KV_C041
Thürlimann, C. M., Dürrenmatt, D. J., Villez, K. (2015). Evaluation of Qualitative Trend Analysis as a tool for Automation. 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering (PSE2015/ESCAPE25), Copenhagen, Denmark, May 31 - June 4, 2015, 2531-2536.

Krist V. Gernaey, Jakob K. Huusom and Rafiqul Gani (Eds.), 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering.
31 May - 4 June 2015, Copenhagen, Denmark.

Evaluation of Qualitative Trend Analysis as a Tool for Automation

Christian M. Thürlimann[a], David J. Dürrenmatt[b] and Kris Villez[a]

[a]*Department of Process Engineering, Eawag, Swiss Federal Institute of Aquatic Science and Technology; Dübendorf, Switzerland*
[b]*Rittmeyer AG, Baar, Switzerland*
kris.villez@eawag.ch

Abstract

Ammonium (NH_4^+) load based aeration control on biological wastewater treatment plants saves costs and enhances nitrogen removal. However, the need for maintenance intensive NH_4^+ sensors hamper the controls application in practice. Alternatives, in the form of soft-sensors are broadly discussed in academia. A soft-sensor recently described in literature exploits the pH effects induced by biological NH_4^+ oxidation. This concept is now further developed by means of qualitative trend analysis (QTA). Previously, the qualitative path estimation (QPE) algorithms was proposed as a fast and reliable QTA algorithm for batch process data analysis. It does not allow online application in continuous flow systems however. In this work, a modification of QPE, call qualitative state estimation (QSE), is proposed as a suitable algorithm for continuous-flow systems. Initial tests indicate that the QSE algorithms is a robust technique for extraction of relevant information in a full-scale environment. At the WWTP Hard in Winterthur, this resulted in cost-saving automation of the aeration system. This contribution summarizes these first results.

Keywords: ammonia control, biological wastewater treatment, hidden Markov model, kernel regression, process monitoring

1. Introduction

Ammonium (NH_4^+) controlled aeration is a well known and widely applied technique (Åmand et al., 2013) for automation of biological wastewater treatment plants (WWTPs). By controlling the ammonium concentration in the effluent, energy costs can be reduced while violation of effluent concentration limits can be avoided. Furthermore, optimization of the oxidation processes ensures that denitrification capacity can be increased and enhanced biological phosphorus (bio-P) removal can take place without the need to increase reactor volumes (Rieger et al., 2014). However, economical application of such ammonium control is only feasible on larger WWTPs, where the energy and cost savings outweigh the NH_4^+ sensors installation and maintenance costs (Winkler et al., 2004; Åmand et al., 2014). Haimi et al. (2013) present numerous studies dealing with NH_4^+ soft-sensors evading the need for a physical NH_4^+ sensor. Importantly, these studies mainly investigate black-box models, which give rise to a series of challenges for widespread full-scale application such as the need to recalibrate the methods for each application, lack of transparency and trust by operators, and potentially difficult implementation and fine-tuning. A soft-sensor based on a mechanistic principle was presented by Ruano et al. (2009). This soft-sensor takes advantage of the acidifying effect of biological NH_4^+ oxidation, which is also known as nitrification. Instead of estimating the NH_4^+ concentration, the soft-sensor monitors the net effect of nitrification (acidifying) and CO_2 stripping (proton-consuming). In locations of a WWTP where nitrification occurs, a net production of protons is typical and causes the pH to drop. Where nitrification is not occurring, a net increase of the pH results due to CO2 stripping. Ruano et al. (2012) manipulated the aeration intensity in an activated sludge system to keep the difference between two pH measurements located at the in- and outlet of an aerated tank sequence at a given setpoint. Practically, the pH difference is as a proxy for the balance between proton production due to nitrification and the proton consumption from CO_2 stripping. The combined effects of hydraulic transport, mixing conditions, oxidation, and stripping contribute to a complex relationship between the ammonia concentration and the pH. This relationship can however be understood qualitatively most of the time so that this concept is relatively easy to use for a diverse set of WWTP configuration. Under steady-state conditions, a certain pH difference corresponds to a certain NH_4^+ effluent concentration. Unfortunately, using a fixed pH difference as a control setpoint assumes perfect pH sensors. In practice, significant signal drift occurs, which can only be kept in check by a prohibitively high maintenance effort. This eliminates the advantage of pH sensors over conventional NH_4^+ sensors for ammonium control. We however claim that the pH difference signal can also be used in a less stringent fashion so that monitoring the pH difference remains useful in practice. Fig. 1 shows the recorded pH difference (top) and the measured NH_4^+ concentration measured (bottom) from the setup at the Winterthur WWTP as described in section Hardware Setup. The qualitative similarity between these two signals is obvious as the maxima in both signals are remarkably synchronous. Consequently, we present in this paper a qualitative trend analysis (QTA) method to use this qualitative similarities for an NH_4^+ load dependent aeration control. This QTA based method is used to detect peak NH_4^+ loads entering the WWTP. This detection allows to adjust the setpoints for the dissolved oxygen (DO) concentration accordingly and thereby optimise the aeration energy costs of the plant. The QTA method used here is referred to as Qualitative State Estimation (QSE) and is based on the earlier Qualitative Path Estimation (QPE) algorithm Villez (2015). The main differences are *(i)* that the Hidden Markov Model (HMM) now represents an ergodic process, as opposed to the linear Markov chain for the QPE algorithm and *(ii)* that the state estimation method is different from the Viterbi algorithm used for QPE.

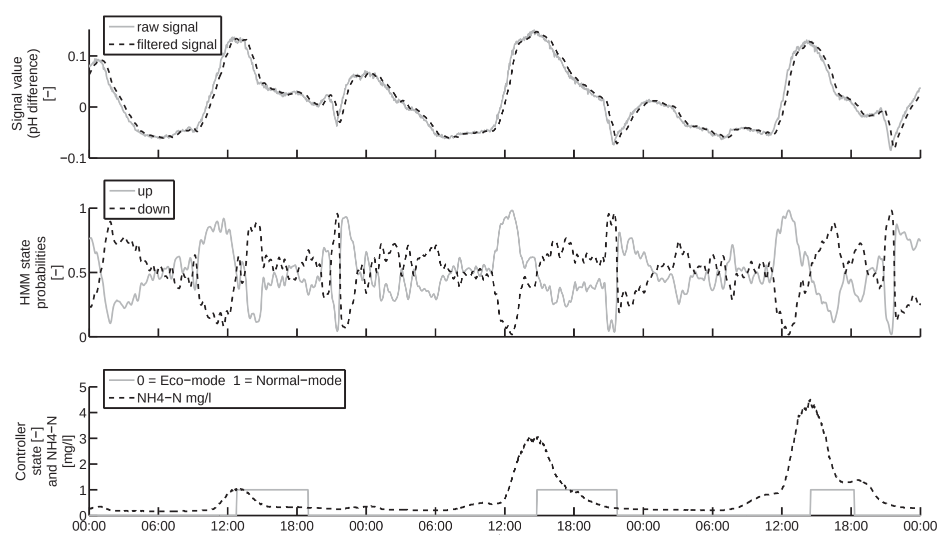

Figure 1: Demonstration of the QSE algorithm: Top – pH difference raw/filtered; Middle – Qualitative trend probabilities; Bottom – Control state and NH_4^+ measurements.

2. Methods

2.1. Hardware Setup

The studied municipal WWTP Hard, Winterthur, Switzerland exhibits one stirred and three aerated activated sludge tanks for oxidation of organic compounds as well as NH_4^+ (cfr. Fig. 2). These are located between the primary clarifier and the secondary clarifier. The signal used in the proposed control system, consists of the difference between a pH measurement in the first aerated tank (upstream, *us*) and the last aerated tank (downstream, *ds*). An ion selective electrode (ISE) measuring the NH_4^+ concentration is placed in the second aeration tank in order to validate and fine-tune the pH difference based control loop.

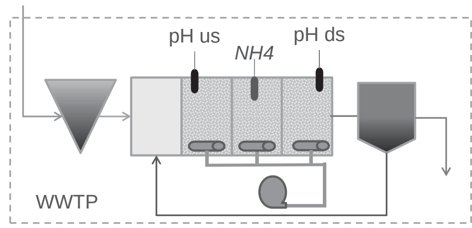

Figure 2: Location of pH sensors (pH *us* and pH *ds*) and ammonium sensor (*NH4*).

2.2. Qualitative Trend Analysis

As mentioned above, QTA comprises a set of algorithms for segmentation of time series. Each segment, referred to as an *episode*, is defined by a start and end time. Within these time points, the sign of one or more of the signal's derivatives is considered constant. In this application only the sign of the first derivative is considered as this is sufficient to define the qualitative features of interest, namely the minima and maxima. A specialised algorithm, called qualitative state estimation (QSE), is developed to enable fast and reliable identification of these extrema. It is based on the QPE algorithm, which was found to be fast and reliable for batch process diagnosis (Villez, 2015). The QSE algorithm consists of two steps.

Step 1 – Qualitative trend probabilities via kernel regression: First, the algorithm estimates the likelihood that the analysed signal is decreasing or increasing at given time points. This assessment is based on local polynomial fit to the data, which consist of pairs of an independent variable, t_j ($j = 1...m$), which is time in our case, and the dependent variable measurement, y_j, which is a pH difference signal in this study. The polynomial coefficients, β_i, are computed for sample index i by minimising the following weighted least squares (WLS) objective function:

$$\min_{\beta_i} \sum_{j=1}^{m} K_{i,j} \cdot (y_j - \mathbf{x}_j^T \cdot \beta_i)^2 \tag{1}$$

$$\text{with } \mathbf{x}_j = \begin{bmatrix} (\mathbf{t}-t_j)^0 \\ (\mathbf{t}-t_j)^1 \\ \vdots \\ (\mathbf{t}-t_j)^p \end{bmatrix}, \quad d_{i,j} = \frac{|t_i - t_j|}{\lambda}, \quad K_{i,j} = \begin{cases} (1-d_{i,j}^3)^3, & \text{if } d \leq 1 \\ 0, & \text{otherwise} \end{cases} \tag{2}$$

The polynomial degree p is 2 or higher. Furthermore, the tri-cube kernel function is used to determine the weighting of the data points. The weights, $K_{i,j}$, are completely specified by a meta-parameter λ. Only data points within the distance of λ to the sample of interest i have a weight larger than zero and contribute to the local model. The data weights decrease as the distance from the considered sample, i, increases. Eq. 1 can be solved analytically as follows:

$$\begin{aligned}\beta_i &= \mathbf{H}_i \cdot \mathbf{y} \\ \mathbf{H}_i &= (\mathbf{X}_i^T \cdot \mathbf{W}_i \cdot \mathbf{X}_i)^{-1} \cdot \mathbf{X}_i^T \cdot \mathbf{W}_i \\ \mathbf{X}_i &= \begin{bmatrix}(\mathbf{t}-t_i)^0 & (\mathbf{t}-t_i)^1 & \cdots & (\mathbf{t}-t_i)^p\end{bmatrix}\end{aligned} \qquad \underset{m\times m}{\mathbf{W}_i} = \begin{bmatrix} K_{i,1} & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots \\ 0 & & K_{i,j} & & 0 \\ \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & K_{i,m} \end{bmatrix} \tag{3}$$

The matrix $\mathbf{X}_i$ is a polynomial basis matrix whereas $\mathbf{W}_i$ is a diagonal sample weight matrix. The polynomial fitting problem is also known as kernel regression and is equivalent to a linear projection. Theoretical point-wise covariance matrices can thus be computed when the measurement errors are assumed to be drawn independently and identically from a Gaussian distribution ($N(0;\sigma_y)$):

$$\Sigma_{\beta_i} = \mathbf{H}_i \cdot \sigma_y \cdot \mathbf{I}_n \cdot \mathbf{H}_i^T \tag{4}$$

The point-wise distribution for the coefficient of the linear term in the polynomial is then:

$$\beta_{1,i} \sim N(\beta_{1,i}(2), \Sigma_{\beta_i}(2,2)) = N(\mu_{1,i}, \sigma_{1,i}) \tag{5}$$

By integration of the probability mass under this density curve over the positive (negative) section of the real axis, one obtains the probability for a upward trend, $P_{u,i}$ (downward trend, $P_{d,i}$). More specifically, one computes these *qualitative trend probabilities* as (Fig. 1 middle):

$$P_{y,i}(1) = P_{u,i} = \int_{u=0}^{+\infty} \frac{1}{\sigma_{1,i}\sqrt{2\pi}} \cdot exp\left(-\frac{(u-\mu_{1,i})^2}{2\cdot\sigma_{1,i}^2} du\right) \qquad P_{y,i}(2) = P_{d,i} = (1-P_{u,i}) \tag{6}$$

Step 2 – Probability integration by means of a Hidden Markov Model (HMM): Discrete state estimation by means of a Hidden Markov Model is used as a filtering step to remove noisy features in the qualitative trend probabilities for the derivative signs as computed in the first step of the QSE algorithm. To this end, the monitored discrete state process is assumed to be represented by a Markov process. Mathematically, a Markov process is described by expressing the likelihood for each of the process states at time i conditionally to the likelihoods of the same states at time $i-1$:

$$\Lambda(\mathbf{s}(i) = t \mid i-1) = \sum_{p=1}^{q} \mathbf{T}_i(t,p) \cdot \Lambda(\mathbf{s}(i-1) = p \mid i-1) \tag{7}$$

The likelihoods, $\mathbf{T}_i(t,p)$, express the chance that the process state will be the target state t at time i conditional to the process being in the state p at time $i-1$. Whereas the QPE method makes use of an upper triangular matrix, $\mathbf{T}$, implying a non-ergodic Markov process, the QSE method proposed here poses no such restrictions. In addition, all transition likelihoods on the diagonal are set to one (1) and the off-diagonal elements are set to an identical and time-invariant value (γ):

$$\mathbf{T}_i(p,t) = \begin{cases} 1, & p = t \\ \gamma_i(t,p) = \gamma, & \text{otherwise} \end{cases} \tag{8}$$

The maximum likelihood (ML) state estimate at time i, $\hat{s}_i$, is now given as:

$$\hat{s} = \underset{t}{\operatorname{argmax}}\, P_{s=t}(i|i) \quad \text{with} \quad P_{s=t}(i|i) = P_{y,i}(t) \cdot \sum_p \mathbf{T}_i(t,p) \cdot P_{s=t}(i-1|i-1) \tag{9}$$

By means of the above recursive equations, one tracks the most likely state at a given time conditional to the evidence gathered until that time and represented by the qualitative trend probabilities computed by Eq. 6. It is this series of ML state estimates that are fed into the controller logic.

3. Results

3.1. Feedback Control Based on QTA

Table 1: Control states and qualitative process properties.

Control Mode	Ammonium Load	Oxygen Setpoint	pH Difference
Eco	Low	Low	Low
Normal	High	High	High

The proposed feedback control based on the QTA is a bang-bang controller. In low load situations (a.k.a. *Eco*-mode) the dissolved oxygen (DO) concentration is lowered in all tanks by reducing the DO setpoint for the corresponding slave proportional-integral (PI) control loops. This slows the nitrification process down, which in turn reduces the oxygen demand and thus the aeration energy and costs. When facing a NH_4^+ peak load (a.k.a. *Normal*-mode), one increases the DO setpoint to speed up the nitrification process so that a violation of the effluent concentration limits is prevented. Proper recognition of peak and normal loads is critical to maintain environmentally safe operation limits while minimising operational costs associated with aeration. QTA is deployed to detect the two modes (Eco and Normal) online (see Table 1). A small width for the support window (λ (cfr. Eq. 1) allows a short response time. However, small oscillations lead to the identification of irrelevant minima and maxima. The HMM-based method was therefore complemented with a number of heuristic quantitative rules, which enable the separation between these small oscillations, which are unrelated to changes in the NH_4^+ concentration, and large trends, which correlated to significant dynamics of the NH_4^+ concentration. Firstly, the recognition of the switch from Eco- to Normal-mode incorporates three rules, which are: *EN1* – At least one minimum, i.e. switch of the HMM state estimate from the downward to upward state, needs to be registered in Eco-mode; *EN2* – The difference between the current pH difference signal value and the lowest minimum registered in the Eco-mode is larger than a critical minimum level, called the *Minimal Difference*; and *EN3* – A maximum, i.e. switch of the HMM state estimate from the upward to downward state, needs to occur after both *EN1* and *EN2* are evaluated as true. These rules ensure *(i)* that the minimum NH_4^+ concentration as occurring during the Eco-mode is recognised properly and *(ii)* a recognised maximum truly corresponds to an NH_4^+ peak load. To switch back from Normal- to Eco-mode, the following heuristic rules are applied: *NE1* – The pH difference signal has to drop below the level defined by the minimum pH difference signal registered in the last Eco-mode plus a tolerance, called *Maximal Difference*. This rule ensures that the nitrification activity is at a similar (low) activity as recorded before; *NE2* – At least one minimum needs to occur after *NE1* is evaluated as true. *NE3* – The Normal-mode needs to be active for a minimal time period. These rules ensure that nitrification activity is always brought to its minimum thereby allowing for proper registration of the minimum NH_4^+ concentration. These rules govern the bang-bang controller, which switches between the Eco-mode, corresponding to low NH_4^+ loads, and the Normal-mode, which corresponds to high NH_4^+ loads.

3.2. Integration into the pre-existing control scheme.

The QTA based bang-bang controller only determines if the plant faces a high (Normal-mode) or low (Eco-mode) NH_4^+ load situation. In the Normal-mode, a high DO setpoint is set for the slave PI controllers regulating the DO concentrations. In Eco-mode, a low DO setpoint is implemented. Because the slave controllers and the aeration system exhibit their own response times, a number of safety rules are implemented to ensure the QTA-based bang-bang controller output is handled well and only when appropriate. One additional rule checks if the plant is facing a high hydraulic load. Detection of peak hydraulic loads are detected faster by means of flow measurements at the inlet of the WWTP and induce a switch to the Normal-mode without further delay. Similarly, a pH sensor at the inlet of the plant can be used as a proxy for toxic, industrial wastewater. By switching to the Normal-mode maximum survival of the sensitive bacterial community is then ensured.

3.3. Experiences and Outlook

The proposed bang-bang controller has been tested on the full-scale WWTP Hard in Winterthur. During this time, the effluent concentration of NH_4^+ did not increase significantly compared to exclusive operation in Normal-mode and remained below the legal limit. Current estimates of the aeration energy savings amount to 15%. Early development and testing was executed jointly with Rittmeyer AG, which has developed a commercially viable version as a module in the RITUNE® software for WWTP supervision and optimisation. Further work is focused on testing and evaluation of the QTA-based controller for other WWTPs. Special attention will be given to *(i)* the ease of implementation and fine-tuning and *(ii)* transparency of the controller to technical operators. QTA methods are being developed to handle *(i)* inflection points, *(ii)* discontinuities (Villez and Habermacher, 2015), as well as *(iii)* multivariate data series.

4. Conclusion

A new method for qualitative trend analysis (QTA) has been developed and tested as part of an advanced control strategy for NH_4^+ removal in biological WWTPs. By means of the QTA method, called qualitative state estimation (QSE), one can differentiate between high and low NH_4^+ load situations on the basis of cheap and reliable pH sensor signals only. Initial tests with this controller delivered reduction in aeration energy requirements of over 10%. As such, the proposed method holds great promise as a robust approach to minimise energy costs in small biological WWTPs.

5. Acknowledgement

This work was supported by the Commission for Technology and Innovation (CTI) of the Swiss Federal Department of Economic Affairs Education and Research (EAER). (CTI project no. 14351. PFIW-IW). The authors thank the staff of the WWTP Hard in Winterthur for the opportunity and assistance with this study.

References

Åmand, L., Laurell, C., Stark-Fujii, K., Thunberg, A., Carlsson, B., 2014. Lessons learnt from evaluating full-scale ammonium feedback control in three large wastewater treatment plants. Water Science & Technology 69 (7), 1573–1580.

Åmand, L., Olsson, G., Carlsson, B., 2013. Aeration control a review. Water Science & Technology 67 (11), 2374–2398.

Haimi, H., Mulas, M., Corona, F., Vahala, R., 2013. Data-derived soft-sensors for biological wastewater treatment plants: An overview. Environmental Modelling & Software 47, 88–107.

Rieger, L., Jones, R. M., Dold, P. L., Bott, C. B., 2014. Ammonia-based feedforward and feedback aeration control in activated sludge processes. Water Environment Research 86 (1), 63–73.

Ruano, M., Ribes, J., Seco, A., Ferrer, J., 2012. An advanced control strategy for biological nutrient removal in continuous systems based on pH and ORP sensors. Chemical Engineering Journal 183, 212–221.

Ruano, M. V., Ribes, J., Seco, A., Ferrer, J., 2009. Low cost-sensors as a real alternative to on-line nitrogen analysers in continuous systems. Water Science & Technology 60 (12), 3261–3268.

Villez, K., 2015. Qualitative path estimation: A fast and reliable algorithm for qualitative trend analysis. AIChE Journal Accepted, In press.

Villez, K., Habermacher, J., 2015. Shape constrained splines with discontinuities for anomaly detection in a batch process. Accepted to the 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering (PSE2015/ESCAPE25), 31 May - 4 June 2015, Copenhagen, Denmark.

Winkler, S., Rieger, L., Saracevic, E., Pressl, A., Gruber, G., 2004. Application of ion-sensitive sensors in water quality monitoring. Water Science & Technology 50 (11), 105–114.