Applying the extended Kalman filter to systems described by nonlinear differential-algebraic equations

Article *in* Control Engineering Practice · March 2001

DOI: 10.1016/S0967-0661(00)00110-6

CITATIONS
127

READS
1,000

3 authors, including:

Victor M. Becerra
University of Portsmouth
193 PUBLICATIONS **2,203** CITATIONS

SEE PROFILE

Graham W Griffiths
City, University of London
54 PUBLICATIONS **762** CITATIONS

SEE PROFILE

PERGAMON

Control Engineering Practice 9 (2001) 267–281

CONTROL ENGINEERING PRACTICE

www.elsevier.com/locate/conengprac

Applying the extended Kalman filter to systems described by nonlinear differential-algebraic equations

V.M. Becerra[a,*], P.D. Roberts[b], G.W. Griffiths[c]

[a]*Department of Cybernetics, University of Reading, P.O. Box 225, Whiteknights, Reading, Berkshire RG6 2AY, UK*
[b]*City University, London, Control Engineering Research Centre, Northampton Square, London EC1V 0HB, UK*
[c]*AspenTech Ltd., Castle Park, Cambridge CB3 OAX, UK*

Received 25 November 1999; accepted 14 August 2000

Abstract

This paper describes a method for the state estimation of nonlinear systems described by a class of differential-algebraic equation models using the extended Kalman filter. The method involves the use of a time-varying linearisation of a semi-explicit index one differential-algebraic equation. The estimation technique consists of a simplified extended Kalman filter that is integrated with the differential-algebraic equation model. The paper describes a simulation study using a model of a batch chemical reactor. It also reports a study based on experimental data obtained from a mixing process, where the model of the system is solved using the sequential modular method and the estimation involves a bank of extended Kalman filters.

Keywords: State estimation; Generalised state space; Large-scale systems; Extended Kalman filters; Process models; Nonlinear systems; Batch reactors

1. Introduction

Systems of coupled differential and algebraic equations (DAEs) often occur as differential equations that are subject to constraints. The constraints may be linear or nonlinear. DAE systems arise frequently as initial value problems in the computer-aided design and modelling of mechanical systems subject to constraints (multi-body systems), circuit simulation, chemical process modelling, and in many other applications. The numerical treatment of DAEs may be more complicated than the numerical integration of ordinary differential equations (ODEs) (Petzold, 1982). Although sometimes it is possible to eliminate the algebraic equations in a DAE to transform it into an ODE, it is not always convenient to do so.

The Kalman filter is a stochastic filter that allows the estimation of the states of a system based on a linear state space model. The extended Kalman filter (EKF) uses local linearisation to extend the scope of the Kalman filter to systems described by nonlinear ordinary differential equations (Maybeck, 1982).

The state estimation problem for *linear* DAEs using the Kalman filter has been studied by several researchers (Nikoukhah, Willsky, & Levy, 1992; Chisci & Zappa, 1992). State estimation for nonlinear DAEs has been studied, for instance, by Albuquerque and Biegler (1997), who used a moving-horizon approach together with model decomposition and nonlinear programming techniques, and by Cheng, Mongkhonsi, and Kershenbaum (1997), who used a variational approach.

Moving-horizon estimation techniques use the measured trajectories over a given period of time and adjust the states of the model along the estimation horizon so that the model trajectories are optimally close in a given sense to the measured trajectories. Parameter estimation for nonlinear DAEs has been studied, for instance, by Tjoa and Biegler (1991), who used simultaneous solution and optimisation via collocation methods and nonlinear programming.

The main advantages of the moving-horizon approach to state estimation over the extended Kalman filter are its capability of handling constraints on the variables and its flexibility with respect to the choice of the estimation criterion. On the other hand, for on-line implementation,

* Corresponding author. + 44(0)118-9318220.
E-mail addresses: v.m.becerra@reading.ac.uk (V.M. Becerra), p.d.roberts@city.ac.uk (P.D. Roberts), graham.griffiths@aspentech.com (G.W. Griffiths).

0967-0661/01/$ - see front matter
PII: S0967-0661(00)00110-6

the computational load carried by the moving-horizon approach becomes too heavy for large-scale models or large horizons. The advantages of the EKF are its simplicity, the fact that it is a recursive algorithm and so its computational load is modest. The EKF is suitable for real-time industrial-scale applications.

The design of observers for nonlinear DAE systems has been addressed by Zimmer and Meier (1997), who transform a regular DAE system into a corresponding explicit ordinary differential equation on a reduced manifold, thus allowing the use of standard observer design techniques.

The EKF has been traditionally applied to state and parameter estimation using models described by ordinary differential equations. A literature search indicates that the problem of state and parameter estimation for nonlinear DAE systems has been addressed using techniques other than the EKF. As far as the authors are aware, the application of the EKF to systems described by nonlinear DAEs has only been treated by themselves in a previous conference paper (Becerra, Roberts, & Griffiths, 1999). The current paper explores the application of the EKF to systems described by nonlinear DAEs and extends the work given by Becerra et al. (1999) with an additional case study, which is laboratory based, and the use of the square root formulation of the EKF (Park & Kailath, 1995), which has better numerical properties than the standard formulation. The aim of this work is to show how a simple extended Kalman filter algorithm can solve the state estimation problem for nonlinear DAE's.

Two case studies are included to illustrate the utility of the work. The first case study consists of a simulated batch reactor (Biegler, Damiano, & Blau, 1986) that was originally provided by the Dow Chemical Company as a challenging test for estimation methods. The second case study is based on experimental data measured from a laboratory mixing rig and a sequential modular model of the process, involving two modules. A bank of two estimators is associated with each module to carry out state estimation. In the sequential modular approach for simulation, the process is represented by a collection of modules where the mathematical description of each item of equipment is encapsulated. Each module is executed and converged individually by a scheduler. With the sequential modular approach very large parallel or distributed simulations are possible, the problem of stiffness may be reduced, the solution and integration algorithms may be tailored to individual modules, and the physical structure of the plant is preserved in the model and its solution (Hillstad & Hertzberg, 1986).

The paper is structured as follows. Section 2.1 introduces the formulation of the differential-algebraic equation model that is considered in this work. Section 2.2 presents the procedure used to linearize the DAE model along a trajectory. Section 2.3 introduces the extended Kalman filter algorithm used and its interface to the DAE model. Section 3 describes a simulation study consisting of a batch chemical reactor. Section 4 describes a study based on experimental data obtained from a laboratory mixing process. Finally, Section 5 states the conclusions derived from this work.

2. Formulation

2.1. DAE model of the process

Consider a process model given by the following set of differential and algebraic equations:

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

and a measurement model given by

$$\mathbf{y}(t_k) = \mathbf{h}(\mathbf{x}(t_k)) + \mathbf{v}(t_k), \tag{2}$$

where $\mathbf{x} \in \Re^{n_x}$ is the vector of differential states, $\mathbf{z} \in \Re^{n_z}$ is a vector of algebraic states, $\mathbf{u} \in \Re^{n_u}$ is a vector of input variables, $\mathbf{y} \in \Re^{n_y}$ is a vector of measured variables, t is a continuous time variable, k is a discrete time index, with sampling time T_s, $\mathbf{f}: \Re^{n_x} \times \Re^{n_u} \times \Re^{n_z} \times \Re \to \Re^{n_x}$ is a mapping of differential equations, $\mathbf{g}: \Re^{n_x} \times \Re^{n_u} \times \Re^{n_z} \times \Re \to \Re^{n_z}$ is a mapping of algebraic equations, $\mathbf{h}: \Re^{n_x} \to \Re^{n_y}$ is a state-output mapping, $\mathbf{w} \in \Re^{n_x}$ is a vector of independent uncorrelated continuous random variables with zero mean and covariance $\mathbf{Q}$, $\mathbf{v} \in \Re^{n_y}$ is a vector of independent uncorrelated discrete random variables with zero mean and covariance $\mathbf{R}$.

Assume that DAE (1) is of index 1. This occurs if and only if the partial derivative matrix $\mathbf{g}_\mathbf{z} = \partial \mathbf{g}/\partial \mathbf{z}$ is nonsingular (Brenan, Campbell, & Petzold, 1996). Also assume that DAE (1) is solvable and that the initial differential state condition is $\mathbf{x}(t_0)$, which is described as a random variable with mean value $\mathbf{x}_0$ and covariance $\mathbf{P}_0$. Notice that if a parameter vector needs to be estimated, state augmentation is normally used.

2.2. Linearisation of the DAE model

In this section, a time-varying linearisation (Campbell, 1995) will be derived for the DAE model (1) and measurement model (2) about a trajectory $\{\dot{\tilde{\mathbf{x}}}(t), \tilde{\mathbf{x}}(t), \tilde{\mathbf{z}}(t), \tilde{\mathbf{u}}(t), t\}$, $t \in [t_0, t_f]$, which satisfies the differential and algebraic equations (1). For the purposes of the linearisation, the stochastic variables $\mathbf{w}$ and $\mathbf{v}$ will be ignored, as they are additive (see Eqs. (1) and (2)).

Define

$$\begin{aligned}\bar{\mathbf{x}}(t) &= \mathbf{x}(t) - \tilde{\mathbf{x}}(t),\\ \dot{\bar{\mathbf{x}}}(t) &= \dot{\mathbf{x}}(t) - \dot{\tilde{\mathbf{x}}}(t),\\ \bar{\mathbf{z}}(t) &= \mathbf{z}(t) - \tilde{\mathbf{z}}(t),\\ \bar{\mathbf{u}}(t) &= \mathbf{u}(t) - \tilde{\mathbf{u}}(t),\\ \bar{\mathbf{y}}(t) &= \mathbf{y}(t) - \tilde{\mathbf{y}}(t),\end{aligned} \tag{3}$$

where $\mathbf{y}(t) = \mathbf{h}(\mathbf{x}(t))$ and $\tilde{\mathbf{y}}(t) = \mathbf{h}(\tilde{\mathbf{x}}(t))$. The linearised equations will have the form

$$\begin{aligned}\dot{\bar{\mathbf{x}}}(t) &= \mathbf{A}(\dot{\tilde{\mathbf{x}}}, \tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{z}}, t)\bar{\mathbf{x}}(t) + \mathbf{B}(\dot{\tilde{\mathbf{x}}}, \tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{z}}, t)\bar{\mathbf{u}}(t),\\ \bar{\mathbf{y}}(t) &= \mathbf{C}(\tilde{\mathbf{x}})\bar{\mathbf{x}}(t),\end{aligned} \tag{4}$$

where $\mathbf{A}, \mathbf{B}$ and $\mathbf{C}$ are matrices of the appropriate dimensions. First, rewrite the set of differential equations as follows:

$$\mathbf{F}(\dot{\mathbf{x}}(t), \mathbf{x}(t), \mathbf{u}(t), \mathbf{z}(t), t) = \dot{\mathbf{x}} - \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{z}(t), t) = 0, \tag{5}$$

where $\mathbf{F}: \Re^{n_x} \times \Re^{n_x} \times \Re^{n_u} \times \Re^{n_z} \times \Re \to \Re^{n_x}$.

Second, assume that the mappings $\mathbf{F}$, $\mathbf{g}$ and $\mathbf{h}$ are sufficiently differentiable in their arguments so that all needed differentiations are possible. A first-order Taylor series expansion of $\mathbf{F}$ and $\mathbf{g}$ about the trajectory $\{\dot{\tilde{\mathbf{x}}}(t), \tilde{\mathbf{x}}(t), \tilde{\mathbf{z}}(t), \tilde{\mathbf{u}}(t), t\}$ gives

$$\begin{aligned}&\mathbf{F}(\dot{\tilde{\mathbf{x}}} + \dot{\bar{\mathbf{x}}}, \tilde{\mathbf{x}} + \bar{\mathbf{x}}, \tilde{\mathbf{u}} + \bar{\mathbf{u}}, \tilde{\mathbf{z}} + \bar{\mathbf{z}}, t)\\ &\quad = \mathbf{F}(\dot{\tilde{\mathbf{x}}}, \tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{z}}, t) + F_{\dot{\mathbf{x}}}\dot{\bar{\mathbf{x}}} + F_{\mathbf{x}}\bar{\mathbf{x}} + \mathbf{F}_{\mathbf{u}}\bar{\mathbf{u}} + \mathbf{F}_{\mathbf{z}}\bar{\mathbf{z}} = \mathbf{0},\end{aligned} \tag{6}$$

$$\begin{aligned}&\mathbf{g}(\tilde{\mathbf{x}} + \bar{\mathbf{x}}, \tilde{\mathbf{u}} + \bar{\mathbf{u}}, \tilde{\mathbf{z}} + \bar{\mathbf{z}}, t)\\ &\quad = \mathbf{g}(\tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{z}}, t) + \mathbf{g}_{\mathbf{x}}\bar{\mathbf{x}} + \mathbf{g}_{\mathbf{u}}\bar{\mathbf{u}} + \mathbf{g}_{\mathbf{z}}\bar{\mathbf{z}} = \mathbf{0},\end{aligned} \tag{7}$$

where all partial derivatives are evaluated at the trajectory $\{\dot{\tilde{\mathbf{x}}}(t), \tilde{\mathbf{x}}(t), \tilde{\mathbf{z}}(t), \tilde{\mathbf{u}}(t), t\}$. Noting that, by definition, $\mathbf{F}(\dot{\tilde{\mathbf{x}}}, \tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{z}}, t) = \mathbf{0}$ and $\mathbf{g}(\tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{z}}, t) = \mathbf{0}$, then it follows that

$$\mathbf{F}_{\dot{\mathbf{x}}}\dot{\bar{x}} + \mathbf{F}_{x}\bar{\mathbf{x}} + \mathbf{F}_{u}\bar{\mathbf{u}} + \mathbf{F}_{z}\bar{\mathbf{z}} = \mathbf{0}, \tag{8}$$

$$\mathbf{g}_{\mathbf{x}}\bar{\mathbf{x}} + \mathbf{g}_{\mathbf{u}}\bar{\mathbf{u}} + \mathbf{g}_{\mathbf{z}}\bar{\mathbf{z}} = \mathbf{0}. \tag{9}$$

Given that $\mathbf{g}_{\mathbf{z}}$ is assumed to be non-singular, Eq. (9) can be solved for $\bar{\mathbf{z}}$:

$$\bar{\mathbf{z}} = -\mathbf{g}_{\mathbf{z}}^{-1}[\mathbf{g}_{\mathbf{x}}\bar{\mathbf{x}} + \mathbf{g}_{\mathbf{u}}\bar{\mathbf{u}}]. \tag{10}$$

Substituting (10) into (8), noting that $\mathbf{F}_{\dot{\mathbf{x}}} = \mathbf{I}_{n_x}$, and solving (8) for $\dot{\bar{\mathbf{x}}}$, gives the linearised state equation

$$\dot{\bar{\mathbf{x}}} = [\mathbf{F}_{\mathbf{z}}\mathbf{g}_{\mathbf{z}}^{-1}\mathbf{g}_{\mathbf{x}} - \mathbf{F}_{\mathbf{x}}]\bar{\mathbf{x}} + [\mathbf{F}_{\mathbf{z}}\mathbf{g}_{\mathbf{z}}^{-1}\mathbf{g}_{\mathbf{u}} - \mathbf{F}_{\mathbf{u}}]\bar{\mathbf{u}} = \mathbf{A}\bar{\mathbf{x}} + \mathbf{B}\bar{\mathbf{u}}. \tag{11}$$

The linearised matrices $\mathbf{A}$ and $\mathbf{B}$ are then defined as

$$\begin{aligned}\mathbf{A} &= \mathbf{F}_{\mathbf{z}}\mathbf{g}_{\mathbf{z}}^{-1}\mathbf{g}_{\mathbf{x}} - \mathbf{F}_{\mathbf{x}},\\ \mathbf{B} &= \mathbf{F}_{\mathbf{z}}\mathbf{g}_{\mathbf{z}}^{-1}\mathbf{g}_{\mathbf{u}} - \mathbf{F}_{\mathbf{u}}.\end{aligned} \tag{12}$$

In a similar way, the measurement function (2) is linearised, resulting in:

$$\bar{\mathbf{y}} = \mathbf{h}_{\mathbf{x}}\bar{\mathbf{x}} = \mathbf{C}\bar{\mathbf{x}}, \tag{13}$$

where $\mathbf{h}_{\mathbf{x}}$ has been evaluated along the trajectory $\tilde{\mathbf{x}}(t)$. Notice that, in the absence of a set of algebraic equations $\mathbf{g}$, matrices $\mathbf{A}$ and $\mathbf{B}$ reduce to the standard state space linearisation $\mathbf{A} = -\mathbf{F}_{\mathbf{x}} = \mathbf{f}_{\mathbf{x}}$ and $\mathbf{B} = -\mathbf{F}_{\mathbf{u}} = \mathbf{f}_{\mathbf{u}}$.

2.3. Extended Kalman filter

For the sake of numerical stability, the conventional square root form of the Kalman filter equations has been used in this work (Maybeck, 1982; Park & Kailath, 1995).

A simplified form of the EKF with discrete measurements is obtained assuming that the linearised matrices $\mathbf{A}$ and $\mathbf{C}$ remain constant between two consecutive sampling instants. This is justified if the process is slow compared with the sampling time T_s.

Assume that the measurements are taken in discrete samples, with a sampling time T_s. Define the state transition matrix $\Phi(k)$, which is obtained by integrating the linearised equation (11) between t_{k-1} and t_k, assuming a constant $\mathbf{A}(k)$ matrix. $\Phi(k)$ is given by

$$\Phi(k) = \mathrm{e}^{\mathbf{A}(k)T_s}, \tag{14}$$

where $\mathbf{A}(k)$ has been computed using Eq. (12) evaluated at $\{\dot{\hat{\mathbf{x}}}(t_{k-1}), \hat{\mathbf{x}}(t_{k-1}), \hat{\mathbf{z}}(t_{k-1}), \mathbf{u}(t_{k-1}), t_{k-1}\}$, where $\dot{\hat{\mathbf{x}}}(t_{k-1})$ and $\hat{\mathbf{z}}(t_{k-1})$ are consistent with $\hat{\mathbf{x}}(t_{k-1})$. The state vectors $\hat{\mathbf{x}}(t_{k-1})$ and $\hat{\mathbf{z}}(t_{k-1})$ are the latest best estimates and so the linearisation to compute $\mathbf{A}(k)$ is carried out about these points.

Define $\mathbf{P}^-(k) \in \Re^{n_x \times n_x}$ as the a priori state covariance, which is a measure of the state estimation error at discrete time k given information up to time $k-1$. Also define $\mathbf{P}(k)$ as the corrected state covariance, which is a measure of the estimation error at discrete time k, calculated using information up to discrete time k. Note that it is not necessary to compute the a priori state covariance $\mathbf{P}^-(k)$ by integrating a Lyapunov equation, as the authors avoid using the continuous time formulation for updating this matrix by defining the state transition matrix $\Phi(k)$, which is based on the linearized $\mathbf{A}(k)$ matrix. This is a valid approximation provided the sampling time is small compared with the characteristic times of the continuous time system.

Define the Cholesky roots (Noble & Daniel, 1988) $\mathbf{S}^-$, $\mathbf{S}$, $\mathbf{L}$ and $\mathbf{D}$ such that $\mathbf{P}^- = \mathbf{S}^-(\mathbf{S}^-)^{\mathrm{T}}$, $\mathbf{P} = \mathbf{S}\mathbf{S}^{\mathrm{T}}$, $\mathbf{Q} = \mathbf{L}\mathbf{L}^{\mathrm{T}}$, and $\mathbf{R} = \mathbf{D}\mathbf{D}^{\mathrm{T}}$.

2.3.1. Square-root-extended Kalman filter algorithm

- *Initialization:* Assume that $\mathbf{x}_0$ and $\mathbf{P}_0$ are given. Set the initial differential state estimate $\hat{\mathbf{x}}(t_0)$ to $\mathbf{x}_0$, and solve the DAE model (17) for the initial algebraic state $\hat{\mathbf{z}}(t_0)$ and state derivatives $\dot{\hat{\mathbf{x}}}(t_0)$ (Here the authors used the nonlinear equation solution algorithm `LMDIF1` from the `MINPACK` software library). Compute the linearized matrix $\mathbf{A}(0)$ about the initial estimate using Eq. (12), and also obtain the state transition matrix

$\Phi(0)$ from Eq. (14). Set the initial state covariance matrix $\mathbf{P}(0)$ to $\mathbf{P}_0$, and compute the corresponding square root $\mathbf{S}(0)$. Set $k = 1$.

Step 1: Assuming that information at time $k-1$ is known, the time update is as follows (Park & Kailath, 1995):

- Form matrix $\mathbf{L}_1$ as follows:

$$\mathbf{L}_1 = [\Phi(k-1)\mathbf{S}(k-1)\ \mathbf{L}]. \tag{15}$$

- Apply the LQ factorization to matrix $\mathbf{L}_1$ (the authors used routine DGELQF from the LAPACK numerical library) to obtain matrix $\mathbf{R}_1$.
- Given matrix $\mathbf{R}_1$, extract matrix $\mathbf{S}^-(k)$ ($\dim \mathbf{S}^-(k) = n_x \times n_x$) from its first n_x columns

$$\mathbf{R}_1 = [\mathbf{S}^-(k)\ \mathbf{0}]. \tag{16}$$

- Compute the a priori state estimate $\hat{\mathbf{x}}^-(t_k)$ by integrating the DAE model

$$\begin{aligned} &\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{z}(t), t), \\ &\mathbf{g}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{z}(t), t) = \mathbf{0}, \end{aligned} \tag{17}$$

over one sampling interval from t_{k-1} to t_k, starting from the latest corrected state estimate $\hat{\mathbf{x}}(t_{k-1})$, using the latest value of the input $\mathbf{u}(t_{k-1})$ (Assuming that the input $\mathbf{u}$ remains constant between sampling intervals).

Step 2: The measurement update is as follows:

- Compute $\mathbf{C}(k)$ using (13) evaluated at the a priori estimate $\hat{\mathbf{x}}^-(t_k)$.
- Form matrix $\mathbf{L}_2$ as follows:

$$\mathbf{L}_2 = \begin{bmatrix} \mathbf{D} & \mathbf{C}(k)\mathbf{S}^-(k) \\ \mathbf{0} & \mathbf{S}^-(k) \end{bmatrix}. \tag{18}$$

- Apply the LQ factorization to matrix $\mathbf{L}_2$ (the authors used routine DGELQF from the LAPACK numerical library) to obtain matrix $\mathbf{R}_2$.
- Partition matrix $\mathbf{R}_2$ as follows and extract from it matrices $\mathbf{W}(k)$ ($\dim \mathbf{W}(k) = n_y \times n_y$), $\bar{\mathbf{K}}(k)$ ($\dim \bar{\mathbf{K}}(k) = n_x \times n_y$) and $\mathbf{S}(k)$ ($\dim \mathbf{S}(k) = n_x \times n_x$):

$$\mathbf{R}_2 = \begin{bmatrix} \mathbf{W}(k) & \mathbf{0} \\ \bar{\mathbf{K}}(k) & \mathbf{S}(k) \end{bmatrix}. \tag{19}$$

- Compute the Kalman gain $\mathbf{K}(k)$ as follows:

$$\mathbf{K}(k) = \bar{\mathbf{K}}(k)\mathbf{W}(k)^{-1}. \tag{20}$$

- Obtain a new output measurement $\mathbf{y}_m(t_k)$ from the process and compute the corrected state estimate $\hat{\mathbf{x}}(t_k)$ as follows:

$$\hat{\mathbf{x}}(t_k) = \hat{\mathbf{x}}^-(t_k) + \mathbf{K}(k) \times (\mathbf{y}_m(t_k) - \mathbf{h}(\hat{\mathbf{x}}^-(t_k))). \tag{21}$$

- Given $\hat{\mathbf{x}}(t_k)$, solve the DAE model (17) for the algebraic state $\hat{\mathbf{z}}(t_k)$ and state derivatives $\hat{\dot{\mathbf{x}}}(t_k)$ (Here the authors used the nonlinear equation solution algorithm LMDIF1 from the MINPACK software library). Compute the linearized matrix $\mathbf{A}(k)$ about the current estimate using Eq. (12), and also obtain the state transition matrix $\Phi(k)$ from Eq. (14). Set $k = k + 1$ and go to Step 1.

3. Simulation study: batch chemical reactor DAE model

This simulation study consists of a kinetic model of an isothermal batch reactor system. The model was presented by Biegler et al. (1986) and later used by Leineweber et al. (1997). The example in its original form was given by the Dow Chemical Company as a challenging test for parameter estimation methods. The desired product AB results from the reaction

$$\mathrm{HA} + 2\mathrm{BM} \rightarrow 2\mathrm{AB} + \mathrm{MBMH}.$$

The reaction starts by adding a catalyst QM to the mixture of reactants. QM is assumed to be completely dissociated to Q^+ and M^- ions. The proposed reaction mechanism involves three slow kinetic reactions,

$$\mathrm{M}^- + \mathrm{BM} \overset{k_1, k_{-1}}{\leftrightarrow} \mathrm{MBM}^-,$$

$$\mathrm{A}^- + \mathrm{BM} \overset{k_2}{\rightarrow} \mathrm{ABM}^-,$$

$$\mathrm{M}^- + \mathrm{AB} \overset{k_3, k_{-3}}{\leftrightarrow} \mathrm{ABM}^-$$

and three rapid acid–base reactions

$$\mathrm{MBMH} \overset{k_1}{\leftrightarrow} \mathrm{MBM}^- + \mathrm{H}^+,$$

$$\mathrm{HA} \overset{k_2}{\leftrightarrow} \mathrm{A}^- + \mathrm{H}^+,$$

$$\mathrm{HABM} \overset{k_3}{\leftrightarrow} \mathrm{ABM}^- + \mathrm{H}^+,$$

which are assumed to be at equilibrium. Also, based on similarities of the reacting species, it is supposed that $k_3 = k_1$ and $k_{-3} = 0.5k_{-1}$. For the other reaction rates k_1, k_{-1} and k_2, an Arrhenius temperature dependence is assumed:

$$k_i = \alpha_i \mathrm{e}^{-E_i/R(T+273)}, \tag{22}$$

where T is the reaction temperature in °C, α_i is the pre-exponential factor, E_i is the activation energy and R is the universal gas constant.

In the model of the batch reactor, the following differential states (denoted as x_i) and algebraic states (denoted as z_i) are assumed: $x_0 = [\mathrm{HA}]$, $x_1 = [\mathrm{BM}]$,

$x_2 = [\mathrm{HABM}], x_3 = [\mathrm{AB}], x_4 = [\mathrm{MBMH}], x_5 = [\mathrm{M}^-]$, $z_0 = -\log([\mathrm{H}^+])$, $z_1 = [\mathrm{A}^-]$, $z_2 = [\mathrm{ABM}^-]$, $z_3 = [\mathrm{MBM}^-]$, where all concentrations $[\cdot]$ are given in gmol per kg of the reaction mixture.

The model consists of six differential mass balance equations:

$$\begin{aligned}
\dot{x}_0 &= -k_2 x_1 z_1,\\
\dot{x}_1 &= -k_1 x_1 x_5 + k_{-1} z_3 - k_2 x_1 z_1,\\
\dot{x}_2 &= k_2 x_1 z_1 + k_3 x_3 x_5 - k_{-3} z_2,\\
\dot{x}_3 &= -k_3 x_3 x_5 + k_{-3} z_2,\\
\dot{x}_4 &= k_1 x_1 x_5 - k_{-1} z_3,\\
\dot{x}_5 &= -k_1 x_1 x_5 + k_{-1} z_3 - k_3 x_3 x_5 + k_{-3} z_2,
\end{aligned} \tag{23}$$

an electroneutrality condition:

$$[\mathrm{Q}^+] - x_5 + 10^{-z_0} - z_1 - z_2 - z_3 = 0 \tag{24}$$

and three equilibrium conditions:

$$\begin{aligned}
z_1 - K_2 x_0/(K_2 + 10^{-z_0}) &= 0,\\
z_2 - K_3 x_2/(K_3 + 10^{-z_0}) &= 0,\\
z_3 - K_1 x_4/(K_1 + 10^{-z_0}) &= 0.
\end{aligned} \tag{25}$$

The output vector is $\mathbf{y_m} = [x_0, x_1, x_2, x_3]^{\mathrm{T}}$. The simulated measurements were sampled with a sampling period of 60 s.

Two DAE models with the same parameters and structure were used in the simulation:

1. A DAE model representing the real process. A Gaussian noise signal was added to each output. The noisy simulated measurements were then fed to the EKF. Recall that this is a simulation case study where a model generates the measured data. The standard deviations of the Gaussian noise signals added to the outputs were: $\sigma_1 = 0.02$, $\sigma_2 = 0.02$, $\sigma_3 = 0.02$, and $\sigma_4 = 0.01$.
2. A DAE model that the EKF uses internally for its calculations. See Section 2.3.

The following parameter values were used in the simulation (Biegler et al., 1986; Leineweber et al., 1997), noting that time is measured in hours: $\alpha_1 = 1.3708 \times 10^{12}$ kg gmol^{-1} h^{-1}, $E_1/R = 9.2984 \times 10^3$ K, $\alpha_{-1} = 1.6215 \times 10^{20}$ h^{-1}, $E_{-1}/R = 1.3108 \times 10^4$ K, $\alpha_2 = 5.2282 \times 10^{12}$ kg gmol^{-1} h^{-1}, $E_2/R = 9.5999 \times 10^3$ K, $K_1 = 2.575 \times 10^{-16}$ gmol kg^{-1}, $K_2 = 4.876 \times 10^{-14}$ gmol kg^{-1}, $K_3 = 1.7884 \times 10^{-16}$ gmol kg^{-1}, $[\mathrm{Q}]^+ = 0.0131$ gmol kg^{-1}.

The initial conditions used for the differential states of the model representing the real process were: $x_0 = 1.5776$, $x_1 = 8.32$, $x_2 = 0$, $x_3 = 0$, $x_4 = 0$, $x_5 = 0.0142$. The initial conditions used for the differential states of the model used by the EKF were: $x_0 = 1.6$, $x_1 = 8.3$, $x_2 = 0$, $x_3 = 0$, $x_4 = 0$, $x_5 = 0.014$. The EKF operated with a sampling period of 60 s. The tuning parameters of the EKF were

$$\begin{aligned}
\mathbf{P}_0 &= \mathrm{diag}(0.003, 0.003, 0.003, 0.003, 0.003, 0.003),\\
\mathbf{Q} &= \mathrm{diag}(0.0001, 0.0001, 0.0001, 0.0001, 0.0001, 0.0001),\\
\mathbf{R} &= \mathrm{diag}(0.0004, 0.0004, 0.0001, 0.0001).
\end{aligned} \tag{26}$$

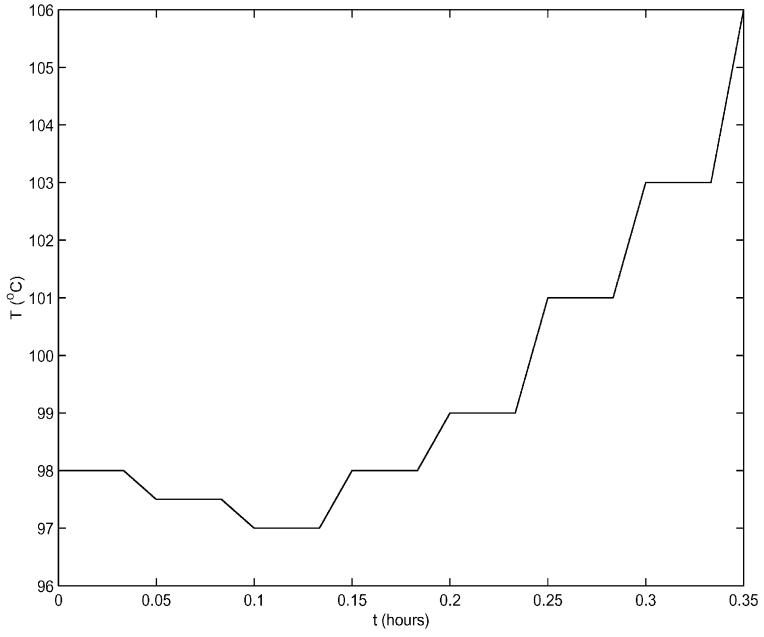

Fig. 1. Temperature profile.

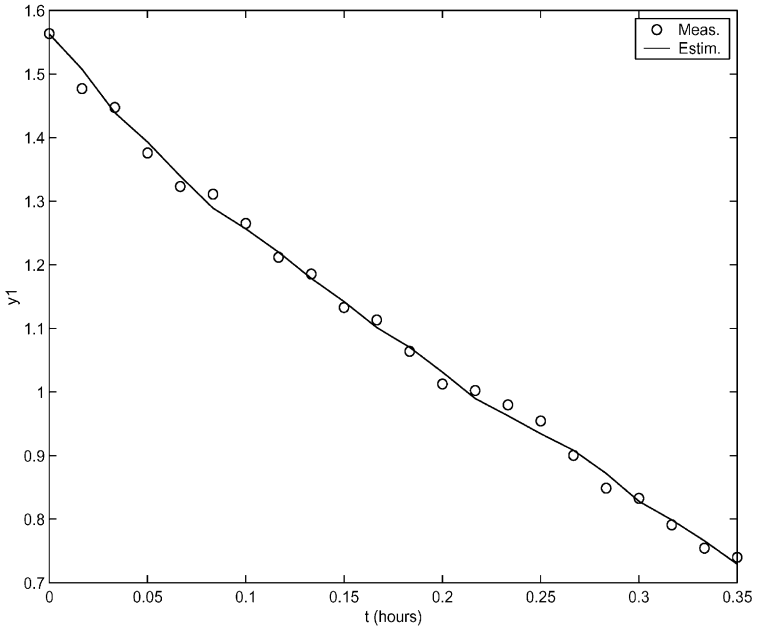

Fig. 2. Measured and estimated output y_1.

The diagonal elements of the output noise covariance matrix **R** were chosen to account for the variance of the noise that was added to each output. The diagonal elements of the process noise covariance matrix **Q** were chosen small and positive in order to prevent the covariance of the state error from becoming zero. The initial covariance of the state error $\mathbf{P}_0$ was chosen to reflect some uncertainty in the initial state estimate.

In order to initialise the model representing the real process and the internal EKF model, the values of the algebraic states **z** were calculated together with the time derivatives $\dot{\mathbf{x}}$ by using the above values of the differential states and then solving the resulting nonlinear Eqs. (17) for **z** and $\dot{\mathbf{x}}$ using the nonlinear equation solution algorithm `LMDIF1` from the `MINPACK` software library. A similar re-initialization is periodically carried out on the internal process model every time the a priori state estimate $\hat{\mathbf{x}}^-(t_k)$ is updated by the EKF. Notice that the number of arbitrarily specifiable conditions in an index one DAE with the structure of (1) is equal to the number of differential equations n_x (Pantelides, Gritsis, Morison, & Sargent, 1988). The DAE integration code DASSL (Petzold, 1983) was used for the numerical integration of the DAE models.

Fig. 1 shows the input temperature profile T. Figs. 2–5 show the simulated measured and estimated output variables. Figs. 6–8 show the true and estimated differential states x_0, x_4 and x_5. Fig. 9 shows the true and estimated algebraic state z_0. Note that the noise in the measurements has been reduced by the EKF. The estimation of differential states is satisfactory, as there is good agreement between the true and estimated responses. Also notice that it is possible to estimate the algebraic states by taking their values from the internal EKF model.

4. Experimental study

A study was carried out using experimental data measured from a two-tank mixing process that is available at City University, London. A section of the process is shown in Fig. 10. Two streams of cold and hot water enter in the first tank, where a motorised mixer operates. These streams are controlled by means of two pneumatic valves equipped with valve positioners and electro-pneumatic transducers. The two tanks are interconnected via a lower pipe with a manual valve that is normally open. The outlet valve from tank 2 is also normally open. The outlet stream from the second tank enters a buffer tank and from there it is pumped to an upper storage tank, which is equipped with an electric heater (Fig. 10 does not show this). The hot water stream is drawn from this tank. The rig is interfaced to a local PC. The four measured variables are the temperatures and levels in both tanks. It is possible to manipulate the opening of the cold and hot water valves via the local PC. Two digital PID algorithms are implemented in software on this PC. The local PC is connected to a more powerful supervisory PC via serial links. The supervisory PC allows remote control and monitoring of the rig. It includes process mimics, PID controller settings, loop decoupling, variable trending, alarm processing and data logging.

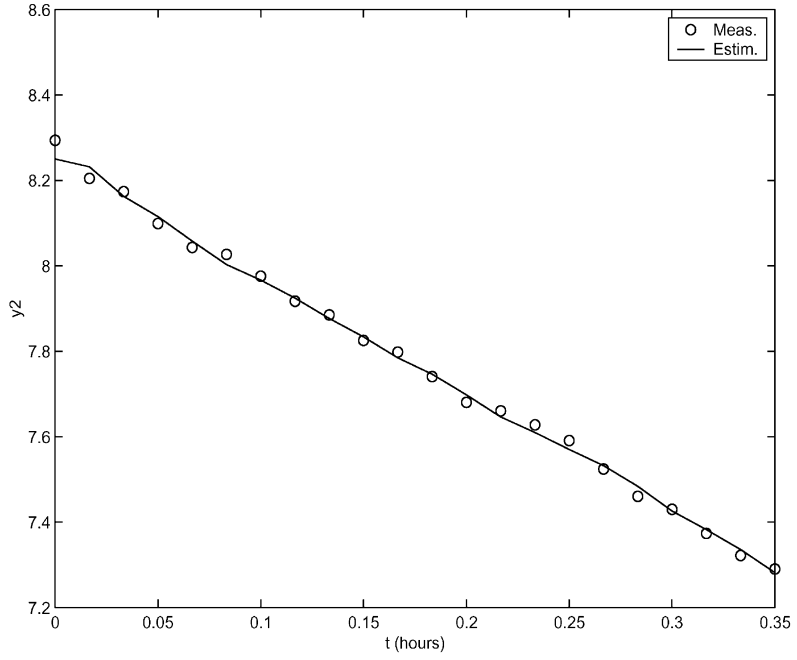

Fig. 3. Measured and estimated output y_2.

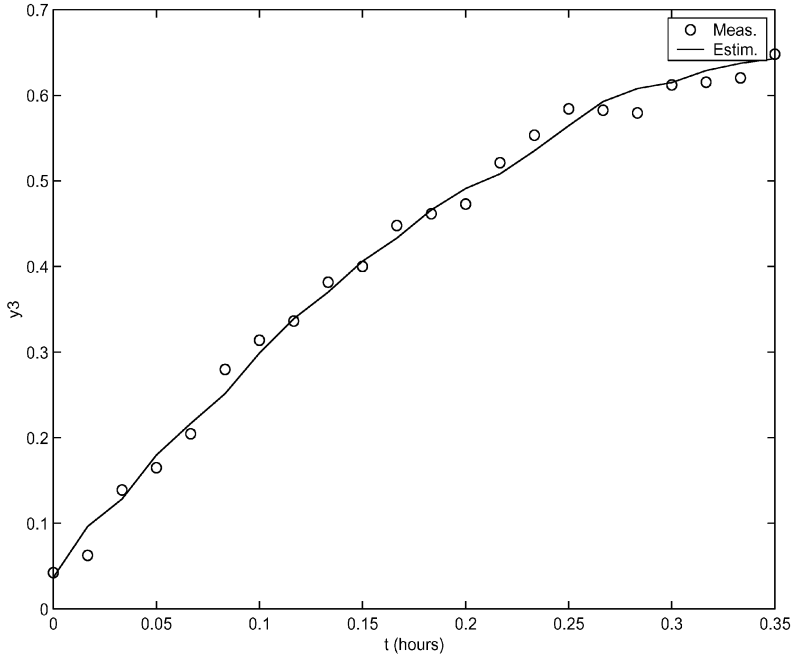

Fig. 4. Measured and estimated output y_3.

The experiment to collect the data was carried out with the PID controllers in the manual position. The opening of the cold and hot water valves were switched randomly as shown in Fig. 11. The sampling time of the signals was 20 s. The experiment lasted for 3800 s. Notice that the studies described here were carried out off-line using the same experimental data set.

The solution of the state estimation problem using a sequential modular model as a whole is a difficult problem, because the calculation of the derivatives with

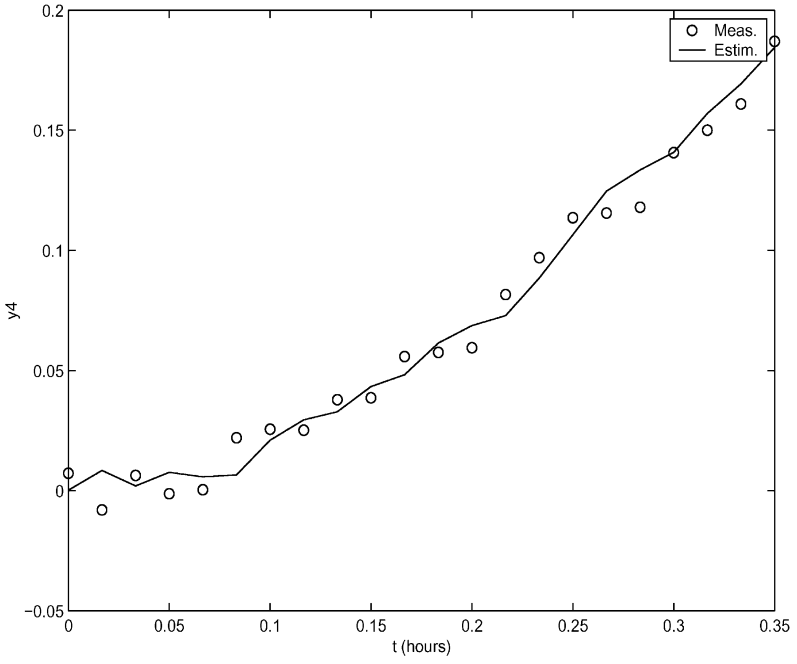

Fig. 5. Measured and estimated output y_4.

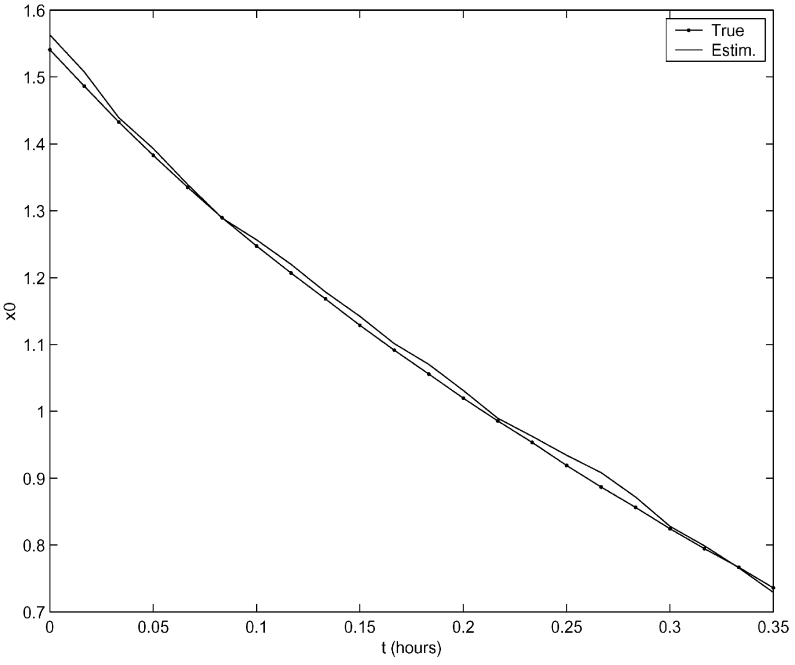

Fig. 6. True and estimated state x_0.

respect to inputs and states becomes difficult due to the interconnections between the modules. A possible way of doing state estimation using sequential modular models is to use a bank of estimators, applying each of them to one relevant module. Fig. 12 illustrates this idea. Another advantage of this approach, particularly for large and sparse systems, is that it is computationally less expensive to use several EKF's of smaller order than to use one EKF of large order.

A simple modular model of the mixing process is described below. The model was obtained from mass and energy balances. The main simplifying assumptions that were taken to derive this model were: (1) the mixing is perfect; (2) heat losses are negligible; (3) the valves have

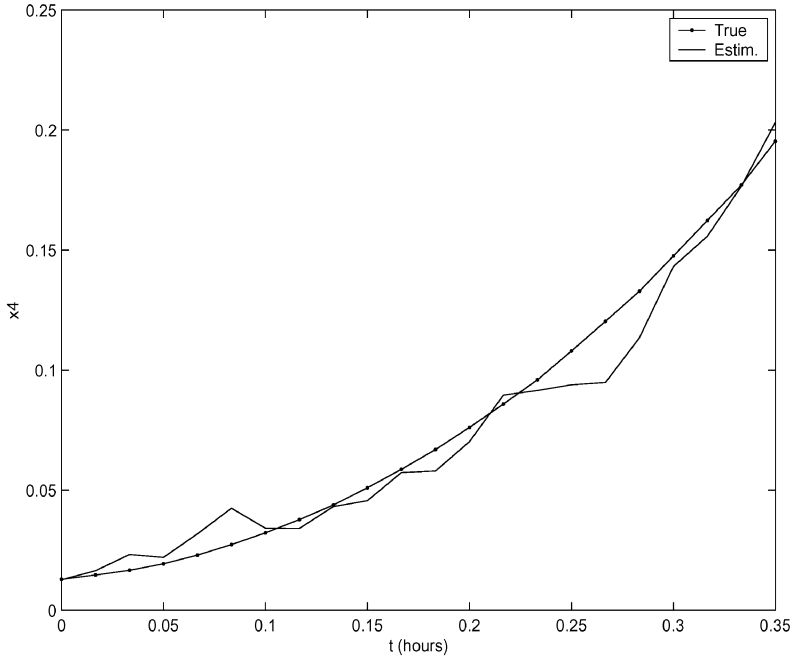

Fig. 7. True and estimated state x_4.

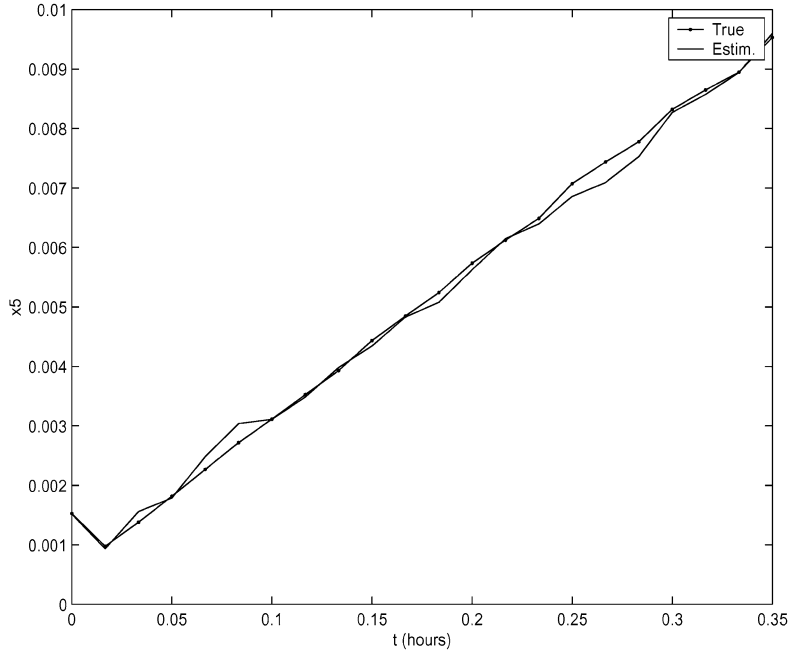

Fig. 8. True and estimated state x_5.

linear characteristics; (4) the temperatures of the cold and hot water streams are constant.

The model for the first tank is given by the following algebraic and differential equations:

$$Q_c = C_c v_c/100,$$

$$Q_h = C_h v_h/100,$$

$$Q_{o1} = K_1\sqrt{h_1 - h_2},$$

$$\frac{\mathrm{d}h_1}{\mathrm{d}t} = (Q_c + Q_h - Q_{o1})/A_1,$$

$$\frac{\mathrm{d}T_1}{\mathrm{d}t} = [Q_c(T_c - T_1) + Q_h(T_h - T_1)]/(A_1 h_1), \tag{27}$$

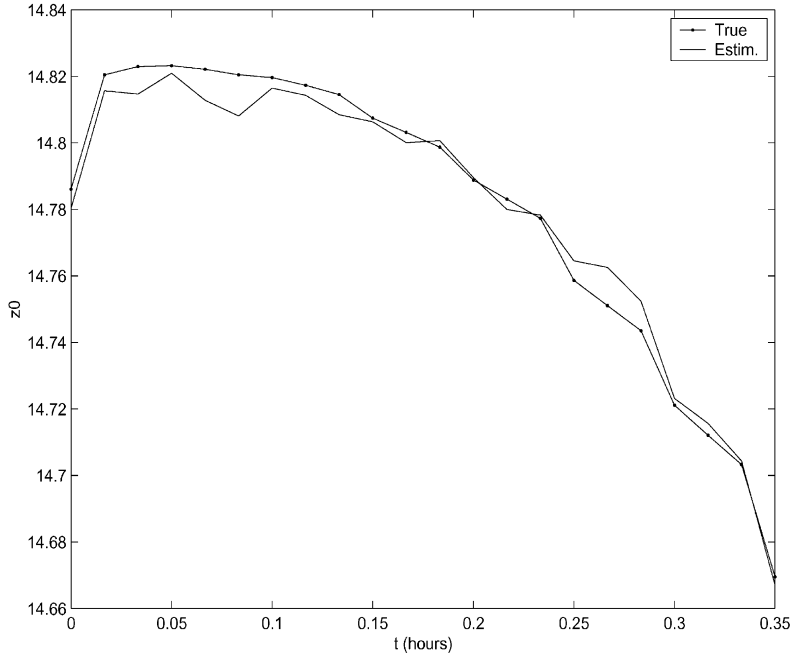

Fig. 9. True and estimated algebraic state z_0.

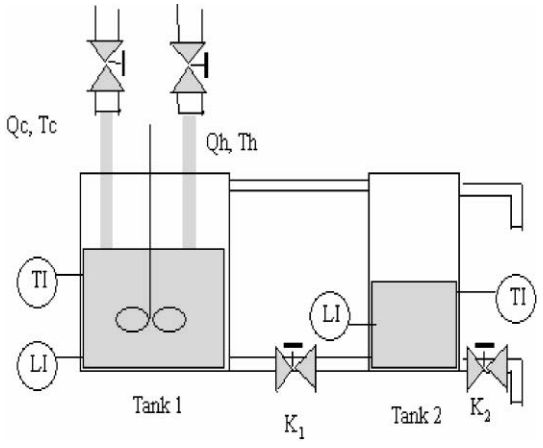

Fig. 10. Schematic diagram of the mixing process.

where v_c is the opening of the cold water control valve (%), v_h is the opening of the hot water control valve (%), C_c is the constant of the cold water control valve (cm^3/s %), C_h is the constant of the hot water control valve (cm^3/s %), Q_c is the cold water flow rate (cm^3/s), Q_h is the hot water flow rate (cm^3/s), Q_{o1} is the outlet flow rate from tank 1 (cm^3/s), h_1 is the liquid level in tank 1 (cm), T_1 is the liquid temperature in tank 1 (°C), T_c is the temperature of the cold water stream (°C), T_h is the temperature of the hot water stream (°C), K_1 is the restriction of the interconnection valve and pipe ($cm^{5/2}/s$), A_1 is the cross-sectional area of tank 1 (cm^2).

The model for the second tank is given by the following algebraic and differential equations:

$$Q_{o2} = K_2\sqrt{h_2},$$

$$\frac{dh_2}{dt} = (Q_{o1} - Q_{o2})/A_2, \tag{28}$$

$$\frac{dT_2}{dt} = Q_{o1}(T_1 - T_2)/(A_2 h_2),$$

where Q_{o2} is the outlet flow rate from tank 2 (cm^3/s), h_2 is the liquid level in tank 2 (cm), T_2 is the liquid temperature in tank 2 (°C), K_2 is the restriction of the tank 2 outlet valve and pipe ($cm^{5/2}/s$), A_2 is the cross-sectional area of tank 2 (cm^2).

The measurement vectors for each module were: $\mathbf{y}_{m,1} = [h_1, T_1]^T$ and $\mathbf{y}_{m,2} = [h_2, T_2]^T$.

The following values were used for the model parameters: $A_1 = 289\ cm^2$, $A_2 = 144\ cm^2$, $C_c = 280.0\,cm^3/s\,\%$, $C_h = 100.0\ cm^3/s\ \%$, $T_c = 20°C$, $T_h = 72°C$, $K_1 = 30\ cm^{5/2}/s$, $K_2 = 30\ cm^{5/2}/s$. The areas A_1 and A_2 could be physically measured, the parameters C_c, C_h, T_c, and T_h were guessed based on the experimental conditions, and the parameters K_1 and K_2 were experimentally measured in previous research (Zhang, 1991).

The modules were integrated using DASSL (Petzold, 1983). Notice that both modules are DAE's that may be reduced to ODE's by direct substitution. An advantage of the DAE approach is that the solution automatically provides estimates of unmeasured algebraic states, such as the flows in this case.

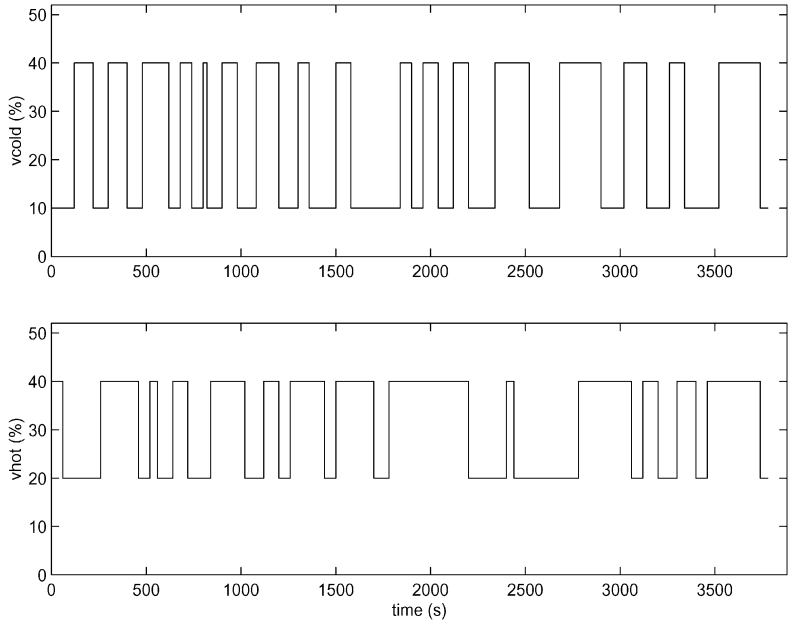

Fig. 11. Opening of cold and hot water valves.

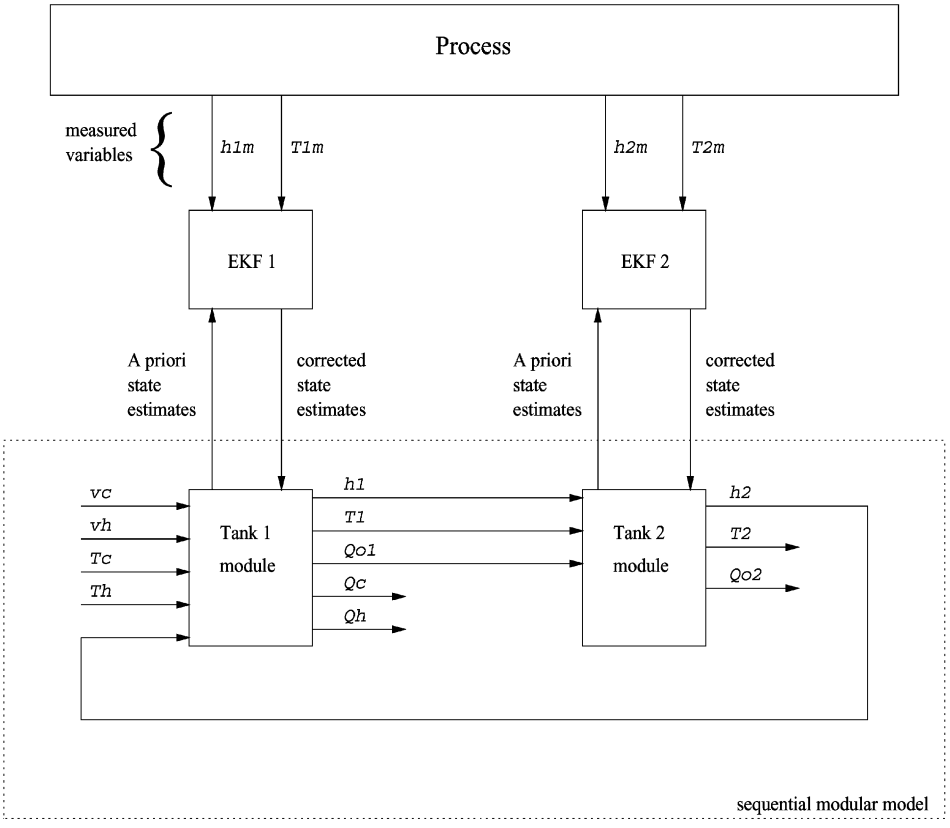

Fig. 12. A bank of estimators applied to the sequential modular model of the mixing process.

The model integration used the parallel approach, which is very simple as it does not require the definition of tear variables or iterations, and can be described as follows:

1. *Initialization*: Initialize all states, inputs and outputs at every module. A common integration horizon H is specified (in this case $H = 1$ s). Set the simulation time $t = 0$.

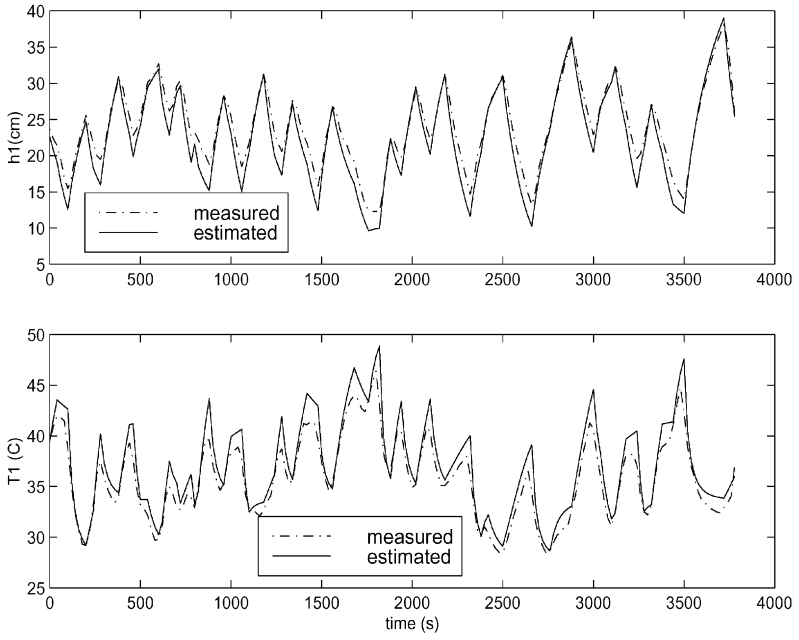

Fig. 13. Open-loop observer: Measured and estimated outputs of tank 1.

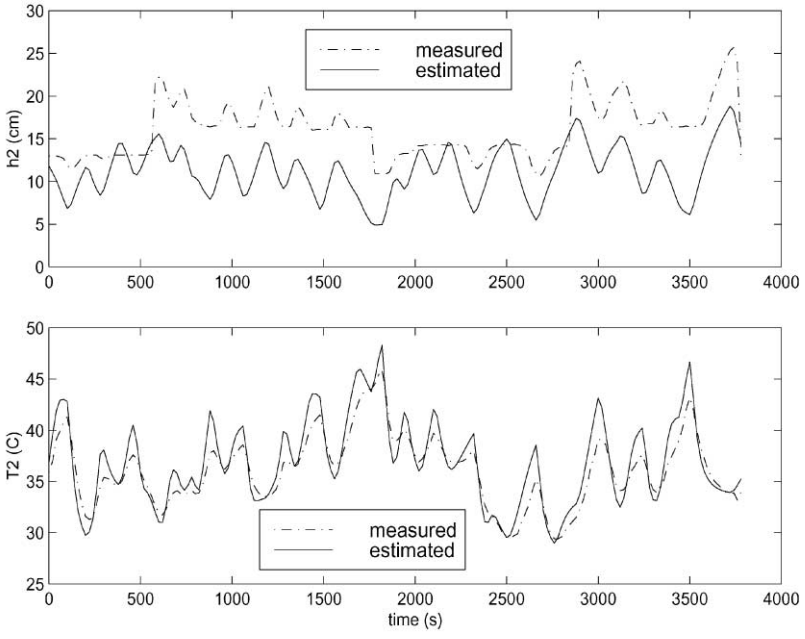

Fig. 14. Open-loop observer: Measured and estimated outputs for tank 2.

2. The scheduler predicts, reads or calculates the independent input variables at time t. In this case these variables are the opening of the cold and hot water valves v_c and v_h, and the temperatures of the cold and hot water streams T_c and T_h.
3. For each module:

(a) The scheduler sets the input of the module based on the independent variables and the outputs of other modules. In this case, the inputs to module 1 (tank 1) were v_c, v_h, T_c, T_h, and h_2. The inputs to module 2 (tank 2) were h_1, T_1 and Q_{o1} (see Fig. 12).

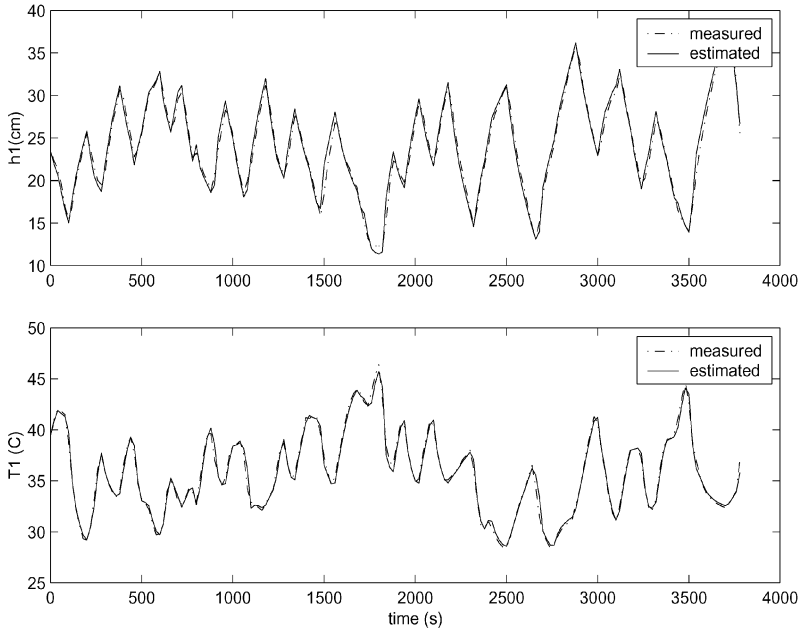

Fig. 15. Measured and estimated outputs for tank 1.

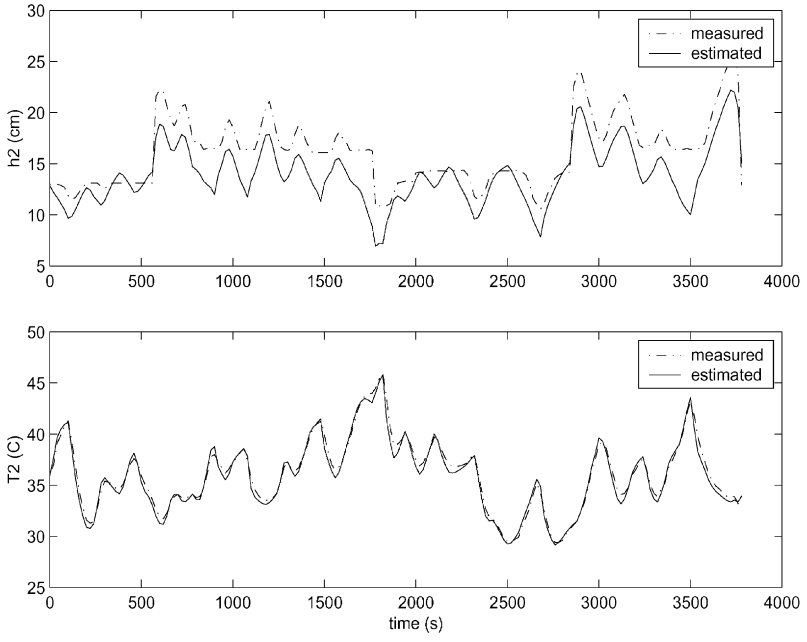

Fig. 16. Measured and estimated outputs for tank 2.

(b) Integrate the module over the required time period $[t, t+H]$. It is assumed that the inputs to the module remain constant during this integration period. In this case, both modules were DAE's and the routine DASSL was used to carry out the integration.

4. Set $t = t + H$ and go back to Step 2.

Figs. 13 and 14 show the response of the model acting as an open-loop observer, compared with the measured variables. Notice the large differences between the estimates and the measurements of the liquid level of tank 2 (see below), as opposed to the close agreement between measurements and estimates in the other three variables.

Two extended Kalman filters were used, one associated with each tank. The following tuning values were used for the two EKF's: $\mathbf{P}_{0,1} = \mathrm{diag}(0.05, 0.05)$, $\mathbf{Q}_1 = \mathrm{diag}(0.002, 0.002)$, $\mathbf{R}_1 = \mathrm{diag}(0.004, 0.004)$, $\mathbf{P}_{0,2} = \mathrm{diag}(0.05, 0.05)$, $\mathbf{Q}_2 = \mathrm{diag}(0.002, 0.002)$, $\mathbf{R}_2 = \mathrm{diag}(0.004, 0.004)$. The diagonal elements of the initial-state error covariance matrices $\mathbf{P}_{0,1}$ and $\mathbf{P}_{0,2}$ were chosen to reflect

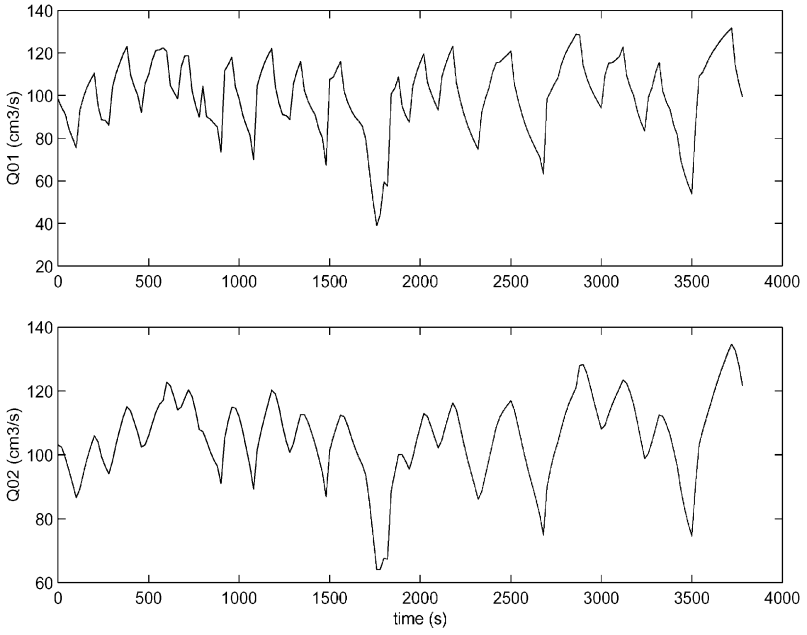

Fig. 17. Estimated values of the unmeasured outlet flow rates.

some uncertainty in the initial-state estimates. The diagonal elements of the process noise covariance matrices $\mathbf{Q}_1$ and $\mathbf{Q}_2$ were chosen greater than zero to reflect the uncertainty on the model used and to prevent the state error covariance from becoming zero. The diagonal elements of the output noise covariance matrices $\mathbf{R}_1$ and $\mathbf{R}_2$ were chosen to reflect the accuracy of the measurements.

Figs. 15 and 16 show the resulting output estimates compared with the measured variables. Notice again the large differences in the liquid level of tank 2. Fig. 17 shows the estimates of the unmeasured outlet flow rates from tanks 1 and 2.

The results indicate that the either measurement or the model are probably in error for h_2, see Figs. 14 and 16. It is however difficult to decide which is wrong without having a redundant measurement.

5. Conclusions

In this paper a method has been presented for the state estimation of nonlinear systems described by a class of differential-algebraic models, using the extended Kalman filter. A time-varying linearisation has been derived for a semi-explicit index one DAE. A simplified square root EKF algorithm has been introduced, and its integration with the DAE model has been described.

A simulation study has been carried out using a DAE model of a batch chemical reactor, consisting of six differential equations and four algebraic equations. This example illustrates how the EKF can be used for noise filtering and the estimation of unmeasured states, including algebraic states, of a system described by a semi-explicit index one DAE.

Furthermore, a study has been presented using experimental data obtained from a mixing process, together with a sequential modular model consisting of two index one DAE's. It was shown how a bank of estimators can be used in conjunction with this sequential modular model in particular to overcome the difficulties in applying a single estimator to the whole model.

Acknowledgements

This work was supported by the UK EPSRC, Grant No. GR/L64478. The authors are grateful to Aspentech Ltd. for supplying the process simulation software Aspen-OTISS™ that was used in this work.

References

Albuquerque, J. S., & Biegler, L. T. (1997). Decomposition algorithms for on-line estimation with nonlinear models. *Computers in Chemical Engineering*, *21*, 283–299.

Becerra, V. M., Roberts, P. D., & Griffiths, G. W. (1999). Dynamic data reconciliation for a class of nonlinear differential algebraic equation models using the extended Kalman filter. *Proceedings of the 14th IFAC world congress 1999*, Vol. L. Beijing, China (pp. 303–308).

Biegler, L. T., Damiano, J. J., & Blau, G. E. (1986). Nonlinear parameter estimation, a case study comparison. *A.I.CH.E. Journal*, *32*(1), 29–45.

Brenan, K. E., Campbell, S. L., & Petzold, L. R. (1996). *Numerical solution of initial value problems in differential-algebraic equations*. Philadelphia, PA: SIAM.

Campbell, S. L. (1995). Linearization of DAE's along trajectories. *Zeit schrift fur Angewandte Mathematik und Physik*, *46*(1), 70–84.

Cheng, Y. S., Mongkhonsi, T., & Kershenbaum, L. S. (1997). Sequential estimation for nonlinear differential and algebraic systems — theoretical development and application. *Computers in Chemical Engineering*, *21*(9), 1051–1067.

Chisci, L., & Zappa, G. (1992). Square root Kalman filtering of descriptor systems. *Systems and Control Letters*, *19*(4), 325–334.

Hillstad, M., & Hertzberg, T. (1986). Dynamic simulation of chemical engineering systems by the sequential modular approach. *Computers in Chemical Engineering*, *10*(4), 377–388.

Leineweber, D. B., Bock, H. G., Schlöder, J. P., Gallitzendörfer, J. V., Schäfer, A., & Jansohn, P. (1997). *A boundary value problem approach to the optimisation of chemical processes described by DAE models*. Technical Report 97-2, IWR, University of Heidelberg, Heidelberg, Germany.

Maybeck, P. S. (1982). *Stochastic models, estimation and control*. New York: Academic Press.

Nikoukhah, R., Willsky, A., & Levy, B. C. (1992). Kalman filtering and Riccati equations for descriptor systems. *IEEE Transactions on Automatic Control*, *37*(9), 1325–1342.

Noble, B., & Daniel, J. W. (1988). *Applied linear algebra*. New York: Prentice-Hall.

Pantelides, C. C., Gritsis, D., Morison, K. R., & Sargent, R. W. H. (1988). The mathematical modelling of transient systems by differential-algebraic equations. *Computers in Chemical Engineering*, *12*(5), 454–459.

Park, P., & Kailath, T. (1995). New square root algorithms for Kalman filtering. *IEEE Transactions on Automatic Control*, *40*(5), 895–899.

Petzold, L. R. (1982). Differential/algebraic equations are not ODE's. *SIAM Journal of Science and Statistical Computing*, *3*(3), 367–384.

Petzold, L. R. (1983). A description of DASSL, a differential-algebraic system solver. In R.S. Stepleman et al. (Eds.), *Scientific computing* (pp. 65–68). Amsterdam: North-Holland.

Tjoa, I. B., & Biegler, L. T. (1991). Simultaneous solution and optimization strategies for parameter estimation of differential-algebraic equation systems. *Industrial and Engineering Chemistry Research*, *30*(2), 376–385.

Zhang, J. (1991). *Expert systems in on-line process control and fault diagnosis*. Ph.D. thesis, City University, London, UK.

Zimmer, G., & Meier, J. (1997). On observing nonlinear descriptor systems. *Systems and Control Letters*, *32*(1), 43–48.