

## COMPARISON OF STATE ESTIMATION TECHNIQUES, APPLIED TO A BIOLOGICAL WASTEWATER TREATMENT PROCESS

Qian Chai \*, Beathe Furenes \*, Bernt Lie \*.<sup>1</sup>

\* Telemark University College, P.O. Box 203, N-3901  
Porsgrunn, Norway

Abstract: In this paper the problem of optimal state estimation in a biological wastewater treatment process (WWTP) is considered. The standard Kalman filter (KF) and its extensions: the extended Kalman filter (EKF) and the unscented Kalman filter (UKF), are used to estimate the unmeasured state. The prediction of the state with the standard KF is poor due to the high nonlinearity of the biological WWTP. Thus, the nonlinear estimation approaches are focused, with a comparison between the EKF and the UKF. The simulation results show that the UKF provides slightly better state estimate than the EKF for both an observable process and an unobservable process. *Copyright © 2007 IFAC*

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### 1. INTRODUCTION

State estimation of dynamic systems is an important prerequisite for safe and economical process operation. There is a wide range of techniques in the literature designed for state estimation in both linear and nonlinear dynamic systems. The *Kalman filter* (KF) (Kalman 1960) is one of the most widely used methods for state estimation and tracking due to its simplicity and robustness. The *standard Kalman filter* is the algorithm of choice in state estimation for linear systems. The approach can be used to reconstruct variables that are not measured and to reduce the effect of noise on the available measurements. However, since most practical systems involve nonlinearity of one kind or another, the problem of nonlinear estimation is extremely important. Therefore, the Kalman filter was early on extended in a somewhat ad hoc way to include nonlinear dynamic models in the *extended Kalman filter* (EKF). For the computation of the filter gain, the EKF simply linearizes the nonlinear models about the current estimate so that the standard Kalman fil-

ter gain computation algorithm can be applied. Although the EKF maintains the elegant and computationally efficient recursive update form of the standard KF, the EKF typically works well only in the region where the first-order Taylor series linearization adequately approximates the nonlinear probability distribution (Crassidis & Junkins 2004). To overcome this limitation, Julier et al. (1995) proposed the *unscented Kalman filter* (UKF) as an alternative to the EKF in nonlinear estimation. The UKF generates a population of so-called *sigma points* based on the current mean and covariance of the state, and permits the direct propagation of the mean and covariance through the actual nonlinear system. The applications and comparisons of the EKF and the UKF have been discussed in a number of studies, e.g. Wan & van der Merwe (2000) and Romanenko & Castro (2004).

In the last decades, due to the increasingly strict requirements on treated wastewater, the need to monitor systems and automatically control biological wastewater treatment processes (WWTPs) is rapidly increasing. To reconstruct the state of the system from the few available measure-

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<sup>1</sup> Corresponding author: Bernt.Lie@hit.no

ments and to control important biological variables, appropriate algorithms have to be developed. Some state estimation algorithms for WWTPs have been described in Dochain & Vanrolleghem (2001), and Olsson & Newell (1999). Also, in Keesman (2002), Boaventura et al. (2001), Lukasse et al. (1999), and Zhao & Kümmel (1995), the EKF has been applied to simplified WWTP models, but the application of the UKF to WWTPs is not studied much in the literature.

The objective of this study is to demonstrate (i) the application of the standard KF, the EKF, and the UKF to state estimation of a biological WWTP and (ii) the differences in performance of these estimation approaches. As an example, a nitrogen removal process described by the Activated Sludge Model No. 3 (ASM3) (Gujer et al. 1999) is considered. The state estimation is carried out for the complete ASM3 model.

The paper is organized as follows. In Section 2, the Kalman filter based state estimation approaches are summarized. In Section 3, the approaches are illustrated on a wastewater nitrogen removal process. The comparison between the EKF and the UKF is shown. Finally, some conclusions are drawn in Section 4.

## 2. STATE ESTIMATION APPROACHES

### 2.1 Standard Kalman filter (KF)

To better understand how nonlinear estimators work, it is useful to focus on the linear case first. A linear system, approximated in discrete time is given as

$$\begin{aligned}x_{k+1} &= Ax_k + Bu_k + Gw_k \\ y_k &= Cx_k + v_k\end{aligned}$$

where  $x_k \in \mathbb{R}^{n_x}$  is the state,  $u_k \in \mathbb{R}^{n_u}$  is the control input, and  $y_k \in \mathbb{R}^{n_y}$  is the controlled output.  $w_k \in \mathbb{R}^{n_w}$  and  $v_k \in \mathbb{R}^{n_v}$  present the process noise and measurement noise, respectively. They are assumed to be zero-mean Gaussian noise processes  $w_k \sim \mathcal{N}(0, Q_k)$  and  $v_k \sim \mathcal{N}(0, R_k)$ .

A standard KF formulation for estimating the process state  $x$ , where  $x$  is assumed to be initially normally distributed with expectation  $\hat{x}_{1|1}$  and covariance  $P_{1|1}$ , is given by:

$$\begin{aligned}\hat{x}_{k+1|k} &= A\hat{x}_{k|k} + Bu_k \\ P_{k+1|k} &= AP_{k|k}A^T + GQ_kG^T \\ K_{k+1} &= P_{k+1|k}C^T (CP_{k+1|k}C^T + R_{k+1})^{-1} \\ \hat{x}_{k+1|k+1} &= \hat{x}_{k+1|k} + K_{k+1}(y_{k+1} - C\hat{x}_{k+1|k}) \\ P_{k+1|k+1} &= (I - K_{k+1}C)P_{k+1|k}(I - K_{k+1}C)^T \\ &\quad + K_{k+1}R_{k+1}K_{k+1}^T,\end{aligned}$$

where  $y_{k+1}$  denotes the actual measurement at step  $k+1$ . The Kalman gain  $K_k$  is chosen to minimize the *a posteriori* estimate error covariance  $P_{k|k}$ . Note that the equation for the *a posteriori* state covariance  $P_{k|k}$  is called the stabilized implementation, because it has better numerical properties than some other frequently used equations for  $P_{k|k}$ , e.g.  $P_{k|k} = (I - K_kC)P_{k|k-1}$ .

### 2.2 Extended Kalman filter (EKF)

For several reasons, state estimation for nonlinear systems is considerably more difficult and admits a wider variety of solutions than the linear problem (Crassidis & Junkins 2004). In this paper, we discuss two different approaches to achieve estimation for nonlinear systems: the method of EKF uses the recursive update form of standard KF by linearizing the nonlinear model at each time step, and the method of UKF uses a set of appropriately chosen weighted points to parameterize the means and covariances of probability distributions.

The nonlinear system is described by the stochastic model

$$\begin{aligned}x_{k+1} &= f(x_k, u_k, w_k) \\ y_k &= g(x_k, u_k, v_k)\end{aligned}$$

where  $x_1 \sim \mathcal{N}(\hat{x}_{1|1}, P_{1|1})$ ,  $w_k \sim \mathcal{N}(0, Q_k)$ , and  $v_k \sim \mathcal{N}(0, R_k)$ .  $\hat{x}_{1|1}$ ,  $P_{1|1}$ ,  $Q_k$ , and  $R_k$  are assumed to be known.

The EKF algorithm can be summarized as the following set of equations:

$$\begin{aligned}\hat{x}_{k+1|k} &= f(\hat{x}_{k|k}, u_k, 0) \\ P_{k+1|k} &= A_kP_{k|k}A_k^T + G_kQ_kG_k^T \\ K_{k+1} &= P_{k+1|k}C_{k+1}^T (C_{k+1}P_{k+1|k}C_{k+1}^T \\ &\quad + H_{k+1}R_{k+1}H_{k+1}^T)^{-1} \\ \hat{x}_{k+1|k+1} &= \hat{x}_{k+1|k} + K_{k+1}(y_{k+1} - g(\hat{x}_{k+1|k}, u_{k+1}, 0)) \\ P_{k+1|k+1} &= (I - K_{k+1}C_{k+1})P_{k+1|k}(I - K_{k+1}C_{k+1})^T \\ &\quad + K_{k+1}H_{k+1}R_{k+1}H_{k+1}^T K_{k+1}^T,\end{aligned}$$

where matrices  $A_k$ ,  $G_k$ ,  $C_k$ , and  $H_k$  are defined as the following Jacobians:

$$\begin{aligned}A_k &= \left. \frac{\partial f}{\partial x} \right|_{\hat{x}_{k|k}, u_k, 0}, \quad G_k = \left. \frac{\partial f}{\partial w} \right|_{\hat{x}_{k|k}, u_k, 0} \\ C_k &= \left. \frac{\partial g}{\partial x} \right|_{\hat{x}_{k|k-1}, u_k, 0}, \quad H_k = \left. \frac{\partial g}{\partial v} \right|_{\hat{x}_{k|k-1}, u_k, 0}.\end{aligned}$$

### 2.3 Unscented Kalman filter (UKF)

We initiate the UKF by

$$x_1 \sim \mathcal{N}(\hat{x}_{1|1}, P_{1|1}).$$

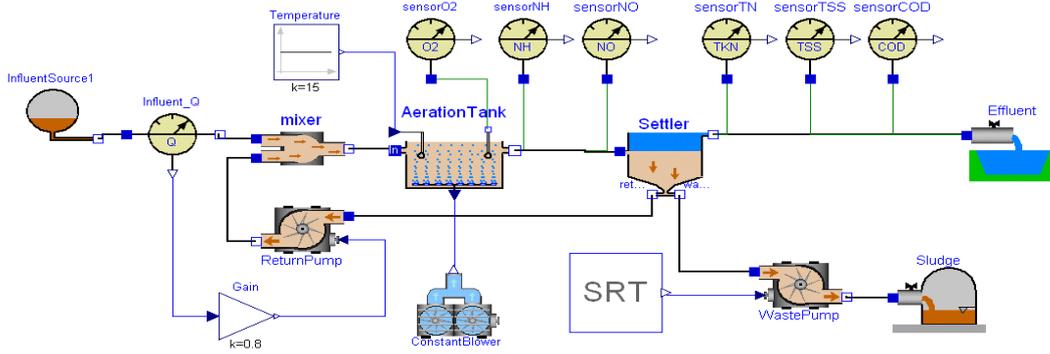


Fig. 1. Model diagram of the nitrogen removal plant implemented in Modelica/Dymola.

First, an augmented state is defined as

$$x_k^a = \begin{bmatrix} x_k \\ w_k \\ v_k \end{bmatrix}.$$

The mean and covariance of the augmented state vector are

$$\tilde{x}_{k|k} = \begin{bmatrix} \hat{x}_{k|k} \\ 0 \\ 0 \end{bmatrix}, \quad \tilde{P}_{k|k} = \begin{bmatrix} P_{k|k} & 0 & 0 \\ 0 & Q_k & 0 \\ 0 & 0 & R_k \end{bmatrix}.$$

The size of  $\tilde{x}_{k|k}$  is  $n_{\tilde{x}} = n_x + n_w + n_v$ . Introduce matrix  $V$  as the Cholesky root of  $(n_{\tilde{x}} + \lambda) \tilde{P}_{k|k}$ :

$$V^T V = (n_{\tilde{x}} + \lambda) \tilde{P}_{k|k}$$

where  $\lambda = \alpha^2 (n_{\tilde{x}} + \kappa) - n_{\tilde{x}}$  is a scaling parameter (typically  $\alpha \in [10^{-4}, 1]$  and  $\kappa = 0$ ). Let  $V_i$  denote column  $i$  of matrix  $V$ .

Next, we define  $2n_{\tilde{x}} + 1$  sigma points  $\tilde{\mathcal{X}}_{k|k}^i$  with corresponding weights  $W_i$  as follows:

$$\begin{aligned} \tilde{\mathcal{X}}_{k|k}^0 &= \tilde{x}_{k|k} \\ \tilde{\mathcal{X}}_{k|k}^i &= \tilde{x}_{k|k} + V_i \quad i = 1, \dots, n_{\tilde{x}} \\ \tilde{\mathcal{X}}_{k|k}^i &= \tilde{x}_{k|k} - V_{i-n_{\tilde{x}}} \quad i = n_{\tilde{x}} + 1, \dots, 2n_{\tilde{x}} \\ W_m^0 &= \lambda / (n_{\tilde{x}} + \lambda) \\ W_c^0 &= \lambda / (n_{\tilde{x}} + \lambda) + (1 - \alpha^2 + \beta) \\ W_m^i &= W_c^i = 1 / [2(n_{\tilde{x}} + \lambda)] \quad i = 1, \dots, 2n_{\tilde{x}} \end{aligned}$$

where  $\beta$  is used to incorporate prior knowledge of the distribution (with Gaussian distribution  $\beta = 2$ ).

Define  $\mathcal{X}_{k|k}^i$  to be the vector of the first  $n_x$  elements of  $\tilde{\mathcal{X}}_{k|k}^i$ ,  $\mathcal{W}_{k|k}^i$  to be the vector of the next  $n_w$  elements of  $\tilde{\mathcal{X}}_{k|k}^i$ , and  $\mathcal{V}_{k|k}^i$  to be the vector of the last  $n_v$  elements of  $\tilde{\mathcal{X}}_{k|k}^i$ . The predicted sigma points  $\mathcal{X}_{k+1|k}^i$  and  $\mathcal{Y}_{k+1|k}^i$  are given by:

$$\begin{aligned} \mathcal{X}_{k+1|k}^i &= f(\mathcal{X}_{k|k}^i, u_k, \mathcal{W}_{k|k}^i), \quad i = 0, \dots, 2n_{\tilde{x}} \\ \mathcal{Y}_{k+1|k}^i &= g(\mathcal{X}_{k+1|k}^i, u_k, \mathcal{V}_{k|k}^i), \quad i = 0, \dots, 2n_{\tilde{x}}. \end{aligned}$$

We then compute the predicted means as

$$\begin{aligned} \hat{x}_{k+1|k} &= \sum_{i=0}^{2n_{\tilde{x}}} W_m^i \mathcal{X}_{k+1|k}^i \\ \hat{y}_{k+1|k} &= \sum_{i=0}^{2n_{\tilde{x}}} W_m^i \mathcal{Y}_{k+1|k}^i, \end{aligned}$$

and the predicted covariances as

$$\begin{aligned} P_{k+1|k} &= \sum_{i=0}^{2n_{\tilde{x}}} W_c^i [\mathcal{X}_{k+1|k}^i - \hat{x}_{k+1|k}] [\mathcal{X}_{k+1|k}^i - \hat{x}_{k+1|k}]^T \\ E_{k+1|k} &= \sum_{i=0}^{2n_{\tilde{x}}} W_c^i [\mathcal{Y}_{k+1|k}^i - \hat{y}_{k+1|k}] [\mathcal{Y}_{k+1|k}^i - \hat{y}_{k+1|k}]^T \\ S_{k+1|k} &= \sum_{i=0}^{2n_{\tilde{x}}} W_c^i [\mathcal{X}_{k+1|k}^i - \hat{x}_{k+1|k}] [\mathcal{Y}_{k+1|k}^i - \hat{y}_{k+1|k}]^T, \end{aligned}$$

where  $E_{k+1|k}$  represents the innovation covariance, and  $S_{k+1|k}$  represents the cross correlation matrix between  $\hat{x}_{k+1|k}$  and  $\hat{y}_{k+1|k}$ .

We can now compute the UKF gain  $K_{k+1}$  as

$$K_{k+1} = S_{k+1|k} E_{k+1|k}^{-1},$$

and finally the updated estimates of state and covariance as

$$\begin{aligned} \hat{x}_{k+1|k+1} &= \hat{x}_{k+1|k} + K_{k+1} (y_{k+1} - \hat{y}_{k+1|k}) \\ P_{k+1|k+1} &= P_{k+1|k} - K_{k+1} E_{k+1|k} K_{k+1}^T. \end{aligned}$$

Compared with the EKF, the UKF features two main advantages: (i) the UKF avoids the computation of the Jacobian matrices, and (ii) the UKF achieves a third order accuracy in the Taylor series expansion of the statistics of the state, whereas the EKF is at most first order accurate.

### 3. APPLICATION TO A NITROGEN REMOVAL PROCESS

#### 3.1 Process model

In this study, a laboratory-scale nitrogen removal plant is considered. More details of the process are given in Chai et al. (2006). The process model consists of an aeration tank model in which oxygen

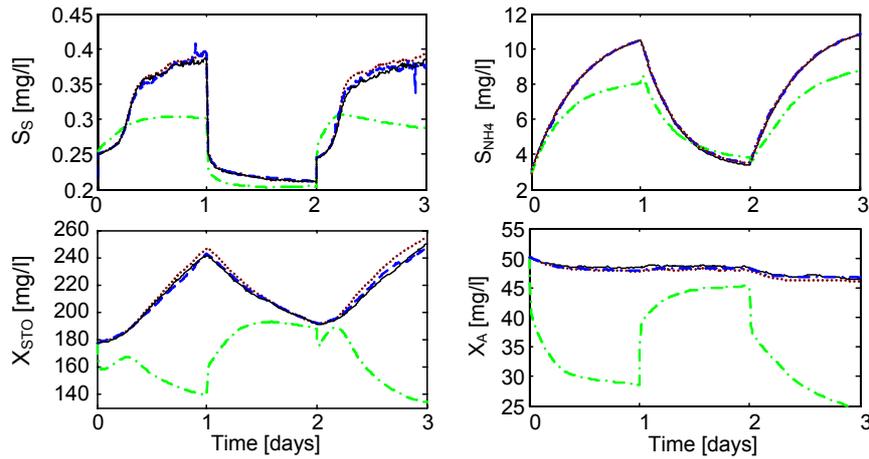


Fig. 2. Simulation results of the standard KF (dash-dot), the EKF (dotted), and the UKF (dashed). The solid line represents the true states.

is supplied, and a settler model where the sludge is separated from the liquid being treated. ASM3 describes the biological processes involved in the aeration tank. The states of the model are grouped into the concentration of soluble components  $S_j$  and particulate components  $X_j$ . The kinetic and stoichiometric parameter values are taken from the typical parameter values suggested in ASM3 publications. Assuming perfect mixing in the reactor, the mass balance in the aeration tank results in:

$$\frac{dx_a}{dt} = \frac{Q_{in}x_{in} + Q_{rs}x_{rs} - (Q_{in} + Q_{rs})x_a}{V_a} + r + e_1 \mathcal{A}_{O_2},$$

where  $x_{in}$ ,  $x_{rs}$ ,  $x_a \in \mathbb{R}^{13}$  contain the concentrations in the influent, in the recycled sludge, and in the reactor, respectively; their components are

$$x_l = [S_{O_2,l} \ S_{I,l} \ S_{S,l} \ S_{NH_4,l} \ S_{N_2,l} \ S_{NOX,l} \ S_{ALK,l} \ X_{I,l} \ X_{S,l} \ X_{H,l} \ X_{STO,l} \ X_{A,l} \ X_{SS,l}]^T,$$

$l \in \{in, rs, a\}$ ;  $r \in \mathbb{R}^{13}$  is the reaction rates of each component (defined in ASM3);  $e_1$  is the standard basis for the first coordinate in  $\mathbb{R}^{13}$ .  $\mathcal{A}_{O_2}$  describes the oxygen transfer:  $\mathcal{A}_{O_2} = K_L a (S_{O_2}^{sat} - S_{O_2,a})$ , where  $K_L a$  is the oxygen transfer coefficient which is the control input variable in this study, and  $S_{O_2}^{sat}$  is the saturated dissolved oxygen concentration.

Assuming that the settler is a perfect splitter, the resulting mass balance equations are as follows:

Effluent concentration:

$$S_{j,eff} = S_{j,a}, \quad X_{j,eff} = 0$$

Recycled sludge concentration:

$$S_{j,rs} = S_{j,a}, \quad X_{j,rs} = \frac{Q_{in} + Q_{rs}}{Q_{rs} + Q_w} X_{j,a}.$$

The dynamic model is implemented in the object-oriented modeling language Modelica (Fritzson

2004) using the Dymola simulation environment (Dymola 2004), see Figure 1, based on modifications of the free Modelica library **WasteWater** (Reichl 2003). Dymola generates a convenient interface to Matlab such that Modelica models can be executed within MATLAB.

### 3.2 Results and discussion

MATLAB is used for implementation of the estimation approaches. To estimate the state, we need measurements from the plant. As an initial study before doing state estimation based on real data from the plant, we choose to check whether reasonable state estimates can be obtained based on response from the simulation model.

Observability is an important concept in dynamic systems in general. Observability depends mainly on the choice of measurement variables. In this case, to ensure that the system is fully observable, the following measurement variables are chosen: the concentration of total nitrogen TN in the effluent, as well as the concentrations of dissolved oxygen  $S_{O_2}$ , dinitrogen  $S_{N_2}$ , inert particulate organics  $X_I$ , and total suspended solids  $X_{SS}$  in the aeration tank<sup>2</sup>. The state and measurement vectors are subject to zero mean additive white noise with covariances

$$Q_k = Q = \text{diag} \left( (x_o \cdot 10^{-3})^2 \right) \text{ and} \\ R_k = R = \text{diag} \left( (y_o \cdot 10^{-4})^2 \right),$$

respectively, where  $(x_o, y_o)$  is the operating point. The chosen noise levels are relatively low in this introductory phase of the study. Larger noise covariances will be considered in future work.

<sup>2</sup> In practice, some of these measurement variables may be difficult to measure; in this study, we assume that they are available.

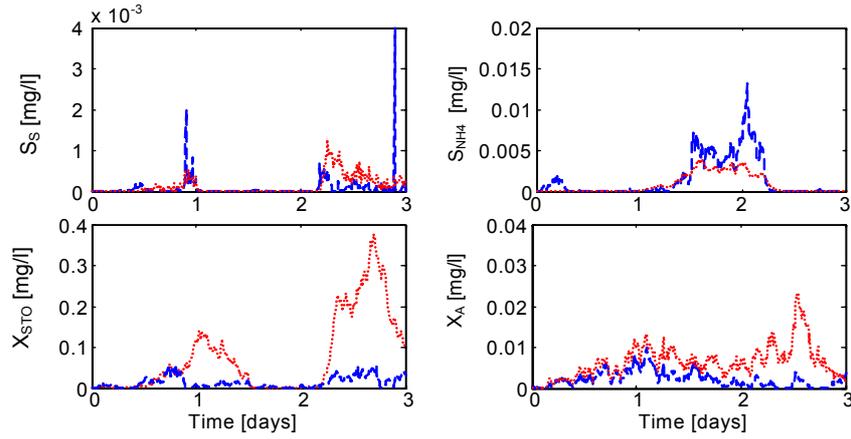


Fig. 3. Comparison of the estimation errors of the EKF (dotted) and the UKF (dashed) for the *observable* process.

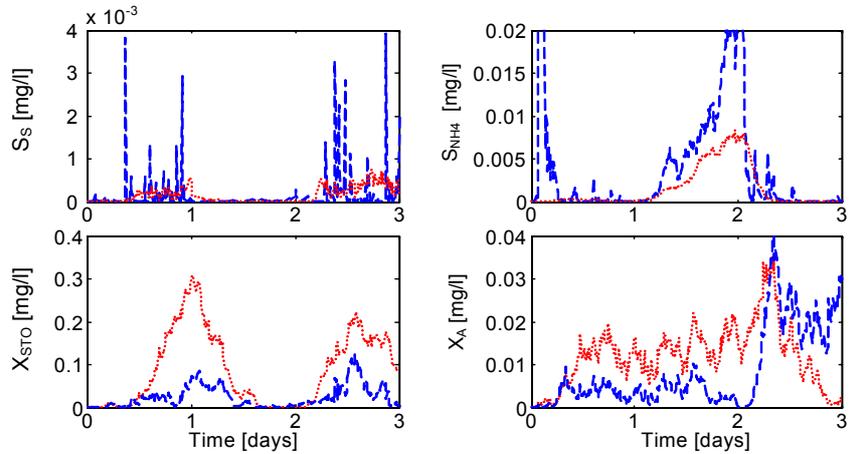


Fig. 4. Comparison of the estimation errors of the EKF (dotted) and the UKF (dashed) for the *unobservable* process.

Figure 2 illustrates the performances of the standard KF, the EKF, and the UKF. Four unmeasured states, which most clearly exhibit the difference of the estimation results between the EKF and the UKF, are shown in the figure: the concentrations of readily biodegradable substrates  $S_S$ , ammonium  $S_{NH_4}$ , organics stored by heterotrophs  $X_{STO}$ , and autotrophic biomass  $X_A$ . The prediction of the states with the standard KF is poor because of the nonlinear characteristics of the biological WWTP dynamics. Nonlinear estimation is therefore imperative for biological WWTPs. In Figure 2, both the EKF and the UKF track all the states of the process; indeed, the performance of the EKF and the UKF are quite similar. To compare the estimation qualities of the EKF and the UKF, Figure 3 plots the relative squared estimation errors of the filters which are relative to the true states. The result shows that the EKF and the UKF give the similar estimation error for the concentrations of the soluble components ( $S_S$ ,  $S_{NH_4}$ ). However, for the concentrations of the particulate components ( $X_{STO}$ ,  $X_A$ ), the superior performance of the UKF is clear.

In WWTPs, measuring most state variables is either difficult or expensive. This time, we assume that only the concentration of total nitrogen TN in the effluent and the concentration of dissolved oxygen  $S_{O_2}$  in the aeration tank are the available measurement variables for the nitrogen removal process. By performing observability analysis of a linearized model, we find that this system is not observable. However, the system is detectable since the dynamics of the filter error is asymptotically stable; detectability guarantees convergence of the filter. Figure 4 depicts the estimation errors of the unobservable process with the EKF and the UKF. By comparing Figure 4 with Figure 3, we find that the estimation errors of the unobservable process are slightly larger than the observable process for both the EKF and the UKF. With the UKF, the state estimates for the unobservable process are more noisy than for the observable process. However, for the unobservable (but detectable) process, the EKF and the UKF still give reasonable estimates for the unmeasured states. Hence, if the available measurements are adequate for the dynamic system's requirements,

Table 1. Mean estimation errors over 3 days.

Method	$S_S$	$S_{NH_4}$	$X_{STO}$	$X_A$
Observable process				
<b>EKF</b>	$1.3 \times 10^{-4}$	$8.5 \times 10^{-4}$	$7.6 \times 10^{-2}$	$6.4 \times 10^{-3}$
<b>UKF</b>	$7.6 \times 10^{-5}$	$1.5 \times 10^{-3}$	$1.4 \times 10^{-2}$	$2.2 \times 10^{-3}$
Unobservable process				
<b>EKF</b>	$1.5 \times 10^{-4}$	$1.5 \times 10^{-3}$	$8.9 \times 10^{-2}$	$1.2 \times 10^{-2}$
<b>UKF</b>	$1.3 \times 10^{-4}$	$4.4 \times 10^{-3}$	$2.5 \times 10^{-2}$	$8.4 \times 10^{-3}$

a fully observable system may not be necessary (Crassidis & Junkins 2004).

Finally, to give an overview of the estimation capabilities of the EKF and the UKF, the mean estimation errors for the aforementioned states over 3 days are summarized in Table 1. For the most states, UKF provides better state estimation than the EKF for both the observable process and the unobservable process (also see Figures 3 and 4).

#### 4. CONCLUSIONS

In this paper, we investigate the use of the standard KF, the EKF, and the UKF in state estimation of a typical biological WWTP and compare the differences in performance of these estimation approaches. First, the general formulations of the Kalman filter based algorithms are introduced. Then, the performances of the estimation algorithms are evaluated by simulation studies. The estimation results show that state estimation with the linear approach (the standard KF) is poor because of the high nonlinearity of the bioprocess. It is therefore important to exploit nonlinear estimation algorithms for biological WWTPs. For the nitrogen removal process, the UKF provides more accurate estimates than the EKF for both the observable process and the unobservable process (see Table 1), which attests to the power of using the UKF for nonlinear systems. In the computation, the EKF takes 8 min, while the UKF takes 23 min, i.e., the computation time of the UKF is about 3 times longer than that of the EKF. The reason for this is that the calculation of the predicted sigma points in the UKF is time-consuming for the nitrogen removal model. Nevertheless, since the UKF avoids the computation of the Jacobian matrices, the UKF is simpler to implement than the EKF.

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