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Incorporating delayed and infrequent measurements in Extended Kalman Filter based nonlinear state estimation

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ABSTRACT

This work deals with state estimation in the presence of delayed and infrequent measurements. While most measurements (referred to as *secondary* measurements) are available frequently and instantaneously, there might be a delay associated with acquiring other measurements (*primary* measurements) due to long analysis times involved. The primary measurements are usually sampled at irregular intervals and the exact delay is also unknown. The traditional fixed-lag smoothing algorithm, which has been applied for a variety of chemical processes systems, can be computationally inefficient for such situations and alternate methods to handle delays are necessary. In this paper, we analyze several existing methods to incorporate measurement delays and reinterpret their results under a common unified framework (for Extended Kalman Filter). Extensions to handle time-varying and uncertain delays, as well as out of sequence measurement arrival are also presented. Simulation studies on a linear distillation column and a nonlinear polymerization reactor are used to compare the performance of these methods based on RMSE values and computation times. A large scale nonlinear reactive distillation column example is also used to illustrate the practicality of the suggested method.

1. Introduction

The idea of incorporating delayed measurements within a Kalman filter framework has been well recognized in the automation industry. In tracking and navigation systems significant time delays get introduced due to complexity of computation or collisions from multiple sensors reporting data to the estimator. The sampling times are of the order of milliseconds and methods proposed in literature to handle delays [2,10,24,9,23,20] primarily rely on fusing the information from the delayed measurement directly into the filter once it arrives.

In chemical process systems, the problem of handling delayed measurements usually arises due to delays in measurement of certain "quality" variables. These measurements (called primary measurements) are sampled infrequently and are available with a delay, while other variables are measured frequently and the measurements are available instantaneously (secondary measurements). For example, in distillation columns the distillate and bottoms compositions often need to be analyzed in a laboratory as the use and maintenance of online analyzers is infeasible due to economic considerations, whereas *secondary measurements* such as tray temperatures are obtained frequently without any time delay. The primary variables are therefore *inferred* from the temperature measurements, which might be inaccurate due to model errors (plant-model mismatch), sensor bias or unmodeled disturbances. In such cases the primary measurements, which are available with a delay due to offline assays, need to be incorporated accurately into the estimator.

Time delays in multi-rate estimation have often been handled in literature for process systems using suitable augmentation of the states. Gudi et al. [7,8] applied multi-rate state estimation techniques with delayed measurements for a fermentation process in a bioreactor. Tatiraju et al. [21] investigated estimation strategies for a polymerization reactor in the presence of delayed measurements of the molecular weight distribution. Mutha et al. [13,14] proposed an algorithm for multi-rate state estimation in a polymerization reactor, that compensates for the slow measurements by making repeated use of the available slow measurements. Amirthalingam et al. [3] augmented the state with past measurements to handle delays in primary measurement for an identified linear model.

The state augmentation approach has been favored in the chemical and biochemical processes because the state-space formulation is retained, which simplifies the extension of delay-handling methods to other approaches, such as moving horizon estimation (MHE) [18,17], nonlinear dynamic data reconciliation (NDDR) [22], Unscented Kalman Filter (UKF), particle filters, etc. In process systems literature, the so-called fixed-lag smoothing algorithm [6] is most popular. Another popular method is to recalculate the filter

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for the entire delay period when the primary measurement arrives [16,11]. In most examples, the time delay for primary measurement was of the order of a few sampling periods (usually one or two samples), was assumed to be constant and known beforehand. Extension to uncertain delays, while conceptually straightforward, has not received enough attention. When time delay is large and/or unknown, both fixed-lag smoothing and filter recalculation methods result in expensive computations. This necessitates the use of alternate methods that can handle irregular and time-varying delays efficiently.

The aim of this paper is to present a critical analysis and to assess through simulation studies the relative merits of various methods to handle measurement delays in multi-rate estimation using Extended Kalman Filter (EKF) for process systems. Since these methods were presented in various different types of applications, presenting them in a unified framework is another aim of this work. We also propose to categorize these methods into two groups: methods that fuse delayed measurements on arrival, and methods that rely on state augmentation. The issue of variable and uncertain time delays is also addressed through a case study of 88-state nonlinear example (Case Study 3). Extension of state augmentation to handle out-of-sequence measurements as well as arrival of multiple measurements at the same time are also provided.

The paper is organized as follows. Section 2 describes the basic system and filter equations in the presence of delayed measurements. In Section 3 various methods to handle measurement delays within the EKF framework are presented. Section 4 presents three case studies for incorporating infrequent delayed measurements: linear example; a simple nonlinear example; and a practical example of a large (88 state) reactive distillation column. Section 5 lists the conclusions and future scope for work.

2. State estimation problem

In this section, we first review standard EKF for a discrete-time nonlinear system. The various methods for handling delays in primary measurement arrival are discussed in the subsequent section.

2.1. System model

Consider the following discrete-time nonlinear system:

$$X(k+1) = f_h(X(k), U(k)) + \varepsilon(k) \tag{1a}$$

$$Y(k) = g(X(k)) + \nu(k) \tag{1b}$$

where $X(k) \in R^n$, $U(k) \in R^l$ and $Y(k) \in R^m$ are the state, input and output variables, respectively. The two noise sources $\varepsilon(k)$ and $\nu(k)$ are assumed to be normally distributed white noise sequences with zero mean and covariance matrices Q and R, respectively. They are also assumed to be independent of each other. Since the contribution of this work is in handling measurement delays in infrequently sampled primary output variables, we have assumed a simpler case of *additive* state and measurement noise. Further, we have assumed $\varepsilon(k)$ and $\nu(k)$ to be white.

The equivalent linear state space model is:

$$\begin{aligned} X(k+1) &= A_k X(k) + B_k U(k) + \varepsilon(k) \\ Y(k) &= C_k X(k) + \nu(k) \end{aligned} \tag{2}$$

where we let system matrices (A_k, B_k, C_k) be time varying, in general.

2.2. Extended Kalman Filter

The Extended Kalman Filter (EKF) is an extension of KF to the nonlinear estimation problem. Starting with filtered state estimates

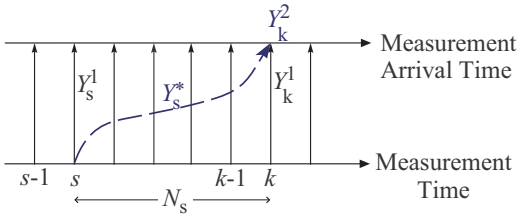

Fig. 1. System with delayed and infrequent primary measurements.

$\hat{X}(k-1|k-1)$ and its error covariance matrix $P(k-1\,|\,k-1)$, the filtered estimates for time k are computed recursively using the EKF equations as summarized below:

$$\hat{X}(k|k-1) = f_h(\hat{X}(k-1|k-1), U(k-1)) \tag{3}$$

$$\hat{X}(k|k) = \hat{X}(k|k-1) + K(k)(Y(k) - g(\hat{X}(k|k-1))) \tag{4}$$

The EKF uses the nonlinear model to compute the state estimates, whereas linear approximation is used for computing the estimate error covariance and the Kalman gain matrices. The Kalman gain matrix, $K(k)$, is given by

$$K(k) = P(k|k-1)C_k^T[C_k P(k|k-1)C_k^T + R]^{-1} \tag{5}$$

and the covariance matrices of errors in the estimates are obtained from:

$$P(k|k-1) = A_k P(k-1|k-1)A_k^T + Q \tag{6}$$

$$P(k|k) = [I - K(k)C_k]P(k|k-1) \tag{7}$$

In the above, A_k and C_k are computed by linearizing the nonlinear model (1) about the current estimate:

$$A_k = \left.\frac{\partial f_h}{\partial X}\right|_{\hat{X}(k-1|k-1),U(k-1)} \qquad C_k = \left.\frac{\partial g}{\partial X}\right|_{\hat{X}(k|k-1)}$$

For a linear system, the above equations reduce to the Kalman filter.

2.3. Delayed primary measurements

Fig. 1 shows a schematic representation of a process with infrequent and delayed primary measurements. Here, k is the current measurement instant, h is the sampling interval, $Y^1(k)$ represents secondary measurements and $Y^2(k)$ represents primary measurements. The time instant at which only secondary measurements become available is known as *minor measurement arrival instance* (or just "minor instance"), and when both primary and secondary measurements become available is known as *major instance*.

In Fig. 1, secondary measurements are represented as vertical arrows, since they are available immediately, without delay. The dashed arrow represents a primary measurement, s being the instance when its sample is taken. This measurement arrives with a delay of N_s intervals. Thus $k = s + N_s$ is a major instance, while $(k-1)$, $(k-2)$, etc. are minor instances. The primary variable is sampled infrequently; the next sample is taken at $s + M_s$, i.e., M_s denotes the number of intervals between two successive primary measurement samplings. The primary variable can be sampled at irregular intervals (M_s is time-varying) and the measurement delay could also vary (N_s is time-varying).

The output equation for secondary measurements is given as:

$$Y^1(k) = g^1(X(k)) + \nu^1(k) \tag{8}$$

Since the primary measurements arriving at time k are related to the state at time s, the output equation for primary measurements

is given by:

$$Y^2(k) = g^2(X(s)) + \nu^2(s) \quad \text{if} \quad k = s + N_s \tag{9}$$

We end this section by noting that the linearized form of the output Eqs. (8) and (9) are given by:

$$C_k^i = \left.\frac{\partial g^i(X)}{\partial X}\right|_{\hat{X}(k|k-1)} \qquad i = \{1, 2\} \tag{10}$$

3. State estimation with delays

For convenience of discussion, we have categorized the various methods for handling delayed measurements into two types: (i) methods that provide a procedure to fuse primary measurements when they arrive, and (ii) methods that rely on state augmentation. Methods in the first category are more popular in tracking and navigation systems than in process systems. We discuss all these methods in a common framework (of nonlinear system), and compare the accuracy and computational tractability of these methods using simulation examples.

3.1. Fusing primary measurements at measurement arrival

3.1.1. Filter recalculation

A straightforward extension of the EKF to handle delays in the primary measurements is to go back to the time step when the sample corresponding to the delayed measurement was taken, incorporate the measurement and recompute the entire trajectory of estimates till the current step [16].

When the primary variable is sampled at time instance s, the state estimate $\hat{X}(s|s-1)$ and covariance of prediction error $P(s\,|\,s-1)$ are stored. Until the arrival of this measurement at major instance $k = s + N_s$, all the secondary measurements $Y^1(s), \ldots, Y^1(k-1)$ are also stored. During this period, only the secondary measurements are fused at minor instances. At the major instance $k = s + N_s$, when both $Y^2(k)$ and $Y^1(k)$ arrive, the state estimates from time s to $s + N_s$ are recomputed. Note that the measurements $Y^1(s)$ and $Y^2(s + N_s)$ are used to update the estimates and their error covariance matrix at time s, and at subsequent time instances, the available secondary measurements are used in the update step.

The main drawback of this method is the large storage cost and computational burden, which increases rapidly as the recalculation period (N_s) becomes longer. This is especially true for nonlinear systems, where one needs to compute A_k and C_k at each sampling instant. This method is therefore impractical for online implementation.

3.1.2. Alexander's method

Alexander [2] proposed a method to handle delayed measurements which utilizes the idea of sequential processing of measurements. Sequential processing of two or more measurements can be performed provided their errors are statistically independent [12]. The measurements $Y^1(k)$ are first fused through the Kalman filter Eqs. (4)–(7), using C_k^1 and $g^1(\cdot)$ in place of C_k, and $g(\cdot)$, respectively. This results in the Kalman gain $K^1(k)$ and $P^1(k\,|\,k)$, which may then be used to compute state estimates $\hat{X}^1(k|k)$. At minor sampling instances, since only $Y^1(k)$ are available, we choose $\hat{X}(k|k) = \hat{X}^1(k|k)$ and $P(k\,|\,k) = P^1(k\,|\,k)$.

However, if the measurements $Y^2(k)$ are available *without any delay*, the Kalman gain and error covariance are updated as:

$$K^2(k) = P^1(k|k)C_k^{2\mathrm{T}}[C_k^2 P^1(k|k)C_k^{2\mathrm{T}} + R_2]^{-1} \tag{11}$$

$$P^2(k|k) = [I - K^2(k)C_k^2]P^1(k|k) \tag{12}$$

The error covariance $P^2(k\,|\,k)$ includes effects of both sets of measurements. The following correction can be added to the state estimates, at major instances, to *sequentially fuse* the measurements $Y^2(k)$:

$$\delta\hat{X}(k) = K^2(k)(Y^2(k) - C_k^2\hat{X}(k|k-1)) \tag{13}$$

If the measurements $Y^2(k)$ are delayed, they cannot be fused simply using (11)–(13). Alexander [2] exploited the fact that for a linear system, the error covariance (and therefore the Kalman gain) is dependent only on the variance of the error in the measurement, and not on the measured value. Thus, even though the primary measurement is not available immediately at time s, one could still use Eqs. (11) and (12) to update the Kalman gain and the error covariance as soon as the primary variable is sampled. Since $Y^2(s)$ is not available, the state estimates continue to be updated using only the secondary measurements. At the major instant ($s + N_s$), the primary measurement is available and the following correction term is added to the filtered state estimate:

$$\delta\hat{X}(s + N_s) = W_s K^2(s)(Y^2(k) - C_s^2\hat{X}(s|s-1)) \tag{14}$$

where $K^2(s)$ is the Kalman gain matrix at time instant s, updated under the assumption that the primary measurement is available immediately (Eq. (11)). Comparing (13) and (14), we note that the matrix W_s

$$W_s = \prod_{i=1}^{i=N_s}(I - K'(s+i)C_{s+i}^1)A_{s+i-1} \tag{15}$$

accounts for the measurement delay. In the above equation, $K'(k)$ is used to distinguish it from $K^1(k)$, where $k \in [s+1,\ s+N_s-1]$: K' implies the Kalman gain and error covariance are updated assuming the primary measurement arrives without a delay.[1] Therefore, the estimates are sub-optimal in this time interval. It can be shown, however, that the above correction gives the optimal state estimate at the major instance $s + N_s$ [2].

Alexander's approach was extended by Larsen et al. [10] for the case where the measurement error variance is unknown at the time when the primary variable was sampled. Alexander's and Larsen's approaches require only the correction term to be stored and requires minimal computational effort. The method can also be used for time varying delays, even if the delay is not known a priori.

3.1.3. Method of parallel filters

Alexander's method gives sub-optimal estimates during the time interval $[s+1,\ s+N_s-1]$ as explained in the preceding section. Optimal estimates can be obtained even during this interval by running another filter in parallel with the current filter, as suggested in [10]. At the sampling instant s, a filter can be started using the updated Kalman gain and error covariance matrix as in Alexander's method. This filter is used only to build up the correct terms ($K'(k)$ and W_s) needed for an optimal measurement update at the major instance. However, during the interim period the second filter, $K^1(k)$, whose Kalman gain and error covariance are updated at time s using only the secondary measurement, will generate optimal estimates when fusing secondary measurements. At time $s + N_s$, the correctly fused optimal estimate of the first filter (which incorporated the delayed measurement) and its covariance is used to re-initialize the second filter. Using this approach optimal estimates are available at all times.

In summary, for $k \in [s,\ s+N_s-1]$, only $K'(k)$ is computed in Alexander's method, whereas both $K'(k)$ and $K^1(k)$ (and

[1] In other words, $K'(k)$ is computed with $P(s\,|\,s) = P^2(s\,|\,s)$, whereas $K^1(k)$ is computed with $P(s\,|\,s) = P^1(s\,|\,s)$.

the corresponding error covariances) are computed in this method.

3.2. State augmentation based methods

These methods rely on augmenting the current state with appropriate past information required for fusing the effect of delayed measurements. The augmented state vector will be represented as $Z(k)$. The state update equation for a linear system can be written in the standard forms as:

$$Z(k+1) = \Phi_k Z(k) + \Gamma_k U(k) + \Psi_k \varepsilon(k) \tag{16a}$$

The measurement equations are given by:

$$Y^1(k) = \Xi_k^1 Z(k) + \nu^1(k) \tag{16b}$$

$$Y^2(k) = \Xi_k^2 Z(k) + \nu^2(s) \tag{16c}$$

State space matrices Φ_k, Γ_k, $\Psi_k Q \Psi_k^T$ and Ξ_k are used in place of A_k, B_k, Q and C_k, respectively, in Eqs. (5)–(7).

Our discussion in this section will be based on a linear model of the above form. For a nonlinear system, the EKF uses the *original nonlinear model* (1) to compute the one-step-ahead prediction (3) and the corrected estimate in (4). For this purpose, the estimates of the original state $\hat{X}(\cdot)$ are obtained by extracting the first n elements of augmented state $\hat{Z}(\cdot)$, i.e.,

$$\hat{X}(\cdot) = [I_{n\times n} \quad 0 \quad \cdots \quad 0]\hat{Z}(\cdot) \tag{17}$$

It is straightforward to see that this state estimate is used to compute $f_h(\hat{X}(k-1|k-1), U(k-1))$ and $g(\hat{X}(k|k-1))$.

The main advantage with all the state augmentation methods is that they retain the 'state-space' description of the system and can be extended to other filters, such as UKF, MHE or particle filters, in a straight forward manner.

3.2.1. Fixed-lag smoothing

The fixed-lag smoothing algorithm is well documented in literature [4,6]. Since the delayed primary measurement affects all states between measurement time s and measurement arrival time $(s+N_s)$, all the information is stored by augmenting the current state with the past N_s states. The augmented state vector is given by:

$$Z(k) \triangleq [X^T(k) \quad X^T(k-1) \quad \cdots \quad X^T(k-N_s)]^T \tag{18}$$

For this augmented state,

$$\Phi_k = \begin{bmatrix} A_k & 0 & \cdots & 0 & 0 \\ I & 0 & \cdots & 0 & 0 \\ 0 & I & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & I & 0 \end{bmatrix} \quad \Gamma_k = \begin{bmatrix} B_k \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$\Psi_k = \begin{bmatrix} I \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \begin{bmatrix} \Xi_k^1 \\ \Xi_k^2 \end{bmatrix} = \begin{bmatrix} C_k^1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & C_s^2 \end{bmatrix} \tag{19}$$

are used to compute Kalman gain and covariance matrices as per (5)–(7).

This method results in smoothing of the past N_s states based on the secondary measurements at the minor time instance. When the delayed primary measurement arrives, both primary and secondary measurements are used to obtain smoothed estimates from s to $s+N_s$.

In case the exact delay is unknown and is time varying, the system can be augmented with the past $N_{\max}$ states where $N_{\max}$ is the maximum possible delay. The measurement equation can be appropriately modified since the actual delay $N_s \le N_{\max}$ will be known at the major instance. The major drawback with this method, however, is the excessive computational load. Since the smoothed estimates are obtained at every sampling instance, the computational load is greater than the filter recalculation method discussed in the previous section.

3.2.2. Measurement augmentation

Often, the number of primary measurements is less than the state dimension. If smoothed estimates of all the states within the delay period are not required (as is the case in most online control and fault detection problems), we only need information about the effect of states on the primary measurements. Therefore, it is sufficient to augment the current state with a transformation given by the measurement model of primary variables for the previous $N_{\max}$ time steps. In this method, the augmented state is given in [5,3] by:

$$Z(k) \triangleq [X^T(k) \quad Y^{*T}(k) \quad \cdots \quad Y^{*T}(k-N_s)]^T \tag{20}$$

where, the transformed state for a linear measurement model is given by

$$Y^*(k) = C_k^2 X(k) \tag{21}$$

Here * indicates the primary output *as if* it were available without any delay or measurement noise. The augmented model is in the same form as (16), with

$$\Phi_k = \begin{bmatrix} A_k & 0 & \cdots & 0 & 0 \\ C_k^2 A_k & 0 & \cdots & 0 & 0 \\ 0 & I & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & I & 0 \end{bmatrix} \quad \Gamma_k = \begin{bmatrix} B_k \\ C_k^2 B_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$\Psi_k = \begin{bmatrix} I \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \Xi_k = \begin{bmatrix} C_k^1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & I \end{bmatrix} \tag{22}$$

The size of the augmented system matrices are smaller than in the state augmentation approach, while being able to maintain the same information. The dimension of the state is now $n + m_2 \times N_s$. However, the computational load can still be significant for large values of N_s.

3.2.3. Sample-state augmentation

Since the delayed measurement is a function of the state $X(s)$, only the information of this state needs to be kept until the measurement arrival time. Instead of augmenting the state with the previous N_s states, it is sufficient to augment the state with the one at time s, when the primary measurement is sampled [23].

The state vector at any time k is augmented with the lagged state $X(s)$:

$$Z(k) \triangleq [X^T(k) \quad X^T(s)]^T \tag{23}$$

where

$$\Phi_k = \begin{bmatrix} A_k & 0 \\ 0 & I \end{bmatrix} \qquad \Gamma_k = \begin{bmatrix} B_k \\ 0 \end{bmatrix} \qquad \Psi_k = \begin{bmatrix} I \\ 0 \end{bmatrix} \qquad \Xi_k = \begin{bmatrix} C_k^1 & 0 \\ 0 & C_s^2 \end{bmatrix} \tag{24}$$

Thus, when the primary variable is sampled, the augmented state estimate is given by:

$$\hat{Z}(s) \triangleq \begin{bmatrix} \hat{X}(s|s) \\ \hat{X}(s|s) \end{bmatrix}. \tag{25}$$

The covariance of the augmented estimate errors is therefore:

$$P^{\text{aug}}(s|s) \triangleq \begin{bmatrix} P(s|s) & P(s|s) \\ P(s|s) & P(s|s) \end{bmatrix} \tag{26}$$

The Kalman filter designed for the augmented process model will therefore update both the current state and the lagged state $X(s)$ during the measurement delay. This can be viewed as a fixed-point smoothing of the lagged state, $X(s)$, using the future measurements $Y^1(s)$, $Y^1(s+1)$, …, $Y^1(s+N_s-1)$. When the delayed measurement arrives at $(s+N_s)$, it is fused with the smoothed estimate of $X(s)$ using Ξ_k as defined in (24). After the primary measurement is optimally fused at $(s+N_s)$, the lagged state $X(s)$ is no longer required and the state is "unaugmented" (i.e., $Z(k) \triangleq X(k)$). If two samples are taken before a measurement arrives, $Z(k)$ would be further augmented with the state at the next sampling instant $s+M_s$.

It has to be noted that the system (Φ_k, Ξ_k^1) is also observable due to the constraint that the sampled state $X(s)$ (which augments the current state) is equal to the current state at time s (as given in Eq. (25)). This method is applicable to the case of uncertain and time-varying delays. The information of the maximum possible delay N_{max} is not required in defining the augmented states.

4. Case studies

The performance of the methods described in the preceding section are compared through three simulation examples. The first is a linear system, which is used to show the equivalence between the estimates provided by the various methods for a linear time invariant (LTI) system. The second example is used to compare the performance of the state estimation methods for a representative nonlinear example. Finally, a large scale reactive distillation column with four species and 22 stages (i.e., 88 states) is used to illustrate the practicality of the chosen method (sample state augmentation). This example also demonstrates the flexibility of this method to handle uncertainty in delay time and the case when the next sample of the primary variable is taken before the arrival of the measurement of the previous sample ($N_s > M_s$). All simulations are done on an Intel Core 2 CPU with 1.73 GHz and MATLAB 7.2.0.

4.1. Linear example

Consider the following discrete-time linear model:

$$X(k+1) = \begin{bmatrix} 0.8499 & 0.0350 & 0.0240 & 0.0431 \\ 1.2081 & 0.0738 & 0.0763 & 0.4087 \\ 0.7331 & 0.0674 & 0.0878 & 0.8767 \\ 0.0172 & 0.0047 & 0.0114 & 0.9123 \end{bmatrix} X(k) + \varepsilon(k) \tag{27}$$

$$Y^1(k) = \begin{bmatrix} 0 & -55.43 & 0 & 0 \\ 0 & 0 & -34.12 & 0 \end{bmatrix} X(k) + \nu^1(k) \quad \forall k \tag{28}$$

$$Y^2(k) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} X(s) + \nu^2(s) \quad \text{if } k = s + N_s \tag{29}$$

This model is obtained by linearizing the nonlinear binary distillation column model of [19]. The state $X = [x_1 x_2 x_3 x_4]^T$ comprises of tray compositions; tray temperatures $Y^1 = [T_2 T_3]^T$ form the secondary measurements and distillate and bottoms composition form primary measurements Y^2.

For this case study, the process is initially at an unsteady state of

$$X(0) = [0.5 \quad 0.5 \quad 0.5 \quad 0.5]^T$$

and the estimator is given an initial guess

$$\hat{X}(0) = [0.2 \quad 0.4 \quad 0.6 \quad 0.8]^T.$$

The process model error covariance, Q, and the initial error in each of the estimates, $P(0)$, are chosen as 10^{-6}. The measurement noise variances are $R_1 = 0.5(^\circ\text{C})^2$ for temperature measurements (secondary), and $R_2 = 10^{-6}$ for composition measurements (primary).

Two different scenarios are considered: scenario A, when there are no primary measurements and the estimates are based only on the secondary temperature measurements and scenario B, when the primary measurements are also included. In scenario B, starting at $t = 1$ min, concentration measurements are taken every 12 min ($M_s = 12$) and available with a delay of 10 min ($N_s = 10$). Both N_s and M_s have been kept constant for ease of comparison. In general, they can be time varying and this is presented in Section 4.3. Fig. 2 shows the tray compositions (estimates and true plant) for the two scenarios. Because of an incorrect initial guess for the compositions, the estimates take around 40 min to reach the plant value in scenario A. In scenario B, the tray compositions are tracked much earlier with the primary measurements also included, in spite of the measurement delay. A noticeable decrease in the estimation error can be observed when the primary measurement arrives (see estimates of x_3 at 11 min).

Averaged root mean square error (RMSE) values and the simulation time taken per sampling instant ($h = 1$ min) are reported for different methods in Table 1. Each simulation was run for a period of 200 min and the results are averaged for 100 such realizations of the noise sequences. Of all methods considered, Alexander's method, which makes an approximation for the error covariance shows a higher RMSE value. All other methods provide exactly the same state estimates (indicated by the same RMSE values) for a linear system.

The fixed-lag smoothing method – perhaps the most popular method in literature for handling delays – is the worst in terms of computational time required, since it involves augmenting the state with past N_s states. Output augmentation fares much better since the state dimension increases to $n + N_s m$ (where m is the output dimension). In several chemical engineering examples, m is much smaller than n, in which case, output augmentation will be more attractive. Alexander's method, which involves no state augmentation has the lowest computational requirement, whereas running parallel filters increases the computational requirement as expected. Finally, the sampled state augmentation method fares better than other augmentation schemes as the state dimension increases to $2n$ during the interval between the sampling time and the measurement arrival time of the primary variable.

It should be noted that for this example, filter recalculation seems very attractive. The computational time required for filter recalculation over N_s steps only increases by a factor N_s. However, the additional computations for filter recalculation is done at major instances, which increases computational time at those instances significantly (without affecting it during minor instances). The situation would get worse for long delays (large N_s) or when the delayed measurements are frequent ($M_s < N_s$). Indeed, in situations like this *linear time invariant* example, filter recalculation is an attractive option. This analysis, though, changes for EKF in the nonlinear case: any method which involves additional integrations and Jacobian evaluations will require more time, as these also add a lot to the computational load.

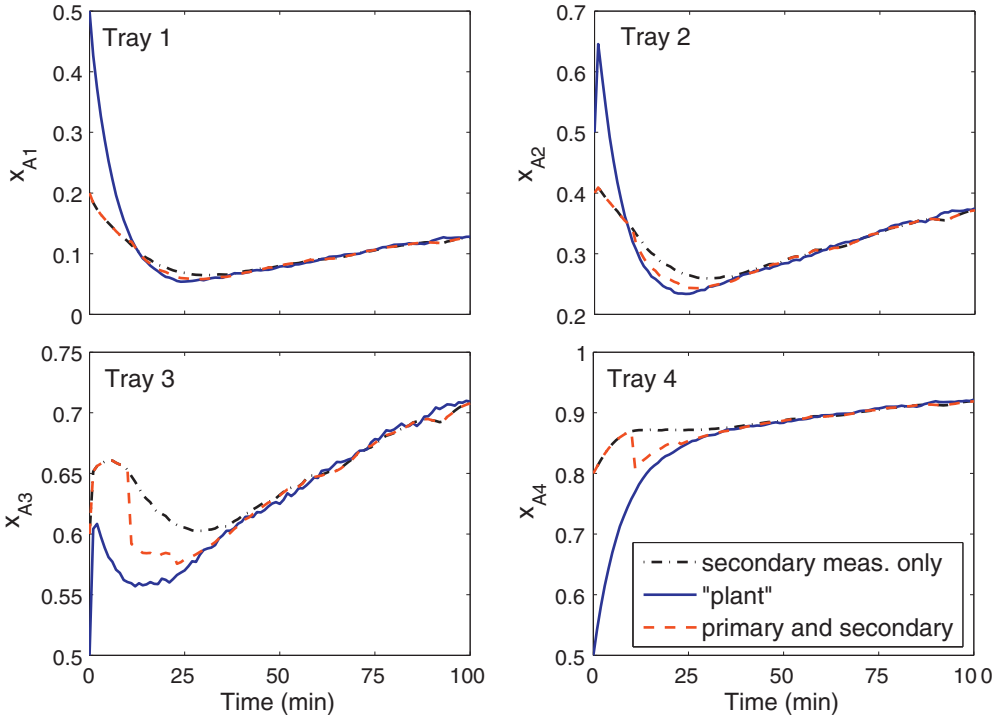

Fig. 2. Estimates of tray compositions for the linear distillation column example.

4.2. Nonlinear example: polymerization reactor

In this section, we compare the various methods using a nonlinear polymerization reactor example. Specifically, the example of free-radical polymerization of styrene in a jacketed stirred tank reactor, described in [21] is used to compare the state estimation methods. Material balances are written for concentrations of the initiator (C_i), monomer (C_m) and solvent (C_s), while energy balances account for the reactor and jacket temperatures (T and T_j). The volume of the CSTR is held constant. Finally, the model equations for 0th, 1st, and 2nd moments of the molecular weight distribution (represented as λ_0, λ_1, and λ_2) are written. Consequently, the state is defined as:

$$X \triangleq [C_i \quad C_s \quad C_m \quad \lambda_0 \quad \lambda_1 \quad \lambda_2 \quad T \quad T_j]^T.$$

The inlet feed to the CSTR consists of initiator, monomer and solvent streams. The inlet streams are all kept at 330 K, while the coolant is at 295 K. The resulting model equations are highly nonlinear. For the sake of brevity, we refer the reader to [21] for a detailed model of the process and the operating conditions.

A sampling time of $h = 1$ min is used. The model is expressed in the standard form: the nonlinear discrete-time state prediction is given by Eq. (1a). The two temperatures and the monomer concentration are measured frequently; thus,

$$Y^1(k) \triangleq [C_m \quad T \quad T_j]^T$$

Table 1
Comparison of different methods with respect to RMSE values and * computational time taken per sampling instant.

	Method	RMSE in X	Time*
1	Filter recalculation	6.7800×10^{-2}	0.20 ms
2	Alexander's method	6.8975×10^{-2}	0.17 ms
3	Parallel filters	6.7800×10^{-2}	0.23 ms
4	Fixed-lag smoothing	6.7800×10^{-2}	0.81 ms
5	Y^2 augmentation	6.7800×10^{-2}	0.37 ms
6	$X(s)$ augmentation	6.7800×10^{-2}	0.19 ms

Tatiraju et al. [21] showed that only four states (C_i, C_m, T, T_j) are observable from the secondary measurements. Thus, the primary measurements are required for obtaining reliable estimates of all the eight states. The measurement of the three moments of the molecular weight distribution require laboratory analysis. Hence, the primary variables

$$Y^2(k) \triangleq [\lambda_0 \quad \lambda_1 \quad \lambda_2]^T$$

are sampled *infrequently* at irregular intervals between 30 and 60 min (i.e., $30 \le M_s \le 60$ varies randomly) and the measurements are available after an uncertain delay of 30–60 min (i.e., $30 \le N_s \le 60$ also varies randomly).

The estimator performances are compared for the estimator settings and initial conditions are given in Table 2. The measurement noise is generated as independent white noise sequences, with covariances of

$$R_1 = \mathrm{diag}[10^{-4} \quad 1 \quad 1]$$
$$R_2 = \mathrm{diag}[10^{-14} \quad 10^{-6} \quad 10^{6}].$$

In this example, state noise is not added in the plant simulations. However, state noise uncertainty is considered in the estimator, with the covariance of the white noise given by:

$$Q = \mathrm{diag}[10^{-8} \quad 10^{-4} \quad 10^{-4} \quad 10^{-8} \quad 10^{-4} \quad 10^{6} \quad 1 \quad 1]$$

Fig. 3 shows the estimates of the number-average and weight-average molecular weights

$$M_n = \frac{\lambda_1}{\lambda_0} \qquad M_w = \frac{\lambda_2}{\lambda_1}, \tag{30}$$

which are the important quality variables for the polymerization process. The circles represent measurements if they were available without any delay and the dots represent the actual measurements when they arrive. Thus, the horizontal distance between open circles and dots is the (uncertain) measurement delay. For example, the arrow in the lower panel shows that the measurement that was sampled at $t = 132$ min is available at $t = 183$ min. The delayed measurements of the leading moments of the distribution help

Table 2
Variables used for the nonlinear polymerization example.

Variable	C_i	C_s	C_m	λ_0	λ_1	λ_2	T	T_j
$X(0)$	5×10^{-2}	5	3	2×10^{-4}	1	5×10^{2}	330	295
$\hat{X}(0)$	2.5×10^{-2}	4	4	5×10^{-4}	5	5×10^{4}	330	295
$P(0)$	10^{-8}	10^{-4}	10^{-4}	10^{-12}	10^{-4}	10^{6}	1	1

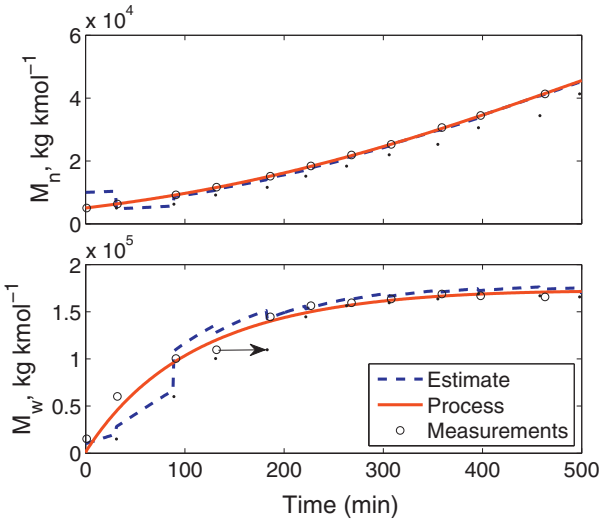

Fig. 3. Actual and estimated values of number- and weight-averaged molecular weights. The dots represent actual measurements when they arrive, whereas the circles denote measured quantities at the time they were sampled.

offset the initial error in the estimates very quickly. For the comparison of the various delay handling methods, averaged RMSE values over the initiator concentration (C_i) and the moments of the distribution (λ_{0-2}) are used. Table 3 shows the results of simulations averaged over 100 noise sequences for a total time period of 500 min.

All the methods considered have similar RMSE values for this example. The filter recalculation method shows marginally better RMSE values than the rest. An important observation is that all the *state augmentation based methods* give exactly the same state estimates. When the measurement model for the primary measurements is linear, there is no approximation made in computing the initial covariance of the estimation errors at the instance when the primary measurement is sampled. In all the three state augmentation methods, the state $X(s)$ or its linear transformation $Y^*(s)$ is smoothed using the same information and the same covariances. As long as the *primary measurement equation* is linear, all the three augmentation-based methods are expected to give identical state estimates.

Thus, the main difference between the various methods is their computational effort. Alexander's method and sampled state augmentation require less computational time than the other methods. Although the computational time for this example is in order of milliseconds, the computational time required is five-fold higher for the fixed-lag smoothing method than sampled-state augmentation method.

Table 3
Comparison of different methods with respect to RMSE values and * computational time taken per sampling instant for the nonlinear polymerization reactor.

	Method	RMSE in X	Time*
1	Filter recalculation	3.2806×10^{-1}	17.31 ms
2	Alexander's method	3.2872×10^{-1}	11.63 ms
3	Parallel filters	3.2864×10^{-1}	17.87 ms
4	Fixed-lag smoothing	3.2840×10^{-1}	55.60 ms
5	Y^2 augmentation	3.2840×10^{-1}	16.04 ms
6	$X(s)$ augmentation	3.2840×10^{-1}	11.55 ms

4.2.1. Summary

The preceding discussion compared the various methods for incorporating measurement delay based on estimation error and computational requirements. The filter recalculation method is attractive for LTI systems, but is not suitable for large delays and scenarios were slow measurements are sampled frequently ($N_s > M_s$). For such situations, Alexander's method will also fail because the state-update of a previously sampled measurement will not affect the multiplier matrix W_s for a subsequent measurement in Eq. (14). The fixed-lag smoothing has large computational requirements and is not feasible for moderate to large delays or state dimension. The method of output augmentation is attractive when the state dimension is much larger than the output dimension. However, it requires computation of $g(F_h(X(k), U(k)))$, which may be cumbersome unless the output equations are linear. Among all the methods, the sample-state augmentation approach appears to provide the best tradeoff between accuracy and computational time.

Additionally, other desirable qualities of delay-handling scheme are extendibility and flexibility. Extension to other estimators such as the MHE, RNDDR, unscented KF, ensemble KF, etc. should be straightforward. All the state augmentation based methods retain the standard state-space formulation, and are therefore extendible. Flexibility means that the estimator should be able to handle irregular and time varying delays (N_s may vary for different measurements), even when no prior information about the delay is known. The output augmentation method requires information of the maximum expected measurement delay ($N_{\max}$); no such prior information is required for sampled state augmentation method.

Based on this analysis and our experience, the sample state augmentation method is recommended over the other methods. In order to demonstrate its applicability to a larger problem, a 88-state nonlinear example is solved in the next section.

4.3. Nonlinear example: reactive distillation

A reactive distillation process described in [1] is considered in this case study. In this section, we present results for implementing sampled state augmentation method. The column has 22 ideal stages with four components in each tray. Fig. 4 shows a schematic of the column. The reversible liquid-phase reaction in the reactive section is:

$$A + B \rightleftharpoons C + D$$

The products C and D are the lightest and heaviest components in the system, respectively. The reactants A and B are intermediate boiling between the products, with A being the lighter of the two reactants. The relative volatilities in the system are of the order

$$\alpha_C > \alpha_A > \alpha_B > \alpha_D.$$

The reactive section contains N_{RX} trays. The fresh feed stream containing reactant A is fed at the bottom of the reactive zone, and that containing reactant B is fed at the top of the reactive zone. The

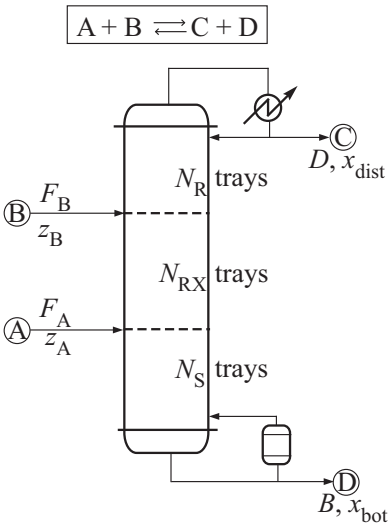

Fig. 4. Schematic of the reactive distillation column. The column contains 22 trays.

rectifying section above the reactive section contains N_R trays, and the stripping section below the reactive section contains N_S trays.

Details of the model derivation are given in [15,1] and the model is described in Appendix A. They are expressed in the standard nonlinear state space model form:

$$\frac{dX(t)}{dt} = f(X(t), U(t)) \tag{31}$$

$$Y^1(t) = g^1(X(t)) \tag{32}$$

$$Y^2(t) = g^2(X(t)) \tag{33}$$

$X(t)$: liquid mole fractions of all 4 components on all 22 trays; $U(t)$: vapor boilup from the reboiler (V_S), reflux flowrate (R), and the fresh feed flowrates (F_A and F_B); $Y^1(t)$: temperatures of the reboiler, condenser and the feed trays; $Y^2(t)$: composition measurements at the reboiler and condenser.

Thus, there are 88 states, 4 secondary temperature measurements and 8 primary composition measurements (distillate and bottoms compositions). The sample state augmentation scheme, described in Section 3.2.3, is chosen.

The noise variances used are as follows. The measurement error covariances for the frequent temperature measurements, $R_1 = 0.1(^\circ\mathrm{C})^2$ and for the delayed concentration measurements, $R_2 = 10^{-8}$; the process noise, $Q = 10^{-6}$. The EKF is started with an initial estimation error $P_0 = 10^{-5}$. The process is initially at an unsteady state and the estimator is given an incorrect starting guess.

Optionally, plant-model mismatch is also considered since an incorrect model affects the estimator performance. Even when a rigorous model is used, incorrect assumptions such as constant relative volatility and/or constant molar overflows could result in the outputs of the model deviating significantly from the real plant. A plant-model mismatch is created by assuming a 10% inaccuracy in α_A (3.6) and α_B (2.2). Both the scenarios A (only secondary measurements) and B (secondary and infrequent/delayed primary measurements) are considered. The estimator performance is tested for: (a) when there is no measurement noise, no process noise and no plant-model mismatch; and (b) in presence of state and measurement noise as well as plant-model mismatch. In these simulations, the lower and upper bounds on the mole fraction estimates and the normalization constraints on the mole fractions were implemented by clipping and re-normalization of the predicted and filtered estimates at each instance. Constrained estimators, such as RNDDR [22] may also be used instead.

The simulations for multi-rate estimation are performed as follows: The plant is assumed to be at an unsteady state at initial time $t = 0$. The secondary temperature measurements are available at every sampling instant ($h = 1$ min) and samples for composition are taken at a regular interval of $M_s = 4$ min, starting from $t = 1$ min. The delay in the measurement arrival is anywhere between 10 and 20 min (i.e., N_s varies randomly between 10 and 20). With this choice of parameters (i.e., the sampling interval for the primary measurement is shorter than the time delay), multiple primary measurements are sampled before the previously sampled measurement arrives. This can also give rise to multiple measurement arriving simultaneously, as well as out of sequence measurement arrival. The code is capable of handling all of these cases.

Case (a): No measurement noise: Fig. 5 depicts the estimates obtained using the multi-rate estimator for case (a) at the condenser. The 'solid' lines represent the plant, the 'dash-dot' lines represent scenario A (secondary measurements only) and the 'dashed' lines represent scenario B (frequent secondary and infrequent/delayed primary measurements). The open symbols in the figures represent the actual primary measurements $Y^2(k)$, which arrive after a delay of 10–20 min.

This example is intended to highlight another feature of the sampled-state augmentation scheme: it has the ability to handle cases where multiple samples are taken before the previously sampled measurement arrives. For example, the primary measurement taken at $t = 1$ arrives at $t = 11$. During this time period, two more samples of the primary variable are taken at $t = 5$ and $t = 9$. This situation is handled by further augmenting the state every time a sample is taken, in order to retain the state information $\hat{X}(s)$ required for estimation when the measurement arrives after the delay. The sampled-state augmentation method can also handle out-of-sequence measurement arrival, and simultaneous arrival of multiple primary measurements sampled at different time instances. To the best of our knowledge, this is the first time these extensions have been demonstrated for a state-augmentation method.

As the figure shows, the estimates agree well with the plant values when the primary measurements are incorporated. If no primary measurements are available, as in scenario A, the estimates converge to the process steady values at a rate comparable to those of process dynamics. With the primary measurements included, the estimates converge to the true process state much faster. For example, in Fig. 5a, until arrival of the first primary measurement (at $t = 11$), the two scenarios have the same estimation error. When the delayed primary measurement is incorporated, the estimation error decreases significantly. This repeats at each major measurement arrival instance. Finally, the simulation results demonstrate an important property of the state augmentation scheme that the estimator provides unbiased state estimates. The average time taken to obtain the state estimates at each sampling interval is 1.83 s. This computational requirement is reasonable because the sampling time is 60 s.

Case (b): With noise and plant-model mismatch: The performance of the estimator in the presence of noise and a plant-model mismatch is shown in Fig. 6. The plant-model mismatch is "unknown" and no online parameter estimation is performed. Even in the presence of plant-model mismatch and large noise, the multi-rate estimator tracks the plant quite well whereas the estimator based on only temperature measurements shows a significant offset from the plant value. In case the mismatch needs to be eliminated completely, online parameter estimation may be performed or an integral action can be added to the estimator. Since the delayed measurements considered are few and far between, they are not sufficient to remove the bias.

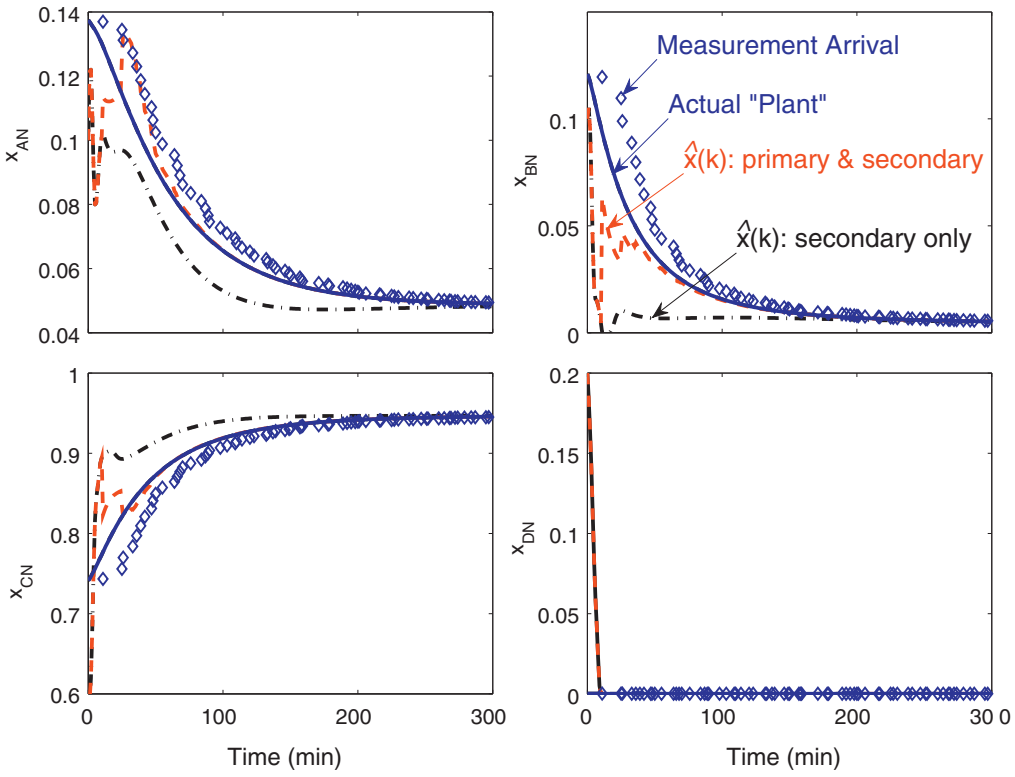

Fig. 5. Plant and estimated values of the compositions at the condenser in the absence of noise and plant-model mismatch.

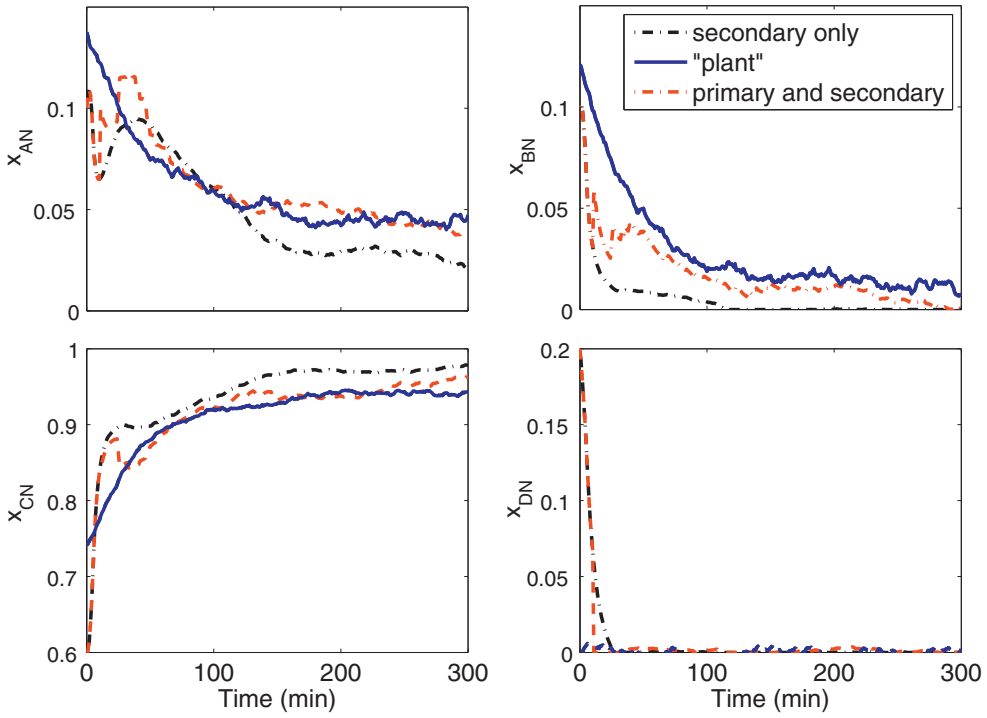

Fig. 6. Plant and estimated values of the compositions at the condenser in the presence of noise and plant-model mismatch.

5. Conclusions

A comprehensive evaluation of different approaches to incorporate infrequent and delayed measurements of the primary variables was presented in this work. These methods were classified into two categories: (i) methods that fuse the delayed primary measurements when they arrive, and (ii) methods based on state augmentation. All the methods were first implemented on a four-state linear example and shown to have identical performance in terms of estimation accuracy. Only the method of Alexander [2], which compromises on optimality for computational time, was marginally poor. However, the more popular state augmentation

Table A.1
Model parameters for reactive distillation.

Flow rates (kmol/s)			
Fresh feed (F_A)	0.0126	Fresh feed (F_B)	0.0126
Reflux (R)	0.0331	Vapour flow (V_S)	0.0285
Distillate (D)	0.0126	Bottoms (B)	0.0126
Column specifications			
Reboiler hold-up (M_1)	10 kmol	Pressure (P)	9 atm
Condenser hold-up (M_N)	30 kmol	Stripping section (N_S)	7 + 1
Tray hold-up (M_i)	1 kmol	Rectifying section (N_R)	7 + 1
		Reactive section (N_{RX})	6
Reaction conditions			
Activation energy (E_F)	30 kcal/mol	k_{Fwd} at 366 K	0.008 s^{-1}
Activation energy (E_B)	40 kcal/mol	k_{Bkd} at 366 K	0.004 s^{-1}
Heat of reaction (λ)	−10 kcal/mol	Heat of vap. (ΔH_v)	6.944 kcal/mol
Relative volatilities			
α_A	4	α_B	2
α_C	8	α_D	1

approach of *fixed-lag smoothing* was shown to be computationally unsuitable for online estimation, even for a linear system example. Likewise, the straightforward approach to fusing delayed measurements by *filter recalculation* was also shown to be computationally unsuitable for nonlinear systems. A nonlinear example of polymerization reactor showed that all the state augmentation methods give the same estimation accuracy if the primary measurement equation is linear. The various methods differed in the computational requirement.

Of all the methods analyzed, the *sample-state augmentation* method was found to have the best tradeoff between estimation accuracy and computational time. This method was then applied to a large scale nonlinear reactive distillation column example. The estimator performed significantly better than the estimator based on only the secondary temperature measurements. The method is flexible to handle unknown (and randomly varying) delays in the measurement arrival time for the primary variable. Since the augmented model is in the standard state-space form, it is extendable to other estimation techniques such as particle filtering techniques and constrained estimators.

Appendix A. Reactive distillation column model

A typical reactive distillation column, shown in Fig. 4, consists of rectification, reaction and stripping sections. The assumptions made are constant liquid hold-up on each tray and equimolal overflow of vapor and liquid flow rates in the rectification and stripping sections. The resulting mass balance equations are written for species $j = \{A,B,C,D\}$ as:

- Reboiler mass balance

$$M_1 \frac{dx_{1,j}}{dt} = L_2(x_{2,j} - x_{1,j}) + V_S(x_{1,j} - y_{1,j}) \tag{A.1}$$

- Stripping section ($2 \le i \le N_S$)

$$M_i \frac{dx_{i,j}}{dt} = L_{i+1}(x_{i+1,j} - x_{i,j}) + V_S(y_{i-1,j} - y_{i,j}) \tag{A.2}$$

- Rectifying section ($N_S + N_{RX} + 1 \le i \le N - 1$)

$$M_i \frac{dx_{i,j}}{dt} = L_{i+1}(x_{i+1,j} - x_{i,j}) + V_N(y_{i-1,j} - y_{i,j}) \tag{A.3}$$

- Condenser ($i = N$)

$$M_N \frac{dx_{N,j}}{dt} = V_N(y_{N-1,j} - x_{N,j}) \tag{A.4}$$

- Reactive section ($N_S + 1 \le i \le N_S + N_{RX}$)

$$M_i \frac{dx_{i,j}}{dt} = L_{i+1}(x_{i+1,j} - x_{i,j}) + V_{i-1}(y_{i-1,j} - y_{i,j}) + V_i(x_{i,j} - y_{i,j}) + R_{i,j} + F_i(z_{i,j} - x_{i,j}) \tag{A.5}$$

where

$$F_i = \begin{cases} F_A & \text{at } i = N_S + 1 \\ F_B & \text{at } i = N_S + N_{RX} \\ 0 & \text{otherwise.} \end{cases}$$

Heat of reaction vaporizes some liquid on each tray in the reactive section. The vapor and liquid flows are then given by

$$V_i = V_{i-1} - \frac{\Delta H_r}{\Delta H_v} R_{i,j}$$
$$L_i = L_{i-1} + \frac{\Delta H_r}{\Delta H_v} R_{i,j}$$

The reaction rate of component j (A, B, C or D) in tray i is,

$$R_{i,j} = M_i(k_{0F} e^{-E_F/RT_i} x_{i,A} x_{i,B} - k_{0B} e^{-E_B/RT_i} x_{i,C} x_{i,D}) \tag{A.6}$$

The VLE equations are:

$$y_{i,j} = \frac{\alpha_j x_{i,j}}{\sum_{k=1}^{N_C} \alpha_k x_{i,k}} \tag{A.7}$$

$$T_i = \frac{B_{vp,1}}{A_{vp,1} - \log(\alpha_1 P / (\sum_{k=1}^{N_C} \alpha_k x_{i,k}))} \tag{A.8}$$

The different parameter values for the column and nominal steady state operating conditions are given in Table A.1.

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