

Soft-sensing nitrite in a urine nitrification system for resource recovery

Kris Villez^{1*}, Christian M. Thürlimann^{1,2}, Chris Brouckaert³, Alma Mašić¹

¹Eawag, Swiss Federal Institute of Aquatic Science and Technology, 8600 Dübendorf, Switzerland

²ETH Zürich, Institute of Environmental Engineering, 8093 Zürich, Switzerland

³School of Chemical Engineering, University of KwaZulu-Natal, Durban, 4041, South Africa

*Corresponding author: kris.villez@eawag.ch

Abstract: The unscented Kalman filter (UKF) has been proposed as general-purpose model-based soft-sensor (i.e. observer) for nonlinear dynamic processes. Prior work focused on use of the UKF with a dynamic model involving all reactions, including chemical speciation and acid-base reactions, as dynamic phenomena in a set of ordinary differential equations (ODEs). This results in an observer that is sensitive to noise. In this work, we present recent results obtained with a reformulated model within which the fast chemical reactions are represented and solved as algebraic equilibria. This leads to an accurate and reliable estimate of the nitrite concentration, which is the key variable for process supervision and control of the urine nitrification process under study.

Keywords: decentralized wastewater treatment, nitrite estimation, observer, resource recovery, soft-sensor, source separation, unscented Kalman filter, urine nitrification

INTRODUCTION

Monitoring and control challenge for decentralized wastewater treatment. The supervision of many decentralized process units for resource recovery comes with additional monitoring and control challenges. This is true for the fertilizer-producing urine nitrification process developed at Eawag (Udert & Wächter, 2012, Fumasoli et al., 2016). A failure occurs when the ratio of the activities of the ammonia oxidizing bacteria (AOB) and nitrite oxidizing bacteria (NOB) causes nitrite to accumulate. Washout of the NOB can occur if this left unmitigated. Recovery then requires washing the biomass with tap water or reactor emptying and start-up. Avoiding NOB-inhibiting nitrite concentrations is thus of paramount interest.

Existing approaches. One approach to tackle the nitrite challenge consists of UV-Vis spectrophotometry (Masic et al., 2015) and is currently tested as an on-line instrument (Thürlimann & Villez, 2016, Thürlimann et al., 2016). This spectrophotometric method remains rather expensive today because measuring a single UV wavelength is not sufficient to estimate the nitrite concentration (0–50 mg NO₂⁻-N/L) in the presence of high nitrate concentrations (2000–3000 mg NO₃⁻-N/L). For this reason, soft-sensing has been adopted as an alternative approach (Masic & Villez, 2014). Soft-sensors comprise a wide array of methods to estimate unmeasured variables on the basis of quantified relationships with measured variables. Soft-sensors are also known as filters or observers if the relationships describe the process mechanistically. The *Unscented Kalman Filter* (UKF) was selected in Masic & Villez (2014) because it does not require differentiation of the rate-of-change expressions, unlike the *Extended Kalman Filter*. The UKF however failed to provide reasonable estimates when more realistic disturbances and noise were added (not reported). This is attributed to the fact that the original model was given as a set of ordinary differential equations (ODE) which include the acid-base and salt speciation reactions.

Novelty of this contribution. With this work, we show that the above problem has been mitigated by reformulating the process model as a differential-algebraic-equation (DAE) system with the algebraic equations expressing the instantaneous equilibrium reactions. We also demonstrate that measurements of temperature, dissolved oxygen (DO), and the pH suffice for nitrite estimation.

MATERIALS AND METHODS

Model used for process simulation and within the observer. All results are based on a dynamic nonlinear model of the urine nitrification process (Fumasoli et al., 2015). This model is used for data simulation and soft-sensing, i.e. there is no mismatch between model and reality. We simulate urine nitrification in a continuous-flow stirred-tank reactor (CSTR) with suspended biomass and intermittent feeding as:

$$t_k \leq t < t_{k+1}: \quad \dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{c}(t), \mathbf{u}(t), \mathbf{v}(t_k)), \quad \mathbf{0} = \mathbf{h}(\mathbf{x}(t), \mathbf{c}(t)), \quad \mathbf{x}(0) = \mathbf{x}_0, \\ \mathbf{y}(t_k) = \mathbf{g}(\mathbf{x}(t_k), \mathbf{c}(t_k)) + \mathbf{w}(t_k), \quad \mathbf{v}(t_k) = \mathcal{N}(\mathbf{0}, \mathbf{Q}), \quad \mathbf{w}(t_k) = \mathcal{N}(\mathbf{0}, \mathbf{R})$$

with \mathbf{x} the $n_x = 8$ differential variables (reactor temperature; 5 component concentrations: oxygen, total ammonia, total inorganic carbon, total nitrate, total nitrite; 2 biomass concentrations: AOB and NOB), \mathbf{c} the algebraic variables which are the species concentrations (e.g., ammonium, molecular ammonia), \mathbf{u} known inputs, \mathbf{v} unknown input disturbances, and \mathbf{w} measurement errors. Both the input disturbances and measurement errors are sampled at regularly spaced times t_k (5 minutes).

The rate of change expressions $\mathbf{f}(\cdot)$ describe the dynamic effects of 4 AOB and NOB growth and decay reactions, 4 gas exchanges (CO_2 , HNO_2 , NH_3 , O_2), and liquid transport (heat, biomass, and components). The algebraic constraints are given as $\mathbf{h}(\cdot)$ and the measured variables are defined with $\mathbf{g}(\cdot)$. The following components are only subject to transport and their influent concentration is assumed constant: K^+ , Na^+ , Ca^{2+} , Mg^{2+} , Cl^- , acetate, inorganic phosphorus, and inorganic sulphate. Consequentially, their reactor concentrations are constant after sufficient time.

The 2 known inputs \mathbf{u} are the expected liquid flow rate and the expected gas flow rate. All $n_v=5$ input disturbances $\mathbf{v}(t)$ are implemented as proportional errors. For instance, the actual feed flow rate is always given as $u_1(t) \cdot (1 + v_1(t))$. The remaining input disturbances are implemented in this manner (influent temperature, gas flow rate, influent ammonia concentration, and influent total inorganic carbon concentration (TIC)). The mean influent ammonia and total inorganic carbon concentrations are known. The $n_y=3$ measured variables, temperature, DO, and pH, are subject to $n_w=3$ independent measurement errors $\mathbf{w}(t)$. \mathbf{Q} and \mathbf{R} are constant, diagonal, and known.

Low-level control. A bang-bang controller sets the feed rate to 70 L/d when the (noisy) pH measurement is below a lower limit. The feed rate is set to 0 L/d when the pH measurement is above an upper limit. The limits are at ± 0.1 around the desired pH value. The air flow is constant.

Unscented Kalman filter. The UKF is based on the generation of $L = n_x + n_v = 13$ Sigma points. These are vectors of the form $\chi = [\mathbf{x}^T \quad \mathbf{v}^T]$, include the differential states and the input disturbances (Wan & van der Merwe, 2000, Wu et al., 2005), and are used to simulate the process from one time step to the next. Our implementation matches the UKF for additive measurement errors in [9] and is tuned conventionally (i.e., $\alpha = 1, \beta = 2, \kappa = 3 - L = -10$).

RESULTS

Scenario 1. The data-generating process is simulated starting from a previously obtained pseudo steady-state operation with pH setpoint of 6.25. At 6 hours into the simulation, the pH setpoint is increased to 6.6 in an attempt to increase the process efficiency. Indeed, such a change increases the available fraction of the ammonia and speeds up the AOB activity. This therefore also increases the produced nitrite, hopefully leading to a matching increase of the NOB activity. In Figure 1, one can

see that this is not the case as nitrite starts to accumulate. After 18 hours following this change, the pH setpoint is reduced back to the original setpoint of 6.25. This is however unsuccessful given that the nitrite concentration keeps increasing and thereby stresses the importance of early detection of nitrite accumulation events. During this time, one can see that the UKF provides a reliable estimate of the nitrite concentration despite absence of a direct measurement.

Scenario 2. A similar scenario is simulated, however increasing the pH setpoint only to 6.5 after 6 hours. In this case, the nitrite accumulation is successfully mitigated after 18 hours by reducing the pH setpoint back to 6.25. The UKF again tracks the nitrite concentration successfully.

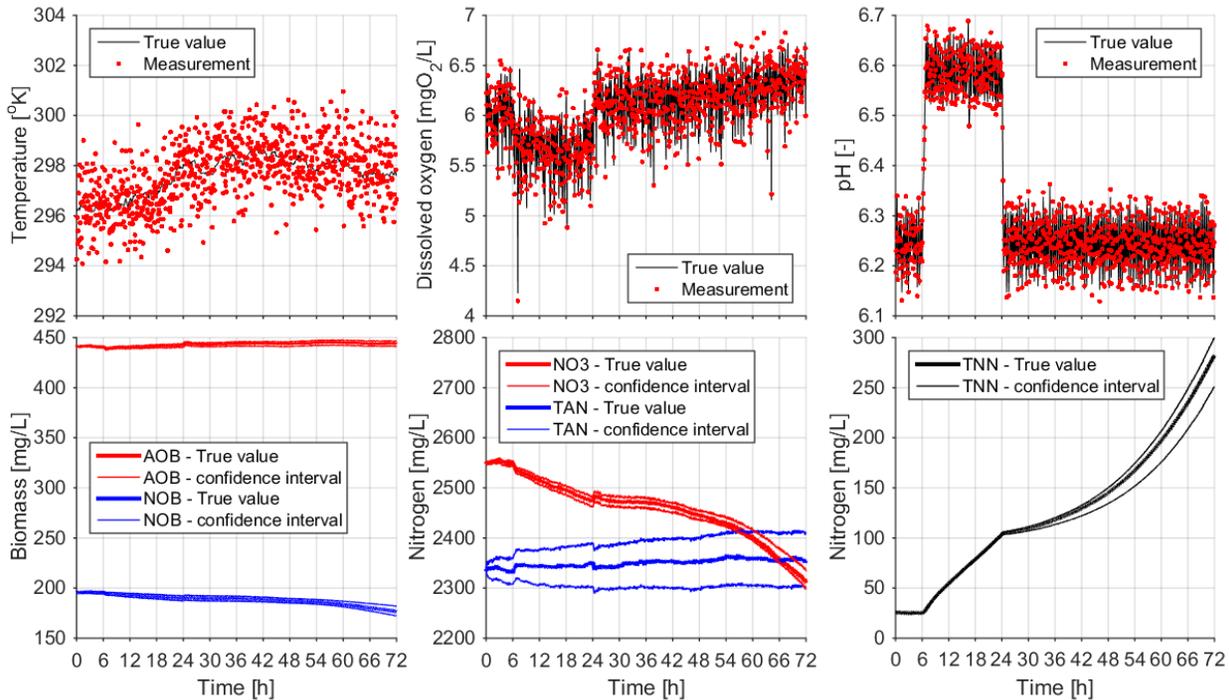


Figure 1. Scenario 1 – Top panels: Measured variables and measurements; Bottom panels: biomass and nitrogen components concentrations and their estimated 99.9% confidence intervals. At all times, the provided confidence interval for nitrite includes the true state value.

CONCLUSIONS

A major obstacle in the use of the UKF for nitrite estimation in a high-rate urine nitrification process has been removed. By means of reformulating the process model as a differential-algebraic equation (DAE), the UKF allows to estimate the nitrite reliably on the basis of three robust and commonly available measurements. Initial results suggest that the UKF can be used for a reliable detection of destabilizing nitrite concentration levels. Continued efforts, to be presented at the conference, are focused on evaluating whether the UKF is also robust to model-reality mismatch.

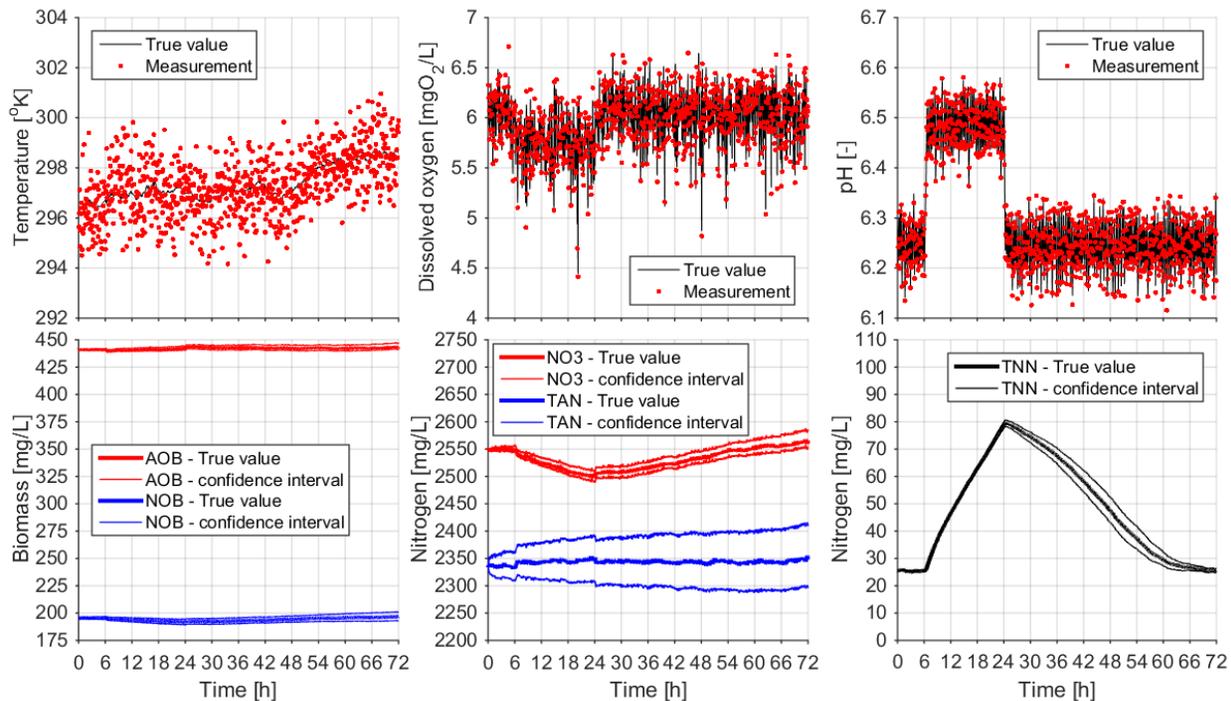


Figure 2. Scenario 2 – Top panels: Measured variables and measurements; Bottom panels: biomass and nitrogen components concentrations and their estimated 99.9% confidence intervals. At all times, the provided confidence interval for nitrite includes the true state value.

REFERENCES

- Fumasoli A, Morgenroth E, Udert K M (2015). Modeling the low pH limit of *Nitrosomonas eutropha* in high-strength nitrogen wastewaters. *Water Research* 83, 161–170.
- Fumasoli A, Etter B, Sterkele B, Morgenroth E, Udert K M (2016). Operating a Pilot-Scale Nitrification/distillation Plant for Complete Nutrient Recovery from Urine. *Water Science and Technology* 73(1), 215–222.
- Masic A, Villez K (2014). Model-based observers for monitoring of a biological nitrification process for decentralized wastewater treatment – Initial results. 2nd IWA Specialized International Conference Ecotechnologies for Wastewater Treatment (EcoSTP2014), Verona, Italy, June 23–25, 2014, 402–405.
- Masic A, Santos A T L, Etter B, Udert K M, Villez K (2015). Estimation of nitrite in source-separated nitrified urine with UV spectrophotometry. *Water Research* 85, 244–254.
- Thürlimann C M, Villez K (2016). In-situ nitrite sensing in a urine nitrification reactor by means of UV-Vis spectrometry. WEF/IWA Nutrient Removal and Recovery 2016 Conference (NRR2016), Denver, CO, USA, July 10–13, 2016, appeared on USB stick.
- Thürlimann C M, Udert K M, Morgenroth E, Villez K (2016). Nitrite sensing in a urine nitrification reactor with in-situ UV-Vis spectrometry. 3rd IWA New Developments in IT in Water Conference, Telford, UK, November 1–3, 2016, presented orally.
- Udert K M, Wächter M (2012). Complete nutrient recovery from source-separated urine by nitrification and distillation. *Water Research* 46(2), 453–464.
- Wan E A, van der Merwe R (2000). The Unscented Kalman Filter for Nonlinear Estimation. *IEEE 2000 Adaptive Systems for Signal Processing, Communications, and Control Symposium*, 153–158.
- Wu Y, Hu D, Wu M, Hu X (2005). Unscented Kalman filtering for additive noise case: augmented vs. non-augmented. *2005 American Control Conference*, 4051–4055.