i=0}^{2nd} w_i \mathbf{e}_{k+1|k,i} \mathbf{e}^T_{k+1|k,i} + \mathbf{R} \tag{B.7}$$

$$\mathbf{e}_{k+1|k,i} = \left(\mathbf{Y}_{k+1|k,i} - \hat{\mathbf{y}}_{k+1}\right) \tag{B.8}$$

$$\mathbf{P}_{xv,k+1|k} = \sum_{i=0}^{2nd} w_i \boldsymbol{\Upsilon}_{k+1|k,i} \mathbf{e}^T_{k+1|k,i}$$

$$\boldsymbol{\Upsilon}_{k+1|k,i} = \left(\mathbf{x}^{aug}_{k+1|k,i} - \mathcal{X}^{aug}_{k+1|k}\right) \tag{B.9}$$

$$\hat{\mathbf{y}}_{k+1} = \sum_{i=0}^{2nd} w_i \mathbf{Y}_{k+1|k,i}$$

(7) The corrected estimates of the differential states are obtained as

$$\hat{\mathbf{x}}_{k+1|k+1} = \hat{\mathbf{x}}_{k+1|k} + \mathbf{K}_{k+1} \left(\mathbf{y}_{k+1} - \hat{\mathbf{y}}_{k+1}\right) \tag{B.10}$$

(8) The algebraic states, $\hat{\mathbf{z}}_{k+1|k+1}$ are computed using the algebraic equations and the updated differential states

$$\mathbf{g}\left(\hat{\mathbf{x}}_{k+1|k+1}, \hat{\mathbf{z}}_{k+1|k+1}\right) = \bar{\mathbf{0}} \tag{B.11}$$

(9) The updated covariance of the differential states is obtained as shown in the UKF algorithm for ODE systems.