Benchmarking soft-sensors for remote monitoring of on-site wastewater treatment plants

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Abstract

On-site wastewater treatment plants are usually unattended, so undetected failures often lead to prolonged periods of reduced performance. To stabilize the good performance of unattended plants, soft-sensors could expose faults and failures to the operator. In a previous study, we developed soft-sensors and showed that soft-sensors with data from unmaintained physical sensors can be as accurate as soft-sensors with data from maintained ones. The quantities sensed were pH and dissolved oxygen (DO), and soft-sensors were used to predict nitrification performance. In the present study, we use synthetic data and monitor three plants to test these soft-sensors. We find that a long sludge age and a moderate aeration rate improve the pH soft-sensor accuracy, and that the aeration regime is the main operational parameter affecting the accuracy of the DO soft-sensor. We demonstrate that integrated design, monitoring, and control are necessary to achieve robust accuracy and to obviate case-specific fine-tuning. Additionally, we provide a unique labelled dataset for further feature and data-driven soft-sensor development. Our approach is limited to sequencing batch reactors. Moreover, nitrite accumulation and alkalinity limitation cannot be detected. The strength of the approach is that unmaintained sensors drastically reduce monitoring costs, enabling the monitoring of plants hitherto unchecked.

Abbreviations

ASM	*activated sludge model*
COD	*chemical oxygen demand*
DO	*dissolved oxygen*
DOC	*dissolved organic carbon*
SL	*standard-liter*
OST	*on-site wastewater treatment plant (small, unstaffed wastewater treatment plant)*
PE	*population equivalent*
SA	*sludge age*
SAC_{254}	*spectral absorption coefficient at 254 nanometers*
SBR	*sequencing batch reactor*
WWTP	*wastewater treatment plant*

1 Introduction

Failing wastewater treatment systems can negatively affect the environment and human health, with potentially dire consequences. Thus, wastewater treatment authorities are under pressure to provide a reliable service. In most OECD countries, such reliability is attained with sewers discharging to a central permanently staffed wastewater treatment plant (WWTP). One reason for the absence of on-site solutions is the lack of an efficient monitoring of overall system performance for large fleets of such on-site wastewater treatment plants (OSTs). Despite the importance of quantifiable treatment performance,[1–3] the authors of this article know of only two published long-term studies of online monitoring of OSTs. Abegglen et al. monitored a membrane biofilm reactor of a 4 population-equivalent (PE) household for 38 months looking at biological phosphorus removal[4] and Straub monitored several on-site wastewater treatment plants with a SAC_{254} sensor.[5] This lack of attention has resulted in OSTs being seen as a stopgap solution.[6]

OSTs have particular characteristics that differentiate them from centralized WWTPs. Among their numerous advantages, we highlight i) a short planning horizon,[7] ii) the potential to rapidly improve urban sanitation in unsewered areas,[8,9] and iii) fewer losses due to cracks in pipes, reported to be 5–20 % of the dry weather flow.[10] Despite these advantages, OSTs face particular challenges related to proximity with dwellings and their decentralized character. Among these are i) high maintenance costs for massively decentralized infrastructures,[11] ii) high inflow variation, iii) low inflow dilution, and iv) faults and failures that do not occur in centralized WWTPs. Examples of such faults from our experiments include undiscovered local power cuts and medication in the inflow suppressing biological activity. These issues are rare in centralized WWTPs, where a power cut would be immediately detected and medication from a single household would be diluted to harmlessness. Moreover, even if a fault is recognized, diagnosis of an OST remains difficult due to a lack of monitoring data.

Herein, we argue that modern monitoring and sensing methods can tackle several of the challenges posed to OSTs. Smart sensing is well established in the energy[12] and drinking water sectors,[13] new types of sensors are constantly emerging,[6,14] and traditional sensors are constantly being improved, such as maintenance-free ion-selective electrodes for clinical diagnostics.[15]

In a previous pilot study, we demonstrated that soft-sensors based on **unmaintained** pH and dissolved oxygen (DO) signals are a feasible solution for remotely monitoring OSTs.[3] The soft-sensors use trend-based feature engineering. This approach applies process knowledge as signal features to predict effluent ammonium concentration above or below 1 $g_N m^{-3}$. An example of using process knowledge is pH feature detection, which relies on the detection of a local minimum in the smoothed pH signal. This minimum is known to occur when ammonium has been fully oxidized.[16] We take a full ammonium oxidation as an indicator of a fully functioning biological treatment process.

Exploiting process knowledge has substantial advantages for the transferability of the methodology over a purely data-driven approach. Data-driven models have free parameters that need adjustment, or at least testing as soon as the setting deviates from the training dataset, such as in new installations and after substantial shifts in operating conditions.[17] Moreover, every adjustment to the same method requires costly measurements of effluent quality, which are used as training labels. However, the hypothesis is that we can transfer feature-based soft-sensors trained on data from unmaintained physical sensors to plants in operation. Until now, to the best of our knowledge, nobody has attempted such a transfer. The grounding of the claim is that feature engineering relying on universal mechanistic process knowledge enables the approach to be transferred. The success of such a transfer would considerably improve the scalability and applicability of soft-sensors based on unmaintained sensors.

The goals of this article are

1. to show that these soft-sensors can be transferred from a pilot plant to a range of full-scale OSTs;
2. to demonstrate that mechanistic process knowledge in the form of synthetic data allows us to define conditions under which the soft-sensors will fail and show which conditions enhance the accuracy of the soft-sensors; and
3. to compare the results with monitoring data from three OSTs in the field, which vary in their treatment performance.

Additionally, we provide a unique dataset from the monitoring of these three OSTs, including high-resolution (10 seconds) pH and DO measurements using inflow and effluent concentration measurements as labels. This labeled dataset is useful for testing further data-driven approaches and a valuable asset for the community at large.

2 Material and Methods

2.1 Soft-sensors and automatic feature identification

Two soft-sensors were developed to monitor a pilot sequencing batch reactor (SBR, for details see Schneider et al.[3]) treating municipal wastewater: an ammonium valley[16] feature detector based on pH data from the aeration phase and an aeration ramp detector in the DO signal (feature is shown in Figure 1). The ammonium effluent concentration serves as the label. If the effluent concentration is below or equal to 1 $g_N m^{-3}$, the label is positive, so the cycle is expected to show the feature; if it is above 1 $g_N m^{-3}$, the label is negative. The only change from the automatic feature detection presented in Schneider et al.[3] is that for this article a variable cycle length was implemented. Figure 1 also shows the slope property of the aeration ramp DO feature. An aeration ramp with a slope lower than the slope tolerance threshold is insufficient and hence discarded. Schneider et al. found an optimal slope tolerance of 21.5° for the maintained soft-sensor and 40° for the unmaintained one.[3] The aeration regime was similar to the “delay” pattern in Figure 1. In this article, we used the slope tolerance for the unmaintained sensor, which is 40°.

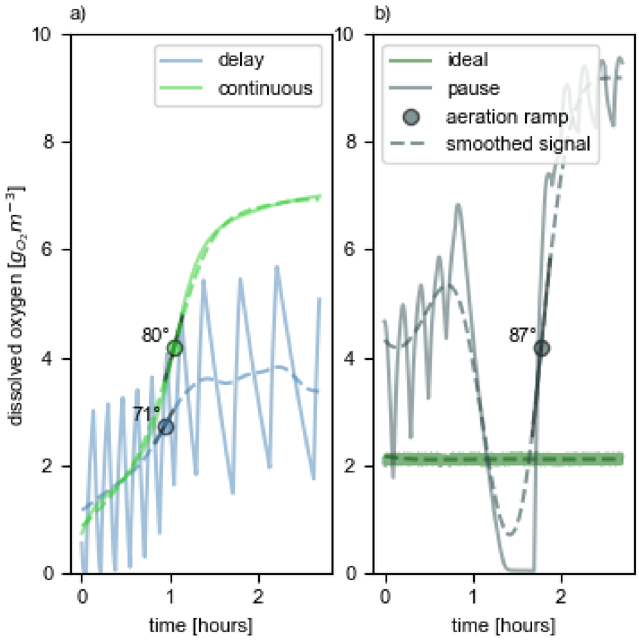

Figure 1: Simulated DO concentrations for different aeration regimes in a nitrifying SBR. Solid lines represent simulated signals. Circles show the location of features detected in the smoothed (dashed) signals. The angles of the ramps are displayed together with the tangent in proportional length. All displayed cycles have a positive label and are expected to display a feature. Ideal *is a close-to-ideal two-point control between 2 and 2.2 $g_{O2}m^{-3}$. Delay is the same two-point control, but with a delay of 5 minutes.* Timed on-off *is time-controlled regular on-off aeration.* Continuous *is continuous aeration.* Pause *is a time-controlled regular on-off aeration that has a pause in the middle of the aeration phase. The only cycle not showing a feature is the one with the close-to-ideal two-point control.*

Classification of the prediction

We use the following definitions to classify the results when comparing the soft-sensors’ predictions with the ammonium effluent concentrations:[3]

- *True positive (TP):* A feature, in this case an ammonium valley for the pH signal and aeration ramp for the DO signal, is detected, and the cycle label is positive.
- *True negative (TN)*: No feature is detected, and the cycle label is negative.
- *False positive (FP)*: A feature is detected despite a negative cycle label.
- *False negative (FN)*: No feature is detected despite a positive cycle label.

2.2 Relevant processes

The pH signal is strongly influenced by the alkalinity of the water, which stabilizes the pH, nitrification, which lowers the pH, and COD removal, which also lowers the pH. In an open system, carbon dioxide is stripped during the aeration of a wastewater treatment process, which increases the pH.[18,19] However, low pH can also restrict nitrification and COD reduction.[20] Schneider et al. hypothesize that the rate of the biological processes and aeration (CO_2 stripping) are confounding factors that affect the reliability of pH soft-sensors.[3] Therefore, a synthetic dataset was produced in which varying sludge ages (SA) inhibited and aided different bacteria and the aeration rate was varied to influence the CO_2 stripping. The DO signal is mainly influenced by the aeration regime and rate. Figure 1 gives some examples of the influence of various aeration regimes on the aeration ramp feature.

2.3 Simulated synthetic data

The dataset was created with Sumo modelling software.[21] The applied model, SUMO1, is based on ASM[22] and additionally estimates the pH from the most relevant chemical speciation and gas exchange processes. The model was used to simulate synthetic pH and DO data at a resolution of 10 seconds and related ammonium effluent concentrations. The reactor was modelled as a 1 m^3 SBR treating 480 liters of wastewater per day and located 200 m above sea level. The total length of a cycle is 4 hours, of which the aeration phase lasts 2.8 hours. The aeration is time controlled, with 6 minutes on and 6 minutes off. A run was performed for 126 cycles in sequence with the same input parameters per run. The inflow concentrations were total chemical oxygen demand of 464.6 $g_{COD}m^{-3}$, total phosphorus of 15 $g_{P}m^{-3}$, and total nitrogen randomly chosen between 100 and 180 $g_{TKN}m^{-3}$. The same inflow pattern of total Kjeldahl nitrogen was defined for one week (42 cycles) and repeated three times per run. Because we did not want to reproduce a specific treatment plant but compare a range of configurations, the parameters defining influent composition, stoichiometry, and kinetics were set to their default values. The exact settings for every run are documented in the data package[23], including model options, modified parameters, input, model, SBR, influent, effluent, and sludge characterization. The results of the simulation are also included in the data package.

Purpose: This synthetic data serves to study the behavior of the soft-sensors. The advantage of generating synthetic data is that reproducible data based on process knowledge is generated, which allows us to explore and explain the boundary operating conditions for the soft-sensors. In particular, we sought design and operating conditions that were likely to lead to a failure of the soft-sensor to deliver accurate predictions about the effluent quality. Based on the simulation results, we then determined design and operating conditions detrimental to OST monitoring purposes.

2.4 Experimental resources for validation

For validation, we monitored three plants in operation. All three plants are SBRs. Three new pH sensors and one new dissolved oxygen (DO) sensor were installed in Plant 1 and subsequently removed and reinstalled in Plant 2 and then Plant 3. An overview of the measured inflow and effluent ammonium concentration in these plants is shown in Figure 2. While the dataset obtained in Plant 2 is the most balanced of the three datasets (36% of ammonium effluent below 1$g_{N}m^{-3}$), the datasets from Plant 1 (4%) and Plant 3 (12%) are clearly imbalanced. Plant schemes, receipts of the phase lengths, and an overview of all sensors are provided in the appendix.

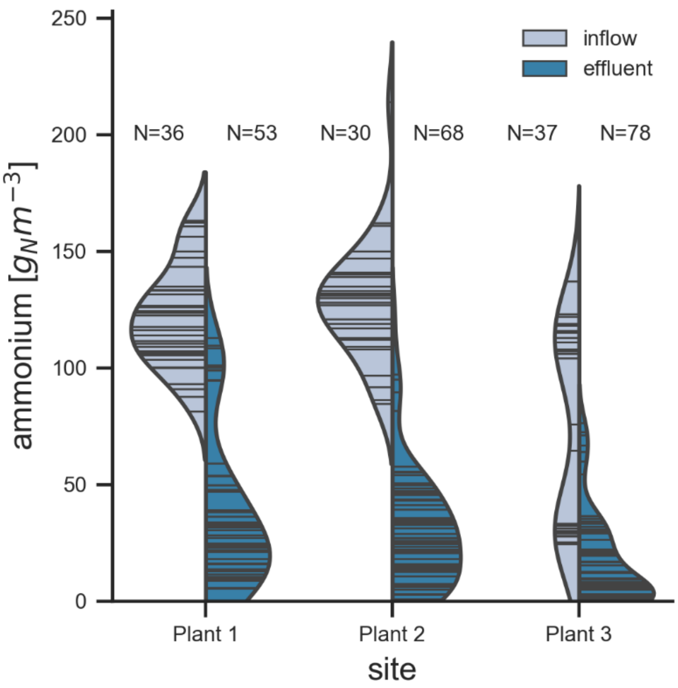

Figure 2: Concentration of ammonium nitrogen measured in the inflow and the effluent of the three case study plants. The horizontal lines within the plots indicate where the individual measurements lie. The outer line of the plot is a kernel density estimation fit to a histogram. Each plot is split into inflow concentration (left) and effluent concentration (right). N is the number of samples analyzed per site. The inflow concentrations of Plants 1 and 2 seem close to Gaussian distributions, while Plant 3 has two hubs in the inflow.

Plant 1: Mountain hut with extreme temperature and irregular aeration regime
Plant 1 is installed in a touristic mountain hut 2328 m above sea level, dimensioned for 25 PE. The hut has 70 beds for overnight stay with a seasonal occupation. Toilets, sinks, showers, kitchen, and washing machines are connected to the SBR. The SBR was constructed in summer 2017 and began operating after the winter break in March 2018. We collected data from mid-March 2018 to the beginning of October 2018, capturing the start-up phase of the new plant. The shortest cycle was 285 minutes, the longest approximately 31 hours. All phases other than the aeration phase have a fixed time length. The aeration phase starts with 4 hours of aeration (15 minutes on, 2 minutes off). Whenever there is little inflow to the SBR, this aeration is followed by a second aeration regime (5 minutes on, 25 minutes off) depending on the water level in the storage tank. Between these two aeration regimes, the aeration is turned off for 45 minutes (as the pause pattern in Figure 1). We expected this pattern to be challenging for the soft-sensors. Plant 1 was chosen for its extremes of temperature, aeration, and yearly seasonality.

Plant 2: Two houses with high ammonium influent concentration, large flow variation, and a regular aeration regime
Plant 2 operates in a rural area at 470 m above sea level. The SBR was designed for 10 PE and built in 2014. During data collection, a total of four people were living in two houses connected to the SBR. Prior to the SBR, which has a tank volume of 3.5 m^3, there is a storage tank of 5 m^3. The site is inhabited all year long and has low seasonal variation. Data was collected from the beginning of November 2018 until end of March 2019. Plant 2 was chosen because of its regular on-off aeration regime (6 minutes on, 4 minutes off).

Plant 3: OST treats the designed load and has a regular aeration regime
Plant 3 treats wastewater from a family in a rural area at 840 m above sea level. The SBR is designed for 6 PE, was built in 2014, and treats the wastewater of four adults and two children. The setup is similar to Plant 2. Prior to the SBR (2.3 m^3), there is a storage tank (3 m^3). We collected data for Plant 3 from the beginning of April to middle of October 2019. Plant 3 was chosen because of its regular on-off aeration regime (7 minutes on, 3 minutes off) and its operation at full capacity.

Sensor installations
Table 1 provides an overview of the installed sensors. All data are stored with a 10 seconds' interval. Unless stated otherwise, the exact same sensors were used for all three plants.

Table 1: Relevant installed sensors at the three plants. 'DO' is dissolved oxygen. The pressure sensors were used for measuring the SBR fill level. A full list of all sensors is given in the appendix.

parameter	Manufacturer	Type	range	number of sensors installed		
				Plant 1	Plant 2	Plant 3
pH	Endress & Hauser	glass CPS91D	0–14 pH	3	3	3
DO	Endress & Hauser	optic COS61D	0–20 gm^{-3}	1	2	2
pressure	Endress & Hauser	Cerabar T PMC131	0–0.2 bar	0	1	1
pressure	Ifm	PS3208	0–0.25 bar	1	1	0

Sensor reference measurements and maintenance

One of the pH sensors and one of the DO sensors were maintained per the manufacturer's recommendations. Two of the pH sensors (last maintenance March 2018) and one DO (last maintenance April 2017) were left unmaintained, and no cleaning or maintenance took place when transferring the sensors from one plant to the next. Unless stated otherwise, the sensor maintenance and reference measurements were executed as described in Schneider et al.[3] The differences were that we did not have automatic cleaning for the unmaintained DO sensor so cleaned it mechanically instead and that we stopped the reference measurements of the unmaintained pH sensors after 14 December 2018 to ensure that no cleaning effects on reference measurements influenced soft-sensor accuracy. The maintained pH sensor started showing instabilities during calibration while installed at Plant 3.

Influent and effluent reference measurements

Grab samples were taken and analyzed for dissolved chemical oxygen demand (COD), dissolved organic carbon (DOC), and nitrogen compounds (ammonium, nitrate, and nitrite). The variables measured and the analytical method can be found in the appendix of this article and in Furrer (2018).

3 Results and discussion

3.1 Simulated, synthetic data

Figure 3 shows the accuracy of the soft-sensor and the treatment performance, represented as ammonium in the effluent below or above 1 $g_N m^{-3}$, for the pH and DO soft-sensors when the sludge age (SA) is varied. The soft-sensor accuracy of the simulated DO signal lies between 85 and 100%, with perfect accuracy for results both for a SA of 1 day and for any SA equal to or longer than 4 days. The soft-sensor accuracy of the simulated pH signal shows its highest accuracy at a SA of 1 day and then falls in accuracy, with its lowest point at a SA of 4–6 days. At a SA of 11 days, the accuracy reaches a ceiling. Figure 3 shows that the treatment performance starts with 0% of full ammonium oxidation at a SA of 1 day and reaches stable nitrification at a SA of 4 days or more.

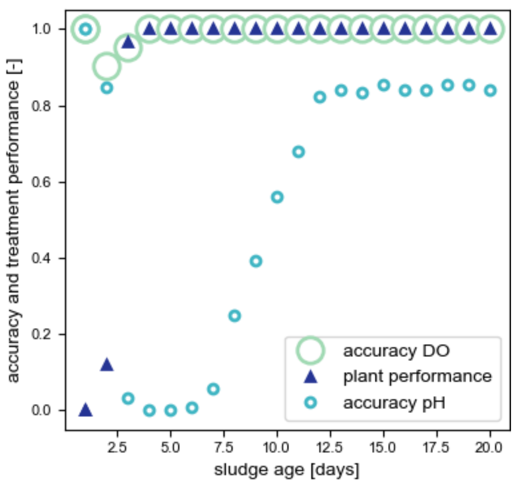

Figure 3: Comparison of accuracy of the pH (small circles) and the dissolved oxygen (DO, larger circles) soft-sensors over increasing sludge ages with synthetic data. The treatment plant performance (triangles) is the fraction of cycles with full ammonium oxidation (effluent < 1 $g_N m^{-3}$) divided by the total number of cycles. In total, 126 cycles are analyzed per data point. The data points are not independent of each other, as the initial conditions were taken from the previous run.

Based on these simulations, we can draw the following conclusions:

i) At 1 day SA, both the pH and the DO soft-sensors exhibit a high accuracy. This type of feature-based soft-sensor can most readily make negative predictions. In order to detect a feature, the signal needs to show exactly the expected behavior, while all other behaviors are classified as nondetection. This is also supported by Figure 3, where the results for treatment plant performance and pH accuracy are mirrored for SAs of 1–5 days. Figure 4 supports this further, as the soft-sensor shows high accuracy as long as nitrification fails. Therefore, detecting a feature provides more information about the actual behavior of the treatment process than nondetection. This behavior is typical of a one-class model and was similarly observed by Villez et al. (2010).

ii) The accuracy of the pH soft-sensor with the given aeration regime is lower than or equal to the DO and generally lower than 100% (except for 1 day SA, for reasons explored in point (i)). This highlights the challenge of the pH soft-sensor, because it is influenced by several competing processes instead of one dominant process, as is the case with the DO soft-sensor (see section 2.2). The pH soft-sensor exploits a very specific feature requiring a well-balanced ratio of positive and negative pH rate changes and demands a more well-tuned set of operating conditions. The feature requires that the aeration phase continues for some minutes after full ammonium oxidation has been reached. Otherwise, no local minimum can be observed, as CO_2 stripping causes the pH to rise again once it becomes the predominant process influencing the pH after all ammonium is oxidized. Figure 4 the effect of increased CO_2 stripping due to the higher aeration rate, which reduces the ability of the biological processes to decrease the pH sufficiently to create a clear feature for the soft-sensor to detect. Higher SA increases the biomass concentration and consequently increases the degradation rates, which in turn increase the probability of producing a clear dip in pH. Any process that has a strengthening effect on the pH feature can improve the soft-sensor. For example, a denitrification phase before the aeration phase increases the initial pH and therefore increases the likelihood of a feature (Table A2 in the appendix). Consequently, any process that dampens the sensitivity of the pH, such as a strong buffer (alkalinity) has a negative impact on pH soft-sensor accuracy.

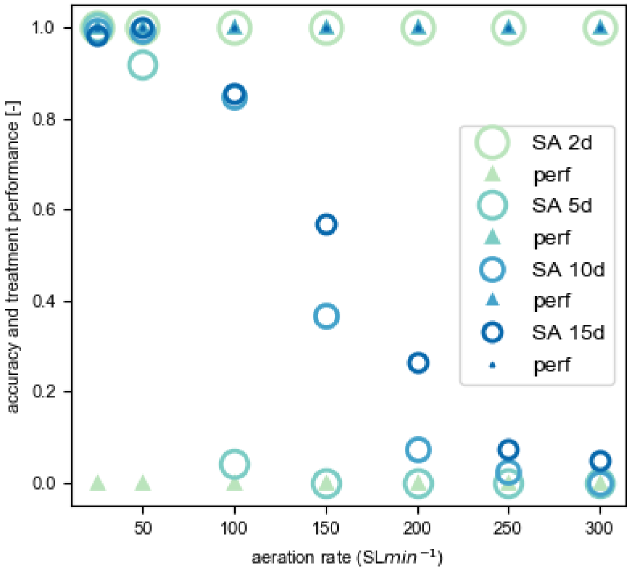

Figure 4: Comparison of pH soft-sensor accuracy (circles) for different sludge ages (SA) and aeration rates in standard–liter (temperature of 273.15 K and absolute pressure of 100 kPa) gas per minute with synthetic data. The ammonium effluent concentration is used as the measure for the treatment plant performance (perf, *triangles), for the same SA as the soft-sensor accuracy. In total, 126 cycles are analyzed per data point, which means that for every SA and aeration rate combination 126 cycles were simulated. The data points are not independent of each other, as the initial conditions were taken from the previous run.*

iii) Consequently, higher SAs in Figure 3 have a positive influence on pH soft-sensor accuracy.

iv) The DO soft-sensor has an overall higher accuracy than the pH one because it is mainly influenced by the aeration state and the respiration rate. Figure 1 shows that the DO feature relies on a detectable increase in the oxygen concentration. This increase in the DO is due to a change in the respiration rate, which is strongly influenced by the end of the nitrification process.

It also shows that the increase depends on the chosen aeration regime, and this in turn has an impact on the slope tolerance, the key parameter used by the soft-sensor to identify the feature.

3.2 Experimental data from three OSTs in operation

Transferability of the soft-sensors

pH soft-sensor: Applying the soft-sensors from Schneider et al.[3] without optimizing any parameters results in an 84% accuracy soft-sensor based on the maintained pH, and 86% and 79% for the two soft-sensors based on unmaintained pH with the dataset from Plant 2 (see Table 2). The input data from Plant 2 provides the most relevant results for soft-sensor accuracy, as it has the most balanced dataset of the three plants (most positive cases, as discussed in section 3.1). This result is in the same range as Schneider et al., who achieved 80% and 85% accuracy with the same type of pH sensor in a laboratory environment and with an optimized cut-off frequency parameter when smoothing the signal. We draw two conclusions: i) The measurement campaign at these three plants supports Schneider et al.'s conclusion that no difference exists between soft-sensor accuracy based on maintained pH signals and on unmaintained ones for this ammonium-valley-based feature detection. Therefore, no further comparison between maintained and unmaintained sensors is required for this specific feature. ii) Interestingly, the pH soft-sensor worked for all three plants without any parameter changes with satisfactorily high prediction accuracy. Even suboptimal aeration regimes, as in Plant 1 with a break during aeration, did not lower the accuracy of the pH soft-sensor.

The DO soft-sensors: The DO soft-sensor has a very low accuracy of 44% with the data collected on Plant 1. For Plants 2 and 3, accuracies of 71% and 88% were reached for the maintained sensors. The dataset for Plant 1 is highly imbalanced, which means that a soft-sensor predicting only negative outcomes would reach an accuracy of 93%, much higher than the DO soft-sensor prediction based on experimental data. This highlights an issue with the prediction for Plant 1. Visual inspection (see Figure A3 in the appendix) of the data shows that the aeration regime of Plant 1, characterized by a pause in the aeration after 4 hours, is suboptimal for aeration ramp detection. Parameter optimization of the slope tolerance improves the accuracy of the DO soft-sensor (see Table 2, last column, for the improved accuracy and Figure A2 in the appendix for the parameter optimization). After the optimization, Plant 2 (87%) and Plant 3 (94%) have a similar accuracy to that achieved by Schneider et al. with a maintained DO sensor signal (92%).

Table 2: Results of automatic feature detection without parameter optimization for the pH soft-sensor and without and with for the DO soft-sensor. Positive means that a feature was detected, negative means no feature was detected. The categories (false positive, false negative, true positives, and true negative) are provided for the soft-sensor without parameter optimization.

		number of false positive	number of false negative	number of true positive	number of true negative	accuracy without optimization	accuracy with optimization of slope tolerance (DO)
Plant 1	pH maintained 1	6	0	3	34	86 %	
	pH unmaintained 1	6	0	3	34	86 %	
	pH unmaintained 2	9	0	3	31	**79 %**	
	DO maintained 1	23	0	2	14	**44 %**	**68 %**
Plant 2	pH maintained 1	6	6	22	43	84 %	
	pH unmaintained 1	5	6	22	44	86 %	
	pH unmaintained 2	4	7	21	45	86 %	
	DO maintained 1	21	1	27	28	**71 %**	87 %
	DO unmaintained 1	20	0	28	29	**74 %**	90 %
Plant 3	pH maintained 1	9	2	6	50	84 %	
	pH unmaintained 1	2	2	6	57	94 %	
	pH unmaintained 2	3	2	6	56	92 %	
	DO maintained 1	6	2	6	53	88 %	94 %
	DO unmaintained 1	19	1	7	40	70 %	84 %

Additional observations from the field study

While monitoring the three plants in operation, we encountered several potentially challenging operating conditions: large variation of nitrogen load, high inflow concentrations of ammonium, nitrite accumulation, and incomplete ammonium oxidation due to alkalinity limitation (observed on Plant 1 and Plant 2). Once the alkalinity is depleted, the pH remains low.[25] This trend results in a failure of the feature detector, leading to both positive and negative classification based on the inability to clearly identify a pH minimum. This limitation could be resolved either by adjusting the current soft-sensor model or by applying process engineering strategies to avoid such limitations. Two attractive solutions to counteract alkalinity limitation would be a solid source of scale or urine separation at the source. The latter could then enable additional process control by dosing urine. This idea seems promising, as intermittent addition of urine has been used to create dynamics that ensure accurate monitoring in other types of plants than SBRs in presence of sensor drift.[26]

3.3 Synthesis from modelling and monitoring

Transferability of the soft-sensors

Comparing the modelling results with the experimental data shows an apparent contradiction: the pH soft-sensor showed much more robust transferability, despite depending on a range of well-balanced process rates, while the DO soft-sensor required specific parameter re-adjustment. However, the results from the synthetic dataset show quite clearly that both soft-sensors require the operational parameters of the plants to be aligned.

The synthetic data (Figure 1) shows that the parameter of the DO soft-sensor depends on the aeration control regime applied. Schneider et al. used the maintained DO signal to control the dissolved oxygen in the SBR between 2 and 2.2 $mg_{O2}L^{-1}$. In contrast, Plants 1–3 are all purely time controlled. Figure 1 shows this aeration regime changes the slope of the aeration ramp feature. This knowledge enables us to estimate the slope tolerance based on the aeration regime without a range of expensive on-site measurements. Therefore, we believe that both soft-sensors show excellent transferability if the plant is operated favorably to the use of soft-sensors. In other words, integral design of soft-sensors and treatment plant is required for successful monitoring of these plants.

Integrated design monitoring and control

These soft-sensors exploit features that are based on a mechanistic understanding of wastewater treatment processes, which enables us to use modelling to explore favorable and disadvantageous conditions for the features. The usage of mechanistic understanding distinguishes feature-based approaches from purely data-driven ones in which the training set defines the transferability and performance of the soft-sensor.

The results highlight how strongly the operating conditions influence the accuracy of the soft-sensors. While the DO soft-sensor is mainly influenced by the oxygen control regime, the pH soft-sensor can be influenced by aeration, alkalinity, sludge age, and denitrification. It is important to emphasize that we mainly identify conditions under which the soft-sensors will fail but cannot prove under which real conditions they will certainly work. However, the study provides strong indications how a plant and its operational parameters should be designed and controlled.

Several articles called for integrated design, monitoring, and control. Olsson et al. argue that an inflexible design cannot be amended by control alone.[27] Vanrolleghem et al. call for a common cost function for design and operation.[28] These approaches show that integrated thinking when considering design, control, and operation improves both process performance and costs. However, the many studies that treat design, monitoring, and control as separate subjects reinforce the old paradigm of building for robustness. This means that in the absence of flexible controls to safeguard and optimize the process online, monitoring and control are conducted post hoc, when the reactor system has already been built. As this article demonstrates, monitoring with unmaintained sensors will only work integrated with design (e.g. by using a mechanical stirrer for the denitrification step instead of blowing low levels of air, as observed at Plant 2) and control (appropriate aeration rate and sludge age). We argue that integrated design, monitoring, and control are not only beneficial but imperative for monitoring and operating OSTs with unmaintained soft-sensors. Interestingly, this holistic approach to control is well established in the field of embodied AI,[29] where plant dynamics are designed and exploited to simplify control.

Monitoring is required to shift OSTs from a stopgap solution to a real, flexible treatment solution and to avoid unnoticed pollution of the environment.[6] We have shown that OSTs of the SBR type can be monitored effectively and remotely with cheap, unmaintained sensors if design, monitoring, and control are implemented appropriately. In turn, we expect the monitoring ability to improve awareness and insights into the performance of entirely OST systems as alternatives to sewer-network-based wastewater systems.

3.4 Limitations

Both these soft-sensors aim to indicate completed nitrification, which is generally a good proxy for well-functioning biological processes. However, the soft-sensors in fact only indicate full ammonium oxidation, not full nitrification. Our experimental work confirmed this. One consequence of this is a trade-off between (a) flexibility in treatment process choice and operational efficiency and (b) information richness of the sensor signals, which in turn influences the accuracy of the soft-sensors.

This kind of trade-off also exists in flow-through wastewater treatment systems[26] and is often used in explore–exploit strategies in robotic applications.[30] Consequently, the soft-sensors used here are only designed for SBRs, as these plants provide the necessary dynamics for the soft-sensors to work.

3.5 Recommendation

Although the operating conditions needed for the pH soft-sensors are stricter than those for the DO soft-sensors, some aspects of the long-term wear-and-tear effects observed at the unmaintained DO sensor are still incompletely understood.[3] Consequently, we think that a pH soft-sensor remains the best option for monitoring the performance of OSTs.

3.6 Data

Several comparisons have been conducted between the micropollutant removal performance of centralized and decentralized WWTPs.[31–33] In addition to online monitoring, data from annual control measurements are collected.[34–36] Overviews are available of types of OSTs in operation[37] and the faults of OSTs[2,38]. Therefore, monitoring techniques and data are needed. In this article, we contribute monitoring data from three OSTs of the SBR type.

The dataset from all three plants is available at https://doi.org/10.25678/000194 (made available upon publication, contact the corresponding author for earlier access)
All python scripts are available at https://gitlab.com/sbrml/integratedmonitoring[39]

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Appendix

Monitored wastewater treatment plants

In the following basic information about the three OSTs is provided.

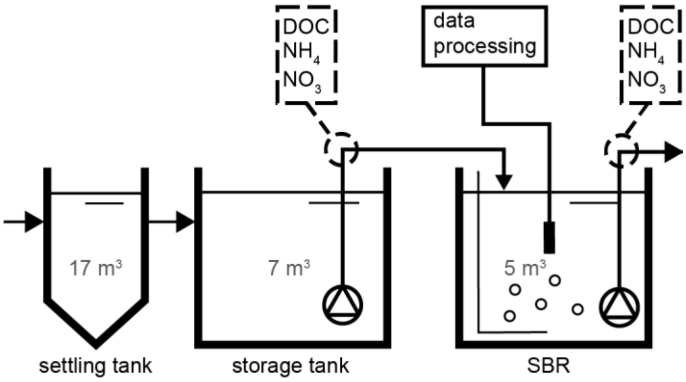

Figure A1: Schematic illustration of the SBR Plants 1 including the experimental setup. Sensors were installed in the SBR and grab samples were taken periodically from the inflow and effluent of the SBR. The volume of the tanks is indicated in m^3.

Table A1: Recipe of different phases of the SBR Plant 1. No stirrer is installed. Total time of one cycle: ≥ 285 minutes.

Phase	Time [min]	Aeration	Comment
Filling	12	No	Approximately 1 m^3 of wastewater is treated per cycle.
Non-aerated phase	33	No	No stirrer, instead 20 seconds aeration in 15 minutes interval.
Aerated phase	≥ 170	Yes	Maximal length dependent on incoming wastewater in storage tank. If no wastewater flows into the storage tank, the SBR keeps aerating. Maximum time of aeration observed was 29 hours.
Settling	58	No	
Decantation	12	No	

Table A2: Recipe of different phases of the SBR Plant 2. No stirrer is installed. Total time of one cycle is 6 hours (355 minutes plus 5 minutes stand bye).

Phase	Time [min]	Aeration	Comment
Filling	12	No	36-599 liter/cycle treated
Aerated phase	30+210	Yes	6 minutes on, 4 minutes off. Per manufacturer, the first 30 minutes were supposed to be non-aerated with 30 seconds' aeration every 9 minutes to mix the reactor. The measured DO concentration was however high. Therefore, we count it to the aeration phase.
Settling	90	No	
Decantation	12	No	
Excess sludge	1	No	Excess sludge is pumped into storage tank

Table A3: Recipe of the SBR Plant 3. No stirrer is installed. Total time of one cycle is 4 hours 48 min, resulting in 5 cycles per day.

Phase	Time [min]	Aeration	Comment
Filling	12	No	48-257 liter/cycle treated
Aerated phase	200	Yes	7 min on, 3 min off
Settling	60	No	
Decantation	12	No	
Excess sludge	3	No	Excess sludge is pumped into storage tank
Idle time	1	No	

Installed sensors

Table A4: Installed sensors at Plant 1, Plant 2, and Plant 3. ORP is oxidation-reduction potential and DO dissolved oxygen. The CO_2 measures off-gas and the magnetic field sensor were used to get information on the *on and off state of the aeration, all other sensors were in the liquid phase. The pressure sensor was replaced in November 2018. The last maintenance of the ORP sensor was in March 2018.*

measured parameter	manufacturer	type	range	number of sensors installed		
				plant 1	plant 2	plant 3
pH	Endress&Hauser	Glass CPS91D	0-14 pH	3	3	3
ORP	Endress&Hauser	Glass CPS72D	-1500 - +1500 mV	1	1	1
DO	Endress&Hauser	Optic COS61D	0-20 mg/L	1	2	2
Turbidity	Endress&Hauser	Optic CUS51D	0-150 gTS/L	1	0	0
Conductivity	Endress&Hauser	Inductive CLS50D	$2\text{-}2*10^6$ µS/cm	1	1	1
CO_2	Pewatron	NDIR	0-5 %	1	1	1
CO_2	Sensirion	NDIR	0-4 %	0	0	1
Ppressure	Endress&Hauser	Cerabar T PCM131	0-0.2 bar	0	1	1
Pressure	Ifm	PS3208	0-0.25 bar	1	1	0
Magnetic field	Extech Instruments	SDL900	0-3000 mT	1	0	0

Reference measurements

At Plants 1, the samples were taken manually. The inflow sample was taken from the primary clarifier during filling and the effluent from a 1 Liter container at the outlet of the plant. At Plants 2 and 3 the samples were taken automatically by two cooled (4 °C) portable samplers (TP5 C, MAXX, 2016). The inflow sample was taken directly from the influent to the SBR. The effluent could be taken from a 1 Liter container at the effluent pipe. All samples were filtered with glass-fiber filters (GF-5, 47 mm diameter, 0.4 µm average retention capacity, MACHEREY-NAGEL) before analyzing.

Table A5: Methods for measuring wastewater composition of inflow and effluent for Plants 1 (mountain hut).

Parameter	Method	Product
$COD_{dissolved}$	Photometric	Hach Dr. Lange LCK 314 and 114
Ammonium	Photometric	Hach Dr. Lange LCK 303 and 304
Nitrate	Photometric	Hach Dr. Lange LCK 339
Total nitrogen	Photometric	Hach Dr. Lange LCK 338
Nitrite	Colorimetric with test strips	Merck MQuant
Alkalinity	Titration with hydrochloric[24]	

Table A6: Methods for measuring wastewater composition of inflow and effluent for Plants 2 and 3.

Parameter	Method
DOC	Nondispersive infrared sensor: TOC-L, Shimadzu.
Ammonium	Flow injection analysis: QC 8500 FIA Series 2 with precision dilutor PDS200, Lachat.
Nitrate	Ion chromatography: IC 761 compact with anion column Metrosep A Supp4 and Supp4/5 Guard, Metrohm.
Nitrite	Ion chromatography: IC 761 compact with anion column Metrosep A Supp4 and Supp4/5 Guard, Metrohm.
Alkalinity	Titration with hydrochloric acid[24]

DO slope tolerance optimization

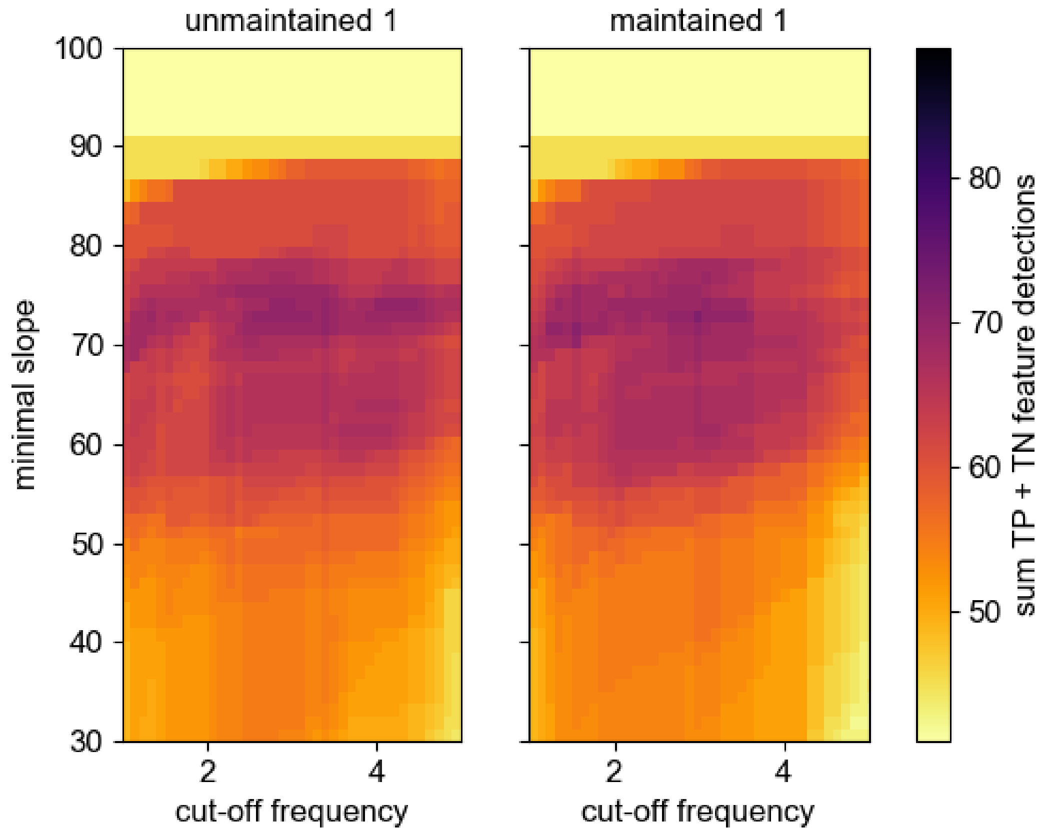

Figure A2: The sum of all true detection for the DO soft sensor's optimization parameters, where TP is true positive and TN is true negative. The parameters are minimal slope and cut-off frequency. The unmaintained sensor and the maintained sensor are displayed. This shows that the cut-off frequency has hardly any influence, while the minimal slope (slope tolerance feature property) influences the true predictions positively.

Table A7: Result of the automatic feature detection with the pH soft sensor processing synthetic data generated with SUMO. The changes in comparison to the previous run are provided. The percent of true predictions as a measure for soft sensor accuracy and of positive (full ammonium oxidation) as a measure for treatment performance are displayed. The two configurations which gave the desired result, 100% accuracy by the soft sensor and 100% treatment plant performance are marked. They represent one possible operation setting. SA stand for sludge age and SL for standard-liter (temperature of 273.15 K and absolute pressure of 100 kPa).

	Model input changed compared to the previous run	**FP**	**FN**	**TP**	**TN**	**accuracy**	**treatment performance**
Denitrification only before aeration phase.	SA 20 days. Denitrification before aeration.	0	18	108	0	86%	100%
	SA 10 days.	0	23	103	0	82%	100%
	SA 5 days.	0	118	8	0	6%	100%
	SA 2.5 days.	0	30	0	96	76%	24%
Best case: Denitrification before and after aeration phase.	SA 20 days. Denitrification before and after aeration.	0	0	84	0	100%	100%
	SA 10 days.	0	0	84	0	100%	100%
	SA 5 days.	1	3	75	5	95%	93%
	SA 2.5 days.	2	0	3	79	98%	4%
Lower load by reducing the inflow.	Low inflow Q. SA 20 days.	1	72	6	5	13%	93%
	SA 10 days.	0	84	0	0	0%	100%
	SA 5 days.	0	84	0	0	0%	100%

	SA 2.5 days.	16	24	0	44	52%	29%
Reduced aeration rate.	50 SLgasmin^{-1}. SA 20 days.	0	23	61	0	73%	100%
	SA 10 days.	0	47	37	0	44%	100%
	SA 5 days.	0	82	2	0	2%	100%
	SA 2.5 days.	0	18	0	66	79%	21%
alkalinity in the inflow	350 $g_{CaCO3}m^{-3}$ in inflow.	13	2	14	55	82%	19%
	500 $g_{CaCO3}m^{-3}$ in inflow.	65	3	16	0	19%	23%
	550 $g_{CaCO3}m^{-3}$ in inflow.	57	4	22	1	27%	31%

3.7 Performance of the three observed OSTs

Table 3: All observed faults and failures during two year of online monitoring on three different OST plants and a pilot scale SBR treating real wastewater.

Observed malfunction	Effects observed	Where observed?	How many times observed?	Additional information for diagnosis.	Estimated duration without intervention	Duration with intervention	Automatic detection with unmaintained sensors[3]
Process stuck during aeration phase	Reduction of NOB activity, resulting in nitrite accumulation	Pilot scale SBR	5	Nitrite reference measurements	> 2 days	0 days	Yes.
All sludge removed manually	No treatment at all or only partial treatment. Resulting in nitrite accumulation	Plant 2	1	Very low ammonium and DOC removal rate; measured TSS very low	> 3 months	0-7 days if sludge is added. Otherwise 1-3 months	Yes.
Alkalinity limitation	Drastic decrease of pH, inhibition of biological activity	Plant 1 and 2	Once on each plant.	pH dropping < 6	> 5 months	Redesign necessary e.g. add denitrification or dosing of calcite	No, not reliably with unmaintained sensors.
Power cut resulting in a complete stop of plant operation	No treatment at all, overflow of storage tank, washout of sludge.	Plant 1	2	No measurement signals	> 4 months	0-5 days depending on the diagnosis	Yes, no data input.
Pump failure (temporary blockage, complete failure)	Depends on which pump: either no inflow, resulting in overflow of storage tank; no effluent resulting in overflow of SBR; no sludge removal resulting in accumulation of TSS	Plant 1 and 2	1 per unit	Visually observation	> 1 month	2-3 days	Yes.
Blockage of outlet pipe	Filling of SBR and probably storage tank	Plant 2	1	Visually observation	> 1 month	0-3 days	Yes.
Excess sludge removal too high resulting in a low sludge age	No full nitrification	Plant 2, Plant 3	Once at each plant	Mass balance calculation	> 3 months	1 week	Yes.

Impact of design and operation on soft sensor accuracy

Figure A3 displays the result of an automatic feature detection with Carbajal and Schneider [39] for selected cycles from Plant 1 and one exemplary cycle of the synthetic data. The synthetic data shows the expected shape of the ramp feature. A visual comparison of the dissolved oxygen signal shows that a human might struggle with the same wrong detections (false positive examples), as the automatic feature classification based on the displayed smoothed signals.

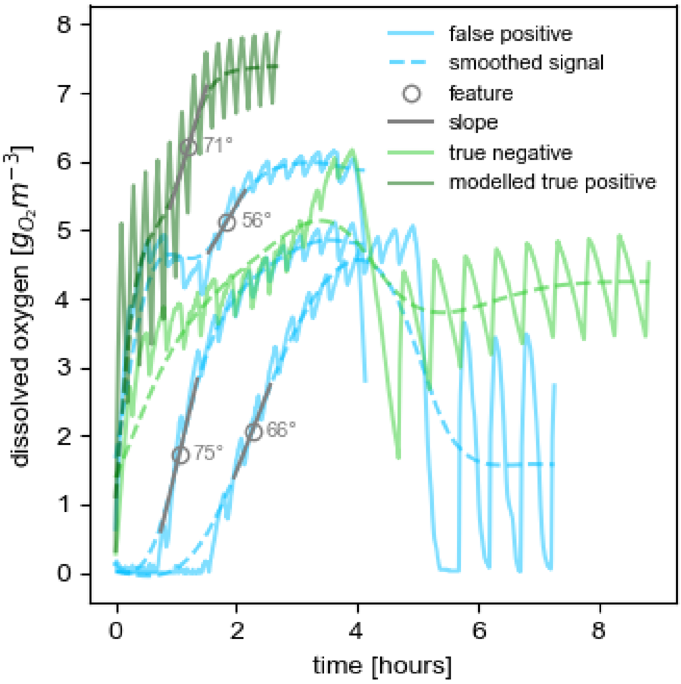

Figure A3: Measured dissolved oxygen concentrations during the aeration phase of cycles. The aeration phase has a different length and the aeration is for 45 minutes off after four hours. The modelled true positive (TP) curve is simulation with the software SUMO and represents the expected dissolved oxygen curve for feature detection.

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