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Qualitative Trend Analysis as a Tool for pH-based Ammonium Soft-Sensor in Full-Scale Continuous WWTP

Christian M. Thürlimann*, David J. Dürrenmatt**, Kris Villez*

* Eawag, Swiss Federal Institute of Aquatic Science and Technology, 8600 Dübendorf, Switzerland
(E-mail: *christian.thuerlimann@eawag.ch; kris.villez@eawag.ch*)
** Rittmeyer AG, 6341 Baar, Switzerland
(E-mail: *david.duerrenmatt@rittmeyer.com*)

Abstract
Ammonium control on wastewater treatment plants (WWTP) reduces costs and increases nutrient removal performances. Despite these advantages its application is bound to maintenance and cost intensive ammonium sensors. Hence, smaller WWTPs do not manage to outweigh their expenditures for the control infrastructure with its cost savings. Soft-sensors could replace the physical sensors and are widely discussed in literature. A mechanistic soft-sensor recently described exploits the acidifying effect induced by nitrification in a continuous flow system. With two pH sensors a difference is measured along the aerated biological reactors, which corresponds qualitatively to the ammonium concentration. Consequently, we propose to use qualitative trend analysis (QTA) tools to establish a two-point controller adapting the oxygen setpoints according to the ammonium load. However, the known QTA algorithms (e.g. qualitative path estimation) are not suitable for online control. Thus, a new algorithm, called qualitative state estimation (QSE), is developed for this purpose. Given the pH difference signal the QSE based controller distinguishes among high and low load situations. At the WWTP Hard in Winterthur, this resulted in a cost-saving automation of the aeration system. This contribution summarises these first results.

Keywords
ammonium control, biological wastewater treatment, observer, process monitoring, qualitative trend analysis

INTRODUCTION

Up to 60% of the total energy consumption of a wastewater treatment plant originates from aeration (Rieger et al. 2008). Significant reduction for aeration energy needs can be achieved with conventional ammonium control (Åmand et al. 2013). Ammonium control adapts the aeration intensity according to the ammonium concentration. A high ammonium concentration asks for a high nitrification performance thus for a high dissolved oxygen (DO) concentration. In low load situations the DO concentration can be reduced so to reduce the aeration intensity and associated costs without risking an effluent concentration limit violation. Apart from the achieved energy savings, ammonium control smoothes the ammonium effluent load, increases the denitrification capacity and enhances the biological phosphorus removal (bio-P) (Rieger et al. 2014). However, the ion selective electrodes (ISE) measuring the ammonium concentration are vulnerable in harsh environments like wastewater and require a high maintenance effort (Winkler et al. 2004). This hampers the economical application on smaller WWTPs, where the cost savings seldom exceed the installation and maintenance expenditures (Åmand et al. 2014). To evade the physical ISE sensor, a whole range of ammonium soft-sensors has been proposed in academia. Haimi et al. (2013) reviewed some of them in their study, but they often suffer from the fact that they rely on black-box models. As these models are neither transparent for operators nor globally valid, their application in practice is challenging. Ruano et al. (2009) presented a soft-sensor based on a mechanistic principle. The pH dynamics caused by nitrification and aeration are used to estimate the required aeration intensity. More concretely, the soft-sensor measures the net balance of the acidifying nitrification and the hydrogen ion neutralising aeration (CO_2-stripping). Nitrification will take place, when ammonium is available and decreases the pH value of the wastewater as more protons are produced than removed from the system. If the nitrification becomes limited or is halted by low ammonium concentrations, the proton balance becomes negative due to the higher CO_2 stripping evoked by over aeration, which in turn causes a rise of the pH. Ruano et al. (2012) exploited this to adjust the aeration intensity so that a stable difference between the first and last aerated activated sludge tank results (cf. Fig. 2). An incoming ammonium load leads to a lower pH in the first tank; consequently the difference to the last aerated reactor rises. When the ammonium reaches the downstream pH sensor, the pH difference drops. Later, the decreasing load enables the plant to nitrify all ammonium in the first two reactors. This evokes net proton consumption in the last reactor, resulting in a pH increase at the downstream sensor. In parallel, the nitrification in the first reactor will last until the peak load has passed resulting in a stable pH value at the upstream sensor. Ruano et al. (2012) smoothed these variations in the pH difference out by continuously adjusting the aeration intensity. This, in turn causes higher or lower CO_2 stripping, which removes protons from the system, keeping its concentration steady (pH = $-\log(H^+)$). For steady state conditions a certain pH difference is linked to a particular ammonium concentration. The mechanistic process behind the soft-sensor is transparent and well understood. This makes it relatively easy to apply this concept on diverse WWTP configurations. However, the control requires accurate pH sensor values, which make this control hard to maintain. This voids the maintenance advantage over conventional ammonium sensors. In this contribution we claim that this mechanistic concept can still be exploited in practice without stringent requirements regarding the pH sensors stability thanks to an automated and intelligent interpretation of the pH difference signal.

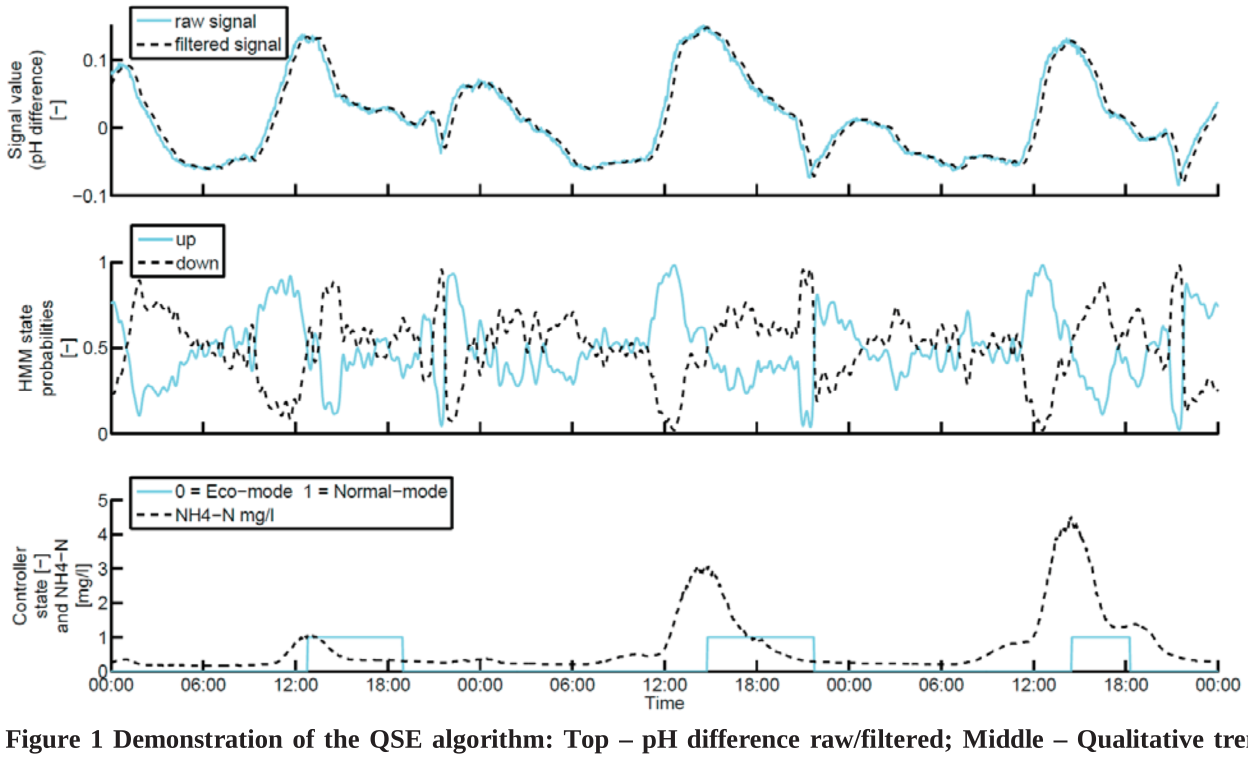

Figure 1 Demonstration of the QSE algorithm: Top – pH difference raw/filtered; Middle – Qualitative trend probabilities; Bottom – Control state and ammonium measurements. (Thürlimann et al., Submitted)

Figure 1 shows the recorded pH difference (top) and the measured ammonium concentration (bottom). The signals share obvious qualitative similarities. For instance, the maxima are particularly synchronous. Hence, we present a qualitative trend analysis (QTA) tool to utilise this qualitative similarities for an ammonium load dependent aeration control. The incoming ammonium peaks are detected by means of automated interpretation of the pH difference. The difference results from the upstream minus the downstream pH value. The extracted information is then used to adjust the setpoints for the DO concentration accordingly and thereby optimise the aeration energy, operational costs and effluent quality of the WWTP. The QTA method used here is called qualitative state estimation (QSE) and is based on the earlier qualitative path estimation (QPE) algorithm developed in Villez and Rengaswamy (2013) and Villez (Submitted). Two main features differentiate the methods *(a)* the hidden Markov model (HMM), representing an ergodic process, as contrasted with the non-ergodic linear Markov chain for the QPE algorithm and *(b)* the Viterbi algorithm used for QPE has fundamental differences to the now applied HMM state estimation method.

METHODS

Plant and Hardware Setup

The studied WWTP Hard in Winterthur, Switzerland treats mainly municipal wastewater from approximately 130'000 population equivalents. It is a conventional activated sludge treatment with a pre-denitrification stage, iron-based phosphorus precipitation and effluent sand filters. Due to the small receiving water body, the plant has strict discharge requirements (e.g. < 1 mg NH_4-N/l). As shown in Figure 2, each biological treatment lane consists of one stirred and three aerated tanks. The pH sensors were placed in the first (pH us) and last (pH ds) aerated reactor. To validate and fine-tune the control loop an ISE was placed into the second aerated reactor to measure the ammonium online (cf. Fig. 1 (bottom) and Fig. 2).

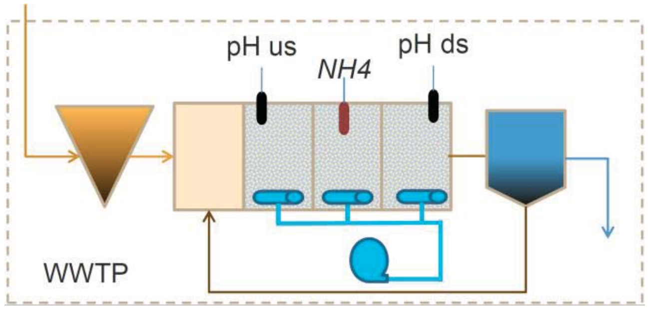

Figure 2 Hardware setup and treatment lane scheme WWTP Hard, Winterthur

Qualitative Trend Analysis

QTA encompasses various sets of algorithms for the segmentation of time series. Each segment is defined by a start and an end time. In between, the sign of signal derivatives are assumed to be constant (e.g. positive or negative). Based on the results shown in Figure 1, it was decided to focus on the first derivative of the pH difference signal as this feature is sufficient to define the qualitative points of interest, namely the maxima and minima. QSE aims for a rapid and reliable detection of these extrema. This algorithm is based on the QPE algorithm, developed for batch process diagnosis (Villez, Submitted).

Step 1 – Qualitative Trend Probabilities via Kernel Regression. In the first step QSE estimates the probabilities that the given signal has a positive or negative first derivative. This is done with a local polynomial fit to the data. The data is composed of the pH difference measurement as the dependent variable (y_j, $j = 1 \ldots m$), and time as the independent variable (t_j). By minimising the following weighted least squares (WLS) objective function (cf. Eq. 1), local polynomial coefficients (β_i) are computed as follows for each sample index (i).

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

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

The used tri-cube kernel function ($K_{i,j}$) defines the weight for each data point. The weights are determined by the parameter λ. Only within a distance λ to the sample of interest (i), data points contribute to the local fit. The weights decay with increasing distance from the considered time point (t_i). The polynomial degree (p) is always larger than one. Eq. 3 shows the analytical solution of Eq. 1 and 2:

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

with the polynomial basis matrix (X_i) and the diagonal sample weight matrix (W_i) specified a priori. In this context, the polynomial local fit is a linear projection and also known as kernel regression. Thus, theoretical point-wise covariance matrices can only be computed under the assumptions that measurement errors are drawn independently and identically from a Gaussian distribution ($N(0,\sigma_y)$):

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

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

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

The probability for an upward trend, ($P_{u,i}$, downward trend: $P_{d,i}$), results from the integration of the probability function from zero to positive (negative) infinity. Eq. 6 shows the formulas for the integration resulting in the qualitative trend probabilities (cf. Fig. 1 middle):

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

Step 2 – Probability Integration trough Hidden Markov Model (HMM): To filter noise from the qualitative trend probabilities (cf. Eq. 6) one estimates discrete states with the hidden Markov model. These discrete states are assumed to follow a Markov process. A Markov process is described by calculating the likelihood for each of the process states at time (t_i) restricted by the likelihoods of the same states at time (t_{i-1}):

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

In Eq. 7, the probability that the process is in state t at sample i conditional to being in state p at sample $i-1$ is expressed as $T_i(t,p)$. This is the point, where the QSE method starts to differ from the known QPE approach: QPE makes use of an upper triangular matrix as the transition matrix *(T)*. This means that a non-ergodic linear Markov chain is assumed. In contrast the QSE method uses a transition matrix with no such restrictions. In practical terms, the diagonal values of T are all set to one; the off-diagonal elements have the identical and time invariant value γ.

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

$\hat{s}_i$, the maximum likelihood (ML) state estimate at time *(i)*, is calculated as follows:

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

The qualitative trend probabilities (cf. Eq. 6) contain all information about the prior states. By taking the qualitative trend probabilities into account, one can tracks the state estimate online. The resulting ML state estimates are fed into the controller logic.

RESULTS

Soft-Sensor Feedback Control

The QTA is set up to distinguish ammonium load states, high and low. In case of a low load situation the feedback control lowers the oxygen input by passing a low oxygen setpoint to the corresponding slave proportional-integral control loop adjusting the airflow. A lower dissolved oxygen (DO) concentration slows down the nitrification process, which in turn reduces the oxygen requirements and eventually the aeration costs. Nevertheless, the nitrification performance is still sufficient to comply with effluent concentration limits. In contrast, an incoming ammonium peak could violate these limits and triggers the control to boost the nitrification process by increasing the DO setpoint. For a proper control behaviour that ensures compliance with effluent limit concentrations but also considerable energy and cost savings, the QTA analysis needs to be complemented with a number of heuristic rules. Currently, the support window (λ in Eq. 1) is kept rather short which allows a fast response time at the expense of a noisy state estimate signal. As a result, the QSE algorithm identifies some irrelevant minima and maxima, which can lead to unwanted disturbances. In the next paragraph all applied rules to prevent this are discussed (cf. **Fout! Verwijzingsbron niet gevonden.**).

Three rules are set for the control state change from Eco- to Normal-mode. Rule 'Eco to Normal 1' (EN1) implies that the QTA has to detect at least one minimum, which means a HMM state change from the downward to an upward trend needs to be recorded. To comply with EN2, the difference between the lowest minimum recorded during the current Eco-mode and the current pH difference signal value is larger than a critical minimum threshold value *Minimal Difference.* EN3 expects a detection of a maximum, i.e. switch from HMM state upward to downward trend, after EN1 and EN2 are evaluated as true. These rules guarantee that the lowest ammonium concentration is registered (EN1), the control only considers relevant ammonium peak loads (EN2) and that the control only switches when the nitrification at the downstream pH sensor speeds up (EN3). The switch back from Normal to Eco-mode (NE) includes three rules as well. The pH difference signal has to fall below the threshold defined by the lowest minimum registered in the last Eco-mode and an additional tolerance *Maximal Difference* (NE1). To comply with NE2 the control needs to detect at least one minimum. The third rule, NE3 checks if the Normal-mode is active for a minimal time length. These rules ensure that the ammonium effluent concentration is close to the global minimum of the last Eco-mode, while permitting drift of the pH signals (NE1-NE2). To prevent oscillatory control behaviour, the controller can not switch back immediately to Eco-mode (NE3).

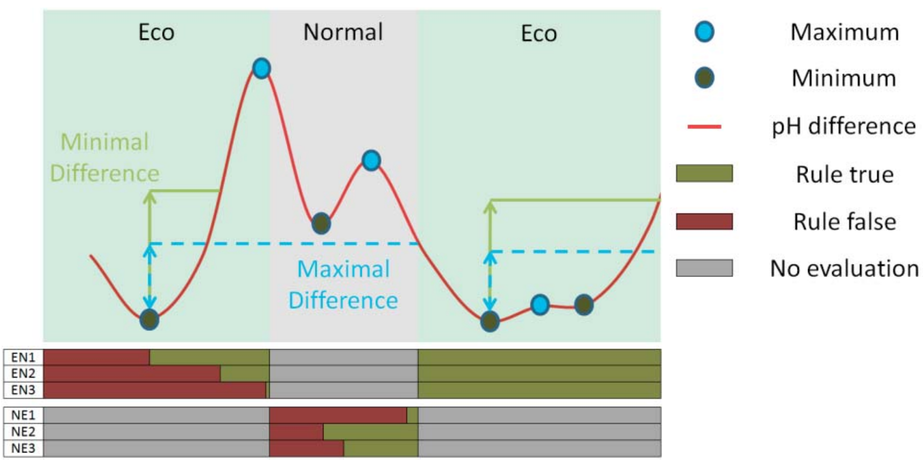

Figure 3 Demonstration of controller behaviour based on qualitative and quantitative rules.

Tuning of the Controller

The control scheme exhibits three possibilities for tuning. It is important to note that tuning is partly challenged because of the interaction between the tuning rules, the nitrification process and the qualitative features (shape) of the pH difference signal. For this reason, initial tests with the control scheme should be tested under close supervision.

The first parameter to tune is the support window length of the Kernel filter (λ in Eq. 1). A larger window includes more data points for the local polynomial fit. This means the signal is filtered more effectively at the cost of a delayed detection of the extrema. In our case λ corresponds to a 60 minutes period. The parameter γ (cf. Eq.8) determines the probability of a sign change in the qualitative trend probabilities. The closer to zero the chosen γ is, the less the algorithm trusts the data-based evidence for changes in the process' state. This will smooth the qualitative trend probabilities and potentially delay the detection of a change in sign. In the tested controller γ is set to 0.5. This choice puts equal weights on the model and the data. On a second tuning level, the presented rules NE1-NE3 and EN1-EN3 can be used for tuning. The quantitative nature of rules NE1 and EN2 make them very attractive for fine-tuning. With EN2 significant peak events can be distinguished from irrelevant ones. The higher the *Minimal Difference* value the fewer events will be considered as relevant by the control. In contrast, the higher the *Maximal Difference* (NE1) the sooner the controller assumes a low load situation. However, the sensitivity of both rules depends on the effectiveness of rules EN3 (maxima) and NE2 (minima) (cf. Fig. 3).

The third tuning level comprises the setting of the DO setpoints for the slave controllers (see below) in Eco- and Normal-mode. Importantly, higher Eco-mode DO setpoints cause a lesser number of peak loads to be relevant for switching to Normal-mode and less energy can be saved. Furthermore, the difference between Eco and Normal DO setpoints should be limited. A too large difference between Eco- and Normal-mode setpoints will increase the response time of the aeration system.

Integration into the Pre-Existing Control Scheme

The controller has been tested successfully to detect high load and low load situations. As mentioned above, the controller output is either Eco- or Normal control mode (cf. Figure 1 bottom) with the corresponding DO setpoint. From this point, the already installed plant supervisory control and data acquisition (SCADA) system takes over. The DO setpoint is passed to a slave PI controller adjusting the airflow according to the derivation of the DO measurement and the DO setpoint value. Additionally, safety rules were implemented to guarantee a safe plant operation in the first experimental phase. In the case one of the safety rules is violated the control will pass a high DO setpoint to the slave controllers independent of the HMM state estimate to ensure a sufficient nitrification capacity at all times. An additional pH sensor at the plant inlet is used as a proxy for toxic, industrial wastewater, which could disturb the pH difference and hamper the sensitive bacterial community. Another set of rules is put in place to register conditions which correlate with high ammonium loads such as high hydraulic loads or sludge digestion water adding periods. In these cases, high load situations are detected faster by means of flow rate measurements rather than on the basis of the QSE algorithm. The faster high loads can be detected, the longer the acceptable response time can be. This allows *(a)* to tune the control towards longer Eco-mode periods and *(b)* to accept larger differences between Eco and Normal DO setpoints.

EXPERIENCES AND OUTLOOK

During the test on the full-scale WWTP Hard in Winterthur, Switzerland, the effluent concentration of ammonium and nitrite did not increase significantly compared to exclusive Normal-mode operations. Within the 200-days test period the strict concentration effluent limits were never exceeded. At the time of writing, the aeration energy savings are estimated to be approximately 15%. The control scheme and software was developed and tested jointly with the WWTP Winterthur and Rittmeyer AG. The latter integrated the controller as a module for its WWTP supervision and optimisation software RITUNE®, which is commercially available (cf. http://www.rittmeyer.com/ritune). Further research and development activities will be directed towards testing and evaluation of the controller on other WWTPs. A key focus is *(a)* to reduce the implementation and fine-tuning effort, *(b)* visualise the algorithm and control behaviour transparent for the technical operator and *(c)* to enhance efficiency gains with algorithm and controller adaptations. Moreover, QTA methods are being developed to cover *(a)* inflection points (Villez, Submitted), *(b)* discontinuities (Villez & Habermacher, Submitted) and *(c)* multivariate data series.

CONCLUSION

A new soft-sensor for ammonium control has been developed and tested. By means of the QTA method, namely the qualitative state estimation (QSE) high and low ammonium loads can be detected by measuring pH with two sensors. The QSE method and the more reliable and inexpensive pH sensors make this soft-sensor robust for drift and thus maintenance friendly. Initial full-scale tests recorded a reduction of over 15% in aeration energy needs. In essence, this enables smaller WWTPs to cost-effectively minimise their energy consumption with a load dependent aeration control.

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