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(P43) Model-based observers for monitoring of biological nitrification of urine in decentralized treatment

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Abstract
Biological nitrification is considered a vital step to enabledecentralized treatment of source-separated urine. However, rapid changes in the load to this process are known to result in rapid build-up of nitrite,which can destabilize the process. A further complication is that no direct, online measurements of nitrite are available. It is for this reason that model-based observers are tested as soft-sensors for online nitrite estimation.
Keywords
Decentralized wastewater treatment; Extended Kalman Filter; nitrification; nitrite; soft sensor; Unscented Kalman Filter.

INTRODUCTION

Nitrification is an aerobic process by which ammonium is biologically oxidized to nitrate in two steps: from ammonium to nitrite by the ammonia oxidizing bacteria (AOB) and from nitrite to nitrate by the nitrite oxidizing bacteria (NOB). Biological nitrification is often part of conventionalwastewater treatment plants.More recently, biological nitrification has been proposed to stabilize decentralized treatment of source-separated urine (Udert and Lienert 2013). The resulting nitrified urine can further be distilled to produce a nitrogen fertilizer and the complete process is geared to urbanenvironments in emerging and developing countries (Udert and Wächter 2012). Under normal circumstances, the AOB are substrate limited as soon as about 50% of the ammonia has been nitrified and the alkalinity in the wastewater is consumed. While this is achievable under stable influent conditions, increases in the ammonia load to the urine nitrification process can result in a rapid accumulation of nitrite. Such accumulation leads to inhibition of NOB, further slowing down the second nitrification step until stopped entirely, with possible complete loss of NOB biomass. Therefore, knowing the nitrite concentration is key to long-term operation under load-changing conditions. However, among today's many online sensors, there is yet none that can measure nitrite continuously and reliably in municipal wastewaters. Moreover, current expectations are that nitrite-nitrogen concentrations can rise up to 200 mgNO_3-N/l in the reactor, which is higher than the range for typical ISE sensors for ammonia and nitrate. The offline method that is currently employed by practitioners, i.e. nitrite strips or sampling, necessitates manpower.A reaction time in the order of hours, possibly days, is required to implement an appropriate action and prevent the reactor from failing, thereby excluding such offline analysis for this purpose.

On the other hand, some key variables such as nitrate nitrogen concentration and pH can be measured reliably today, and others are likely to exist within the near future (ammonium nitrogen concentration). These signals are considered to contain indirect information about the nitrite concentration. For this reason, soft sensing is a promising approach to obtain a reliable, online estimation of the nitrite concentration. Soft sensors denote a subset of observers, which are used to estimate unmeasured quantities by utilizing information from additional process parametersand existing measurements. Typical applications for soft sensors include process monitoring and control(Vargas *et al.* 2000)as well as fault detection and identification(Prakash*et al.*2005, Villez *et al.*2013). In this contribution, we demonstrate the potential of observers for nitrite estimation in the absence of a direct measurement. Our ultimate goal is to test the developed soft-sensorsin a real case scenario with an operational reactor

and with a set of online sensors (Udert and Wächter 2012, Hug *et al.* 2013).

MATERIALS AND METHODS

In this paper, we use a very simplified version of a model describing a nitrification reactor (Hug *et al.* 2013) in order to test and demonstrate the selected observers.Here, we assume that the system is defined by the three state variables: S_{NH3}ammonia concentration, S_{HNO2}nitrite concentration, and S_{NO3}nitrate concentration, and the two processes: growth of AOB, and growth of NOB. Furthermore, it is assumed that the oxygen concentration, the volume of the reactor and the biomass activity are kept perfectly constant. The nitrifying reactor is modeled as a system of three ordinary differential equations expressing the rate of change in the concentrations of ammonia, nitrite and nitrate:

$$\frac{dS_{NH3}}{dt} = -\frac{S_{NH3}}{K_{NH3}+S_{NH3}} \times \frac{I_{HNO2,AOB}}{S_{HNO2}+I_{HNO2,AOB}} \times A_{AOB} \quad (1)$$

$$\frac{dS_{HNO2}}{dt} = \frac{S_{NH3}}{K_{NH3}+S_{NH3}} \times \frac{I_{HNO2,AOB}}{S_{HNO2}+I_{HNO2AOB}} \times A_{AOB} - \frac{S_{HNO2}}{K_{HNO2}+S_{HNO2}+\frac{S_{HNO2}^2}{I_{HNO2,NOB}}} \times A_{NOB} \quad (2)$$

$$\frac{dS_{NO3}}{dt} = \frac{S_{HNO2}}{K_{HNO2}+S_{HNO2}+\frac{S_{HNO2}^2}{I_{HNO2,NOB}}} \times A_{NOB} \quad (3)$$

where K_{NH3} and K_{HNO2} denote the affinity constants for NH_3 and HNO_2, respectively, $I_{HNO2,AOB}$and $I_{HNO2,NOB}$denote the non-competitive inhibition constants for HNO_2 for AOB and NOB and A_{AOB} and A_{NOB} denote the biomass activities. The constants are given in Table 1. Note that A_{AOB} and A_{NOB} have been taken as averages of the values used in Hug *et al.* (2013).

Table 1. Kinetic constants for the microbial processes (Hug *et al.* 2013).

Constant	Value	Unit	Constant	Value	Unit
K_{NH3}	0.50	mg NH_3-N/l	$I_{HNO2,NOB}$	0.06	mg HNO_2-N/l
K_{HNO2}	0.0004	mg HNO_2-N/l	A_{AOB}	57	mg COD/(l·day)
$I_{HNO2,AOB}$	1.61	mg HNO_2-N/l	A_{NOB}	6.5	mg COD/(l·day)

The Kalman filter algorithm is used to find statistically optimal estimates of both measured and unmeasured variables that are described as internal states in a linear dynamic system (Welch and Bishop 2006). The Extended Kalman Filter (EKF) is the equivalent algorithm for nonlinear dynamic systems. The main disadvantages of using the EKF are the requirement of an explicit Jacobian for the linearizationand the possibility of algorithm divergence when the system is highly nonlinear (Julier *et al.* 2000). The Unscented Kalman Filter (UKF) was introduced as a different approach to nonlinear estimation, tackling the issues of the EKF and avoiding the need for linearization, resulting in a more accurate and easier implemented algorithm (Julier and Uhlmann2004). Among the several existing versions of the UKF, we chose the algorithm presented by Wan and van der Merwe (2001), howeverusing a continuous formulation of the state equation and a discrete measurement equation.

All equationswere implemented in Matlab. First, the system (1)-(3) was simulated from time 0 to 50 days, using the initial values

$$S_{NH3}(0) = 100, S_{HNO2}(0) = 0, S_{NO3}(0) = 0. \quad (4)$$

The simulated concentrations of ammonia and nitrate were considered to be measurements and given as input to the EKF and UKF, respectively, therein assuming that nitrite was not measured. For both EKF and UKF, the following values were used:

$$Q = \begin{pmatrix} 0.01 & 0 & 0 \\ 0 & 0.01 & 0 \\ 0 & 0 & 0.01 \end{pmatrix}, R = \begin{pmatrix} 10 & 0 \\ 0 & 0.2 \end{pmatrix}, P_0 = \begin{pmatrix} 150 & 0 & 0 \\ 0 & 150 & 0 \\ 0 & 0 & 150 \end{pmatrix} \quad (5)$$

$$\hat{S}_{NH3,0} = 150, \hat{S}_{HNO2,0} = 40, \hat{S}_{NO3,0} = 5 \quad (6)$$

where Q is the system noise covariance matrix, R the measurement noise covariance matrix,P_0 the initial

error covariance and $\hat{S}_{NH3,0}$, $\hat{S}_{HNO2,0}$ and $\hat{S}_{NO3,0}$ are the initial guesses for the state variables. For this specific test case, we opted for a medium-large covariance in P_0 and a relatively small covariance in Q. The different values in R indicate that nitrate measurements can be trusted more than ammonia measurements, and is based on currently available real-life experience with such sensors. For the UKF, the following scaling parameters were used:

$$\alpha = 10^{-3}, \beta = 2, \kappa = -5, \quad (7)$$

where α is set to a small positive value, $\beta=2$ is optimal for Gaussian distributions, and $\kappa=3-L$,Ldenoting the length of the augmented state vector (Wan and van der Merwe 2001).The above simple tests are currently extended to test for (1) more complex models, including pH and oxygen dynamics and (2) conditions in which the simulated system model and the model observer are not necessarily the same.

PRELIMINARY RESULTS

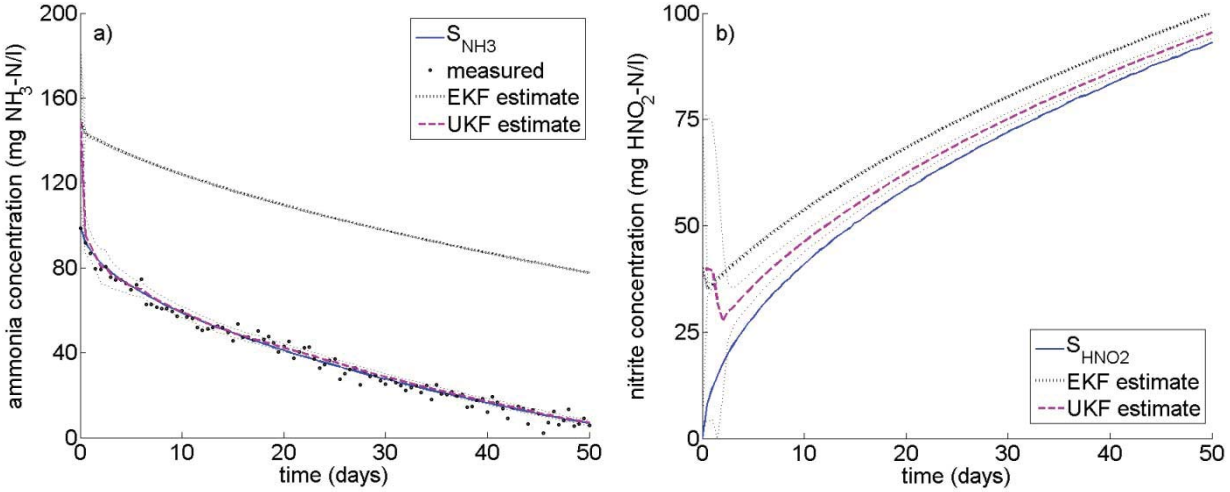

Figure 1. **a)** Ammonia concentration (solid, blue), measured ammonia (solid w. marker, dark red), EKF estimate of ammonia (dash-dot, dark gray), and UKF estimate of ammonia (dashed, magenta) as functions of time; **b)** nitrite concentration (solid, blue), EKF estimate of nitrite (dash-dot, dark gray), and UKF estimate of nitrite (dashed, magenta) as functions of time.

Both the EKF and UKF were tested on the same, simulated data. These data were obtained as discussed above. Most importantly, there is no direct measurement of nitrite concentration and the observers are set up to estimate its value. Figure 1a shows the internal state ammonia, the simulated measurement of ammonia and the estimates obtained with EKF and UKF, respectively. The estimates are also plotted with three standard deviations. In Figure 1b we see the internal state nitrite with the two estimates from EKF and UKF. The divergence of the EKF is most visible for ammonia, where the EKF-estimate never really estimates the state to a satisfying degree. The UKF on the other hand is able to track the states reliably, therefore showing a robustness against ill-defined prior means at time zero. Nitrite, as an unmeasured state, is estimated better with the UKF than with the EKF, i.e. the estimate obtained with the UKF converges faster and is closer to the true values.

CONCLUSIONS AND PERSPECTIVES

The EKF and UKF algorithms were both successfully implemented and applied to a simulated test case, which describes a simplified nitrification reactor. Under the assumption that nitrite, one of the three state variables, was unmeasured, and using the same initial data for both algorithms, the UKF performed better than the EKF. The UKF results in a reasonable estimate of the nitrite concentration, despite ill-defined initial guesses. Furthermore, the EKF lacks robustness to ill-guessing of initial states. The UKF, on the other hand, requires tuning of the scaling parameters, which is not yet completed.

As future work, we will test the same simplified observer model, as described in this paper, with a more complex simulated system as well as with full-scale data obtained from an operating reactor. Additionally, we will include pH and oxygen in the observer model if that is necessary to obtain reliable estimates. Moreover, we envision e.g. an evaluation of the effect of the model simplification, comparison of different sensor sets and evaluation of the importance of an online ammonia sensor.

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