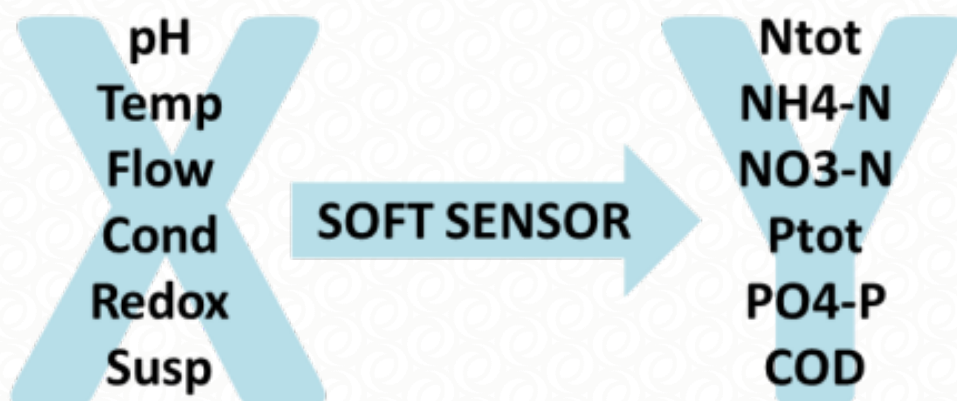




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Synthesis report on soft sensor activities at Hammarby Sjöstadsverk

Sara Nilsson, Anders Björk and Christian Baresel

Authors: Sara Nilsson, Anders Björk, Christian Baresel (IVL Swedish Environmental Research Institute)

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IVL Swedish Environmental Research Institute Ltd.

P.O Box 210 60, S-100 31 Stockholm, Sweden

Phone +46-(0)10-7886500 // +46-(0)10-7886590 // www.ivl.se

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Preface

A common problem in monitoring and control of chemical or biochemical processes is that some important process properties can only be measured accurately by means of manual sampling and laboratory analyses or by expensive and labour intensive automatic probes or analysers. One way to generate online process information is to use soft sensors instead. This report summarizes the results from projects on development of soft sensors for sewage treatment plants at the R&D facility Hammarby Sjöstadswerk during 2013-2017.

We thank all contributors, especially the master thesis workers Elin Ottosson and Sandra Abrahamsson, and Mila Harding, Linda Åmand and Magnus Rahmberg from IVL Swedish Environmental Institute.

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List of abbreviations

BR	Bioreactor
DO	Dissolved oxygen (mg/L)
COD	Chemical oxygen demand - indirect measure of amount of organic matter (mg/L)
COD _f	Dissolved COD (mg/L)
MBR	Membrane bioreactor
NH ₄ -N	Ammonium nitrogen - nitrogen in the form of ammonium (mg/L)
NO ₃ -N	Nitrate nitrogen - nitrogen in the form of nitrate (mg/L)
tot-N	Total nitrogen (mg/L)
PCA	Principal component analysis
PLS	Partial least squares - regression method
PO ₄ -P	Phosphate phosphorous - phosphorous in the form of phosphate (mg/L)
tot-P	Total phosphorous (mg/L)
SBR	Sequencing batch reactor
TSS	Total suspended solids - solid particles in suspension (mg/L)
TTF	Time to filter - sludge filterability (s)
TTF _{norm}	Time to filter normalized with TSS (s10 ⁻⁴ /(mg/L))
WWTP	Wastewater treatment plant

Summary

Many process parameters at a wastewater treatment plant are expensive, difficult or even impossible to measure online, limiting the possibilities for efficient process monitoring and control. One way to provide wastewater treatment plants with online process information is so-called soft sensors. A soft sensor is a virtual sensor in the form of a mathematical model that estimates the value of a parameter whose value is unknown, e.g. a parameter that is hard to measure online, solely based on values of other parameters whose values are known, e.g. parameters that are easier to measure online.

This report summarizes results from IVL's soft sensor related activities at Hammarby Sjöstadsvverk. It very briefly mentions two previous projects and focuses on the results from two master theses and two more recent soft sensor projects.

The parameters for which soft sensors were developed within the projects were typically different fractions of phosphorous, nitrogen, organic matter and suspended solids in various process steps. All soft sensor models were PLS-models calculated on laboratory data as y-values and online process data from the control system as x-values. The most recent projects also included data from acoustic sensors.

The performance of the soft sensors varied significantly and some of them showed promising results. The soft sensors that were based on acoustic data had in most cases comparable or better performance than corresponding models based on process data, suggesting that acoustic measurements is a promising approach. Furthermore, it was concluded that a crucial factor for successful soft sensor model development was access to large data sets from reliable online sensors and laboratory analyses. The data should represent a wide range of water characteristics and process conditions and there must also be enough for external validation of the models. It was also pointed out that well-maintained online sensors, automatic monitoring of model validity and re-calibration of models when necessary is important for well-functioning soft sensors when they are implemented in the process.

Future considerations such as stricter effluent regulations, more extreme weather conditions and a change of focus from just treating the wastewater to viewing it as a resource are predicted to further increase the need for better monitoring and control of the wastewater treatment processes. The rapid progress of information technology and further improvements of both acoustic measurements and model development will probably facilitate the development of reliable soft sensors and make it a potential approach to meet wastewater treatment plant's current and future needs for process monitoring.

Sammanfattning

Många processparametrar i ett reningsverk är dyra, svåra eller till och med omöjligt att mäta online, vilket begränsar möjligheterna för effektiv övervakning och styrning av processen. Ett sätt att tillhandahålla reningsverk med sådan information i realtid är genom så kallade soft sensorer. En soft sensor är en virtuell sensor i form av en matematisk modell som uppskattar värdet på en parameter, t.ex. en parameter som är svår att mäta online, enbart baserat på värden på andra parametrar vars värden är kända, t.ex. parametrar som är lättare att mäta online.

Denna rapport sammanfattar resultaten från soft sensor-relaterade projekt på Hammarby Sjöstadswerk. Rapporten nämner kort två tidigare projekt och fokuserar på resultat från två examensarbeten och två nyare soft sensor-projekt.

Parametrarna som soft sensorer utvecklades för var olika fraktioner av fosfor, kväve, organiskt material och suspenderade ämnen i olika processteg. Soft sensorer modellerna beräknades på laboratoriedata som y-värden och online-processdata från styrsystemet som x-värden. I de senaste projekten användes även data från akustiska sensorer.

Soft sensorernas prestanda varierade kraftigt och en del av dem visade på lovande resultat. De soft sensorer som baserades på akustiska data hade i de flesta fall jämförbar eller bättre prestanda än motsvarande modeller baserade på enbart processdata, vilket tyder på att akustiska mätningar är ett lovande angreppssätt. Det konstaterades även att en viktig faktor för utvecklingen av soft sensorer är tillgång till en stor mängd data från tillförlitliga onlinesensorer och laboratorieanalyser. Data ska täcka in ett brett spektrum av olika vattensammansättningar och processvariationer och ska även räcka för att göra extern validering av modellerna. Man drog också slutsatsen att välunderhållna onlinesensorer, automatisk övervakning av modellernas validitet och omkalibrering av modeller när behovet uppstår är viktigt för välfungerande soft sensorer när de sedan implementeras i processen.

Framtida omständigheter såsom strängare utsläppskrav, mer extrema väderförhållanden och en förändring av fokus från att bara rena avloppsvattnet till att se det som en resurs förutspås öka behovet av bättre övervakning och kontroll av avloppsreningsprocesserna. Den snabba utvecklingen inom informationsteknologin och ytterligare förbättringar av både akustiska mätningar och modellutveckling kommer förmodligen underlätta utvecklingen av tillförlitliga soft sensorer och göra dem till ett attraktivt alternativ för att tillgodose avloppsreningsverkens nuvarande och framtida behov av processövervakning.

1 Introduction

This report summarizes the results from four projects at Hammarby Sjöstadsvverk related to so-called soft sensors. A soft sensor is a mathematical model that estimates a quantity using information from other sensors, instead of measuring it directly. In the projects addressed in this report, soft sensors have been developed for different fractions of phosphorous, nitrogen, organic matter and suspended solids in various process steps. On-line process data, and in some cases acoustic data, have been used as input values to the soft sensors.

1.1 The challenge

The composition and flow of wastewater entering a wastewater treatment plant (WWTP) varies greatly on many levels: from hour to hour, daily, between seasons, depending on weather conditions etc. Due to its heterogeneity and the harsh environment it constitutes for sensors, some of the parameters of interest for the treatment results, such as phosphorous, nitrogen and COD (chemical oxygen demand) can be difficult to measure with online sensors. The physical sensors available on the market are usually very expensive and in need of continuous maintenance. Therefore, these parameters are usually analyzed manually as daily or weekly composite samples in a laboratory, sometimes several days after the samples were taken. Consequently, it is very difficult to control the wastewater plant based on those parameters and to make needed adjustments in time. This also implies increased costs and environmental impact due to inefficient use of chemicals and energy. The even stricter effluent and resource consumption requirements are further incentives to address the challenge.

1.2 Soft sensors - the potential solution

A soft sensor is a virtual sensor in the form of a mathematical model that estimates a new quantity whose value is unknown, based on values of other parameters whose values are known. This requires that the parameters are somewhat dependent. The method for calculating the soft sensor models referred to in this report is PLS (partial least squares). In the WWTP case, the unknown parameters are hard to measure online, for example tot-N, NH₄-N, NO₃-N, tot-P, PO₄-P or COD, and the known parameters are measured online, for example pH, temperature, flow, conductivity, redox or suspended solids. Thus, the soft sensors are models/equations that use the parameters that are easy to measure as x-values to determine the values of parameters that are hard to measure. This is shown schematically in Figure 1.

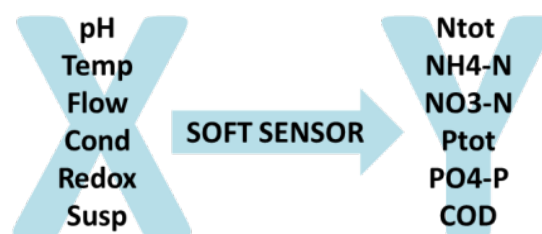


Figure 1. A soft sensor predicts unknown y-values based solely on known x-values.

1.3 The development environment

One of the pilot treatment lines at the R&D-facility Hammarby Sjöstadsvverk was used for development of the soft sensors. It is a copy of Stockholm's largest WWTP, Henriksdal, and

receives the same water as the Henriksdal WWTP, but has a capacity of 150 pe (population equivalents). The inflow can be static or dynamic with the option to either select a preferred setpoint or to correlate it to the actual variations into the Henriksdal WWTP. All effluents (including sludge) are returned to the inlet of the Henriksdal WWTP, which implies that no emission limitations affect the activities at the pilot plant. Furthermore, the line is fully instrumented and connected to a control system.

Two different setups of the pilot plant were used during the soft sensor projects (see Figure 2). During the first two projects (presented in chapter 3 and 4), the pre-sedimentation and subsequent unaerated and aerated bioreactors were followed by an after-sedimentation basin, and during the two more recent projects (presented in chapter 5 and 6) a membrane bioreactor (MBR) replaced the after-sedimentation. Also, the recirculation outtake was changed from bioreactor 6 to bioreactor 5.

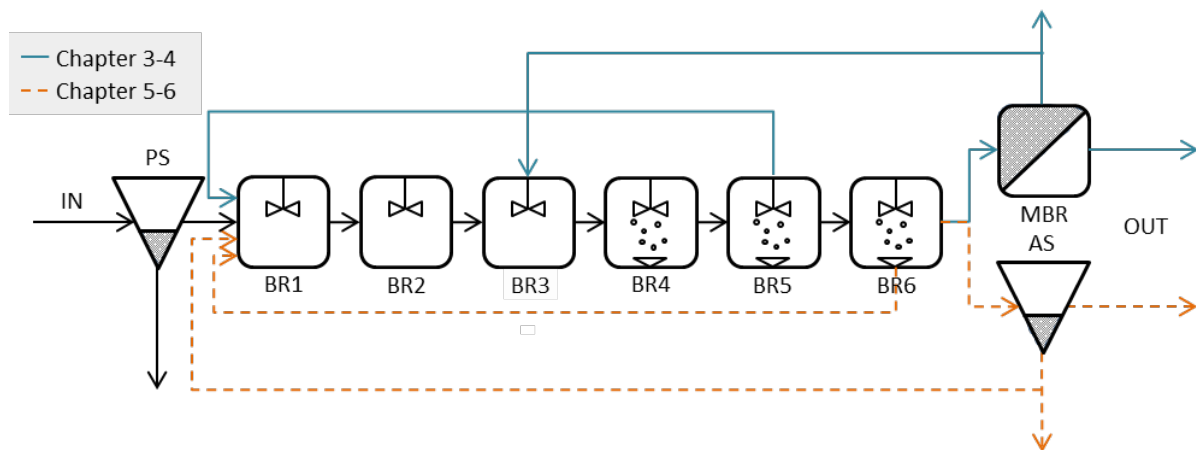


Figure 2. Schematic overview of the two different process setups used during the soft sensor projects. After pre-sedimentation (PS) the wastewater passed through three unaerated bioreactors (BR 1-3) and three aerated bioreactors (BR 4-6). During the two first projects the bioreactors were followed by after-sedimentation (AS) and the aerated water was recirculated from BR6 to BR1. During the last two projects the bioreactors were followed by a MBR and the aerated water was recirculated from BR5 to BR1.

1.4 Previous related soft sensor activities

1.4.1 Resource efficient wastewater treatment, 2002-2007

One of the subprojects of the project “Resource efficient wastewater treatment” (“Resurseffektiv avloppsvattenrening”) concerned implementation of soft sensors at the Henriksdal WWTP as an alternative to conventional measurements.

It was concluded that it should be possible to implement soft sensors for COD, tot-N, $\text{NH}_4\text{-N}$, tot-P, $\text{PO}_4\text{-P}$ in incoming water based on flow, conductivity, TSS and pH. The average prediction error of the soft sensor models developed in the project was between 13 % (for tot-N) and 31 % (for COD) (Nilsson et al., 2007).

1.4.2 Holistic Integrated Process CONTROL, HIPCON, 2003-2006

The aim of this three-year project (2003-2006) was to develop methodology and technology for holistic process management from a life cycle perspective. One of the more specific goals was to develop models that could describe the properties of the incoming water at the Henriksdal WWTP.

Soft sensors for prediction of COD, phosphorous and nitrogen in incoming water were developed. The soft sensors were based on online measurement of TSS, conductivity, flow and pH. They were installed at the Henriksdal WWTP for monitoring purposes and were concluded to be reliable. The use of the soft sensors for control of precipitation chemical dosage was estimated to have the potential to reduce the precipitation chemical consumption with 30 %, corresponding to 630 00 SEK/yr. It would also result in better sludge quality since the sludge would contain less heavy metals originating from the precipitation chemicals. (Röttorp and al., 2007)

2 Introduction to methods used

2.1 Laboratory analysis

COD, COD_f, tot-N, tot-P, NH₄-N, NO₃-N and PO₄-P were analyzed with Hach Lange or WTW cuvette tests approved for accredited analyses. In the master theses, all above-mentioned parameters were measured on samples that had been filtered before analysis. In the other projects analysis of COD_f, NH₄-N, NO₃-N and PO₄-P was made on filtered samples, while COD, tot-N and tot-P was analyzed on unfiltered samples.

In the cases where TSS was not measured online, it was analyzed by filtering a known volume of sample through a filter with a known weight. The filter was then dried in 105°C at least 1hr and weighed again to determine the amount of TSS in mg/L.

The sludge filterability was measured in terms of time to filter (TTF), i.e. the time in seconds required for a certain volume of sample to pass a 90 mm glass microfiber filter (Grade 934-AH RTU, Whatman, GE Healthcare) with a vacuum of 15 mmHg. This was done according to the method specified in GE Water & Process Technologies, 2009. In addition, a TTF value normalized with TSS was calculated according to the following equation:

$$TTF_{norm} = \frac{TTF}{TSS/10^4} \quad (1)$$

2.2 Online process data

The treatment line used for the soft sensor development was equipped with standard online sensors during all projects addressed in this report.

Online process data, and in some cases acoustic data, were collected during the time of the sampling campaigns. Mean values for each online parameter were calculated, corresponding to the samples collected for laboratory analysis.

MATLAB was used for preparing data from the control system for modelling.

2.3 Acoustic measurements

By attaching an accelerometer directly to a process steel reactor or to a constriction through which a side stream of the fluid is pumped, vibrations can be measured, typically in the frequency range 0-50 kHz. In this way, the characteristics of the turbulence of the fluid can be captured in the acoustic signal. Many physical and chemical properties such as particle size, viscosity and density influence the turbulence and thus the acoustic signal. For a more detailed discussion on acoustic measurements and acoustic chemometrics, see (Björk, 2007).

Before useful information can be extracted from the accelerometer signal, it has to be further processed. To reduce irrelevant noise and to make the signal ready to be analyzed, it is amplified, filtered, converted to a digital signal and transformed (e.g. by fast Fourier transform, FFT). The pre-processing results in an acoustic spectrum for each measurement. In the work presented in this report, the generated spectra were analyzed with multivariate data analysis. The procedure of acoustic analysis is illustrated in Figure 3.

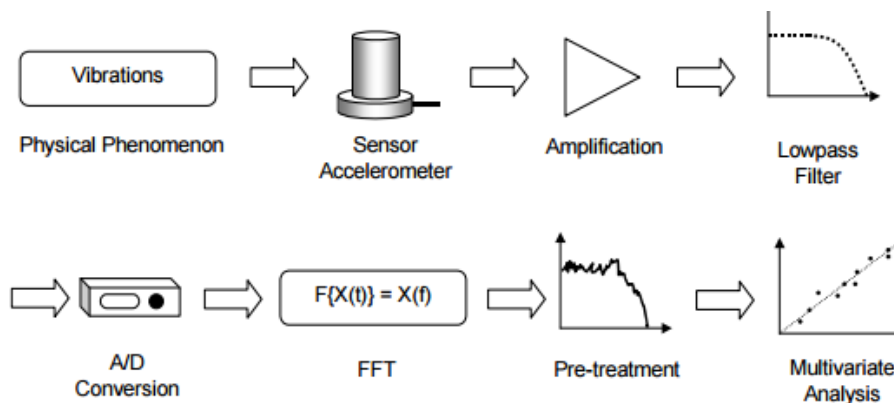


Figure 3. Visualization of steps used for characterization of a fluid with acoustic measurements.

2.4 Multivariate statistics

Data from laboratory analyses, from the control system and from acoustic measurements were used to develop the soft sensor models. First data were pre-processed, then the majority was used to calibrate models and the rest of the data were used for external validation of the models. The software used for all modelling steps was different versions of SIMCA from Umetrics.

2.4.1 PLS and PCA

The multivariate statistical regression method used for calculation of the soft sensor models was PLS, which is short for Partial Least Squares or Projection to Latent Structures (Geladi and Kowalski, 1986, Martens and Naes, 1989). With PLS, the aim is to establish the relationship between input (x) variables, and output (y) variable(s). This is done by reducing the multidimensional data set to lower dimensions by calculating so-called principal components that summarize the data. The number of principal components is often decided by an iterative process where the predictive ability of the principal components is tested and the procedure is stopped when the increase in prediction ability is no longer significant (Eriksson et al., 2001). A PLS model is calculated in such a way that it describes as much variance as possible in the data, while at the same time maximizing the covariance between the x-variables (e.g. the parameters that are measured online) and the y-variables (e.g. the soft sensor parameters). The result is an equation expressing y as a linear combination of the x-variables:

$$y = a_0 + a_1x_1 + a_2x_2 + \dots + a_nx_n, \quad \text{where } n \text{ is the number of } x\text{-variables}$$

PCA (principal component analysis) also summarizes the dataset by creating principal components that describe as much variance as possible in a data matrix (Jackson, 2003). (Martens and Naes, 1989). Unlike PLS PCA it is not a regression method. (Martens and Naes, 1989)

2.4.2 Pre-processing

To be able to use variables of different sizes and variances to calculate models, data are often centered and scaled before modelling. Each variable is centered around its mean value by subtracting each value with the mean value and is thereafter scaled to unit variance by dividing each value with the standard deviation of that variable. The pre-processing is illustrated in Figure 4.

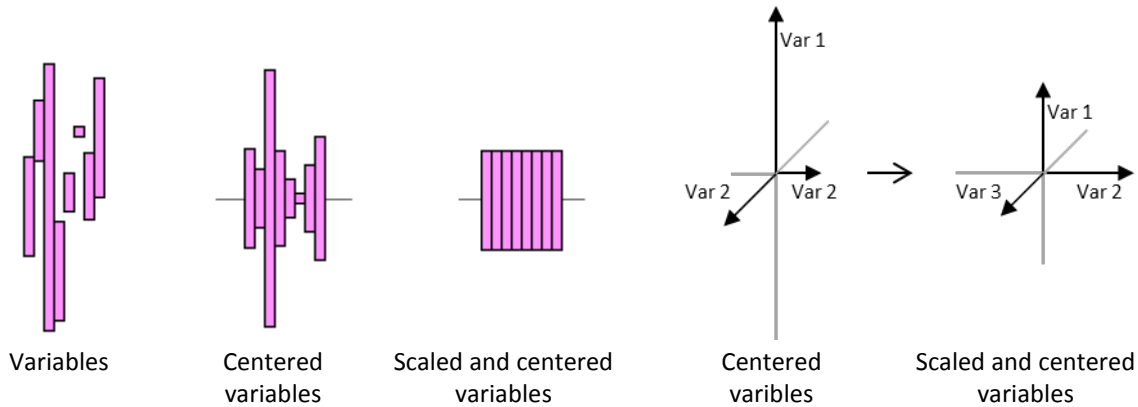


Figure 4. Scaling and centering of variables prior to modelling

2.4.3 External validation

A relatively reliable way of validating the predictive ability of a model is by external validation. When externally validating a PLS-model, data that have not been involved in the calculation (calibration/training) of the model is used. The external validation data set consists of the same x- and y-variables as the calibration data set, but with observations that are new to the model. The PLS-model is fed with the values of the x-variables and is allowed to calculate (predict) the corresponding y-value(s). The predicted y-value(s) can then be compared to the corresponding “real” y-value(s), giving an estimate of the predictive ability of the model.

2.4.4 Measures of model performance

The quality of a PLS-model can be represented in several ways. Quality measures mentioned in this report are:

- R^2 is the part of the variance explained in the calibration data, thus, it is a measure of how well the model fits the calibration data. Note that it does not give information about model performance for new observations. If R^2 is 1, the model explains the data perfectly, if R^2 is zero the model performance is not better than just guessing a random number.

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (2)$$

where $(y - \hat{y})$ refers to the fitted residuals for the observations in the calibration set and n refers to the number of samples.

- Q^2 is an estimate of the predictive ability of the model and is calculated by cross-validation. If Q^2 is 1, the model predicts the data perfectly.

$$Q^2 = 1 - \prod \left(\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \right)_a \quad (3)$$

where $(y - \hat{y})$ refers to the predicted residuals for the observations in the calibration set during cross-validation, n refers to the number of samples and a refers to the principal components.

- **RMSE_{cv}** (root mean square error of cross validation) is an estimate of the predictive power of the model based on cross validation. It has the same unit as the y-variable.

$$RMSE_{cv} = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}} \quad (4)$$

where $(y - \hat{y})$ refers to the predicted residuals for the observations in the calibration set during cross-validation and n refers to the number of samples

- **RMSEP** (root mean square error of prediction) is a measure of the predictive power of a model. It is calculated similarly to standard deviation and can be used roughly as a standard deviation of the predictions. Thus, the lower the value, the better the prediction. It has the same unit as the y-variable.

$$RMSEP = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}} \quad (5)$$

where $(y - \hat{y})$ refers to the predicted residuals for the observations in the external validation data set and n refers to the number of samples.

- **relRMSEP** is a measure of the relative predictive power of a model. Given in %.

$$relRMSEP = 100 \frac{RMSEP}{y_{max} - y_{min}} \quad (6)$$

where $(y - \hat{y})$ refers to the predicted residuals for the observations in the external validation data set, n refers to the number of samples and $y_{max} - y_{min}$ to the range of the y-variable in the calibration set.

- **RMSEP_{true}** is a measure of the prediction error of the model after adjusting for the measurement error and sampling error. It has the same unit as the y-variable.

$$RMSEP_{true} = \sqrt{RMSEP^2 - (ME^2 + SE^2)} \quad (7)$$

where $RMSEP$ refers to the prediction error of the model, ME to the measurement error and SE to the sampling error.

- **relRMSEP_{true}** is a measure of the relative prediction error of the model after adjusting for the measurement error and sampling error. It is given in %

$$relRMSEP_{true} = 100 \frac{\sqrt{RMSEP^2 - (ME^2 + SE^2)}}{y_{max} - y_{min}} \quad (8)$$

where $RMSEP$ refers to the prediction error of the model, ME to the measurement error, SE to the sampling error, $y_{max} - y_{min}$ to the range of the y-variable in the calibration set.

3 Pilot study of soft sensors based on multivariate data analysis

This section is based on work presented in the Master thesis “Prediction of parameters in wastewater using multivariate analysis” (Ottosson, 2013).

3.1 Aim

The purpose of this study was to investigate the possibility of developing soft sensors for COD, tot-N, tot-P, NH₄-N, NO₃-N and PO₄-P in various stages in the pilot-line 1 at Hammarby Sjöstadsværk (incoming water, last anaerobic bioreactor (BR3) and last aerobic bioreactor (BR6)).

3.2 Generation of data

3.2.1 Sampling

53 samples were collected with automatic samplers placed at the incoming wastewater, the last anaerobic bioreactor (BR3) and the last aerobic bioreactor (BR6). The samples were 2 h composite samples and were collected over a period of 5 days during the autumn of 2012. For each sample, corresponding average values for relevant online process parameters in the control system were gathered from the control system. These samples were later used for the training of the models.

6 samples were collected for the external validation of the models. The samples were randomly distributed over a period of 5 days during the winter of 2012.

3.2.2 Parameters

The parameters that the soft sensors were to be calculated for were analyzed by laboratory analyses. The parameters were:

Incoming

- COD_f
- tot-N
- NH₄-N
- tot-P
- PO₄-P
- TSS

Bioreactor 3 (last anaerobic bioreactor)

- NO₃-N

Bioreactor 6 (last aerobic bioreactor)

- NH₄-N
- NO₃-N
- TSS

Note that all lab analyses, including COD, tot-P and tot-N, were made with wastewater that had been filtered through a 1.6 µm filter.

2-hour average data corresponding to the collected samples were calculated for the process parameters of interest. The following online process parameters were used:

Incoming (IN)

- Flow rate (m³/h)
- Temperature (° C)
- pH (pH)
- Redox (mV)
- Cond (µS/cm)

Bioreactor 5 (BR5)

- DO (mg/L)
- Air valve position (%)
- Air flow (m³/h)

Bioreactor 1 (BR1)

- pH (pH)
- Redox (mV)

Bioreactor 4 (BR4)

- DO (mg/L)
- Air valve position (%)
- Air flow (m³/h)

Bioreactor 6 (BR6)

- DO (mg/L)
- Air valve position (%)
- Air flow (m³/h)

Other

- Total air flow(m³/h)
- Precipitation chemical (g Fe/h)

3.2.3 Time lagging of data

Retention times were used to lag data from previous process steps to be able to use those data for models describing parameters in BR3 and BR6.

3.3 Modelling results

3.3.1 Training of models

Models for all parameters measured with lab analyses were calculated on 47 samples. The best models were achieved for PO₄-P and tot-P, both with R²-values over 0.6 and Q²-values over 0.5.

Table 1. Properties of the models calculated for parameters in the incoming water (IN), in bioreactor 3 (BR3) and bioreactor 6 (BR6).

	Parameter	R ²	Q ²
IN	COD	0.45	0.37
	tot-N	0.19	0.095
	NH ₄ -N	0.44	0.308
	PO ₄ -P	0.63	0.561
	tot-P	0.70	0.636
BR3	NO ₃ -N	0.45	0.262
BR6	NO ₃ -N	0.35	0.110
	NH ₄ -N	0.27	0.003

The training resulted in the following equations for tot-P and PO₄-P:

$$\begin{aligned} \text{tot-P}_{\text{IN}} = & 1.8123 + 0.270976 \cdot \text{TSS}_{\text{IN}} + 0.358956 \cdot \text{Temp}_{\text{IN}} + 0.0189042 \cdot \text{pH}_{\text{IN}} \\ & + 0.151619 \cdot \text{Redox}_{\text{IN}} + 0.0508265 \cdot \text{Kond}_{\text{IN}} \end{aligned} \quad (9)$$

$$\begin{aligned} \text{PO}_4\text{-P}_{\text{IN}} = & 1.54872 + 0.182581 \cdot \text{TSS}_{\text{IN}} + 0.344069 \cdot \text{Temp}_{\text{IN}} + 0.00269488 \cdot \text{pH}_{\text{IN}} \\ & + 0.171185 \cdot \text{Redox}_{\text{IN}} + 0.0551863 \cdot \text{Kond}_{\text{IN}} \end{aligned} \quad (10)$$

3.3.2 External validation of models

The external validation was only done for PO₄-P and tot-P since they were the models that gave the most promising results. The validation set consisted of six samples. The coherence of the predicted PO₄-P values and tot-P values and the corresponding values from the lab analyses was poor. This result was most likely mainly caused by a change of the inlet water to the treatment plant, resulting in a significant change of the conditions.

3.4 Discussion and conclusions

Best models could be calculated for tot-P and PO₄-P in the incoming water. These models showed that the input data could be relatively well described by the models and that they provided relatively good predictions. For the other parameters, the models were not good enough. The external validation showed poor conformity between the predicted values and corresponding observed values. This was probably due to the considerable change of the properties of the incoming water that occurred between the collection of samples for training of the models and of the external validation.

In addition, the number of samples used for external validation was low, giving the validation less significance. Despite a poor validation performance, it was, based on this and previous studies, concluded that it could be possible to create and implement soft sensors for tot-P and PO₄-P in incoming water at Hammarby Sjöstadswerk/the Henriksdal WWTP.

4 Pilot study of soft sensors using varying flowrate

This section is based on work presented in the Master thesis “Design of soft sensors for wastewater with multivariate analysis methods” (Abrahamsson, 2013).

4.1 Aim

The purpose of this study was to investigate the possibility of creating soft sensors for COD, tot-N, tot-P, NH₄-N, NO₃-N and PO₄-P in incoming water, in the last anaerobic bioreactor (BR3) and in the last aerobic bioreactor (BR6). A controlled variation in the incoming flow rate was used.

4.2 Generation of data

4.2.1 Sampling

On March 11-15 2013, 2 h flow proportional samples were collected from incoming water, bioreactor 3 and bioreactor 6. 53 samples were collected from each sampling point. No separate sampling campaign for generation of data for external validation was performed, but eight out of 53 samples were used for validation of the models.

4.2.2 Parameters

The following parameters were analyzed on the samples collected during the sampling campaign:

Incoming water

- CODf
- tot-N
- NH₄-N
- tot-P
- PO₄-P
- TSS

Bioreactor 3 (last anaerobic bioreactor)

- NO₃-N

Bioreactor 6 (last aerobic bioreactor)

- NH₄-N
- NO₃-N
- TSS

Note that all lab analyses were made with water that had been filtered through a 1.6 µm filter.

Online process data were collected during the time of the sampling campaign. 2 h mean values for each online process parameter were calculated, corresponding to the samples collected and analyzed. The following online process parameters were used:

Incoming water (IN)

- Temperature (° C)
- pH (pH)
- Redox (mV)
- Conductivity (µS/cm)
- Suspended solids (mg/L)

Bioreactor 3 (BR3)

- Temperature (° C)
- pH (pH)
- Redox (mV)

Bioreactor 4 (BR4)

- DO (mg/L)
- Air valve position (%)

Bioreactor 5 (BR5)

- DO (mg/L)
- Air valve position (%)

Bioreactor 6 (BR6)

- DO (mg/L)
- Air valve position (%)
- Temperature (° C)
- pH (pH)
- Suspended Solids (mg/L)

Other

- Recirculation flow (m³/h)
- Return sludge flow (m³/h)

4.2.3 Controlled flowrate

Normally, the incoming flowrate at Hammarby Sjöstadswerk Line 1 is relatively constant at approximately 1.25 m³/h. To introduce more variations, the flow rate was instead manually changed once a day, creating controlled flow variations between 0.9 and 1.5 m³/h during the sampling campaign. The ratio between incoming flow and recirculation flow was kept at 1:4 and the ratio between incoming flow and sludge recirculation flow was 1:1.

4.2.4 Time lagging of data

To be able to combine process data from several process steps, i.e. to use information collected during earlier process steps, data were lagged. The lag was determined by using calculated values for retention time for each process basin, which were assumed to be filled to 90%.

$$T = \frac{0.9 V}{Q} \quad (11)$$

where T = retention time [h], V = total volume of the process basins up to the measurement point [m³], Q = flow rate [m³/h]. The lagging of the data was then made accordingly.

4.3 Modelling results

4.3.1 Training of models

PLS models for phosphorus, nitrogen and COD in incoming water, and nitrogen in the bioreactors were calculated. The models were based on 35 (fractions of nitrogen in incoming water), 43 (COD and fractions of phosphorous in incoming water) or 45 (fractions of nitrogen in bioreactors) observations. In Table 2, only the models for COD and tot-N in incoming water had a Q² over 0.5, i.e. a decent predictive ability. The models for the nitrogen fractions in the bioreactors had Q²-

values under 0.2 and were therefore not presented or further evaluated. The model equations for the parameters are presented in Table 3.

Table 2. Properties of the best models calculated for each parameter in the incoming water (IN). Q²-values for the parameters in bioreactor 3 (BR3) and bioreactor 6 (BR6) were very low and the model characteristics were therefore not reported.

	Parameter	R ²	Q ²
IN	COD	0.600	0.575
	tot-N	0.558	0.526
	NH ₄ -N	0.457	0.426
	PO ₄ -P	0.517	0.460
	tot-P	0.345	0.256
BR3	NO ₃ -N	-	-
BR6	NO ₃ -N	-	-
	NH ₄ -NBR6	-	-

Table 3. Modell Equation for the different properties estimated

Modell equation

$$\text{COD}_{\text{IN}} = 3.14 + 0.42 \cdot \text{Kond}_{\text{IN}} + 0.42 \cdot \text{TSS}_{\text{IN}} \quad (12)$$

$$\text{tot-N}_{\text{IN}} = 6.82 + 0.32 \cdot \text{Kond}_{\text{IN}} + 0.32 \cdot \text{TSS}_{\text{IN}} - 0.3 \cdot \text{pH}_{\text{BR6}} \quad (13)$$

$$\text{NH}_4\text{-N}_{\text{IN}} = 6.89 + 0.27 \cdot \text{TSS}_{\text{IN}} - 0.32 \cdot \text{pH}_{\text{BR6}} \quad (14)$$

$$\text{tot-P}_{\text{IN}} = 5.34 + 0.31 \cdot \text{pH}_{\text{IN}} - 0.34 \cdot \text{Redox}_{\text{IN}} \quad (15)$$

$$\text{PO}_4\text{-P}_{\text{IN}} = 3.95 - 0.4 \cdot \text{Redox}_{\text{IN}} - 0.4 \cdot \text{pH}_{\text{BR6}} \quad (16)$$

4.3.2 External validation of models

External validation of the models was made with 6 (nitrogen) or 8 (phosphorous and COD) randomly selected observations. The results from the external validation are presented in Table 4 below.

Table 4. Results from external validation of the soft sensor models.

	Parameter	R ²
IN	COD _{IN}	0.32
	tot-N _{IN}	0.86
	NH ₄ -N _{IN}	0.86
	PO ₄ -P _{IN}	0.68
	tot-P _{IN}	0.51
BR3	NO ₃ -N	-
BR6	NO ₃ -N	-

4.4 Discussion and conclusions

Promising models could be calibrated for tot-N and NH₄-N in the incoming water. The external validation confirmed the promising results. The model for COD in the incoming water was also

good, but the external validation indicated that its predictive ability was very low. However, the selection and number of observations for external validation was not optimal.

Mentioned factors that could have affected the results were:

- More samples were needed to calculate reliable models
- The number of observations for external validation was too low
- There should have been a separate sampling campaign to collect data for external validation, rather than randomly selecting observation from the same sampling campaign intended for the training of the models
- The lagging of data from previous sampling points was a rough approximation
- There were some changes/disturbances in the process during the sampling campaign, which might have affected the results

5 Application of acoustic and soft sensor based monitoring

This section is based on work presented in the article "Feasibility study on passive acoustic and soft sensor based monitoring of biological wastewater treatment processes" (Nilsson et al., 2017).

5.1 Aim

The aim of the study was to develop soft sensors for a number of parameters at five different process steps in line 1 at Hammarby Sjöstadswerk, and to evaluate acoustic measurements for generation of input variables to soft sensors.

5.2 Generation of data

The data used for modelling, originated from laboratory analysis of samples collected during a sampling campaign and corresponding process values and spectra from acoustic sensors.

5.2.1 Sampling

During 13 days (October 5th to 18th 2014), grab samples were collected from incoming (untreated) wastewater, BR 1, BR5, BR6 and from the MBR. Which parameters to analyze were selected based on their relevance in each process step. Samples for analysis of PO₄-P, NH₄-N, NO₃-N and COD_f were manually collected every fourth hour between 08:00 and 16:00 on weekdays and were filtered through a 0.45 µm syringe filter within 2 minutes after collection. Samples for analysis of tot-P, tot-N, TSS, COD and sludge filterability (TTF) were collected with automatic samplers (6712 Portable Sampler, Isco) every fourth hour around the clock every second day. The samples were stored in the partially ice-filled insulated samplers and/or in a +4⁰C fridge until analyzed.

5.2.2 Parameters

The following parameters were manually analyzed in the samples collected during the sampling campaign:

Incoming water:

- PO₄-P
- tot-P
- NO₃-N
- NH₄-N
- COD
- COD_f
- tot-N
- TSS

Bioreactor 1 (first anaerobic bioreactor)

- PO₄-P
- tot-P
- NO₃-N
- NH₄-N
- COD
- COD_f
- tot-N
- TSS

Bioreactor 5 (second aerobic bioreactor)

- NO₃-N
- NH₄-N

Bioreactor 6 (last aerobic bioreactor)

- NO₃-N
- NH₄-N
- TSS

Membrane bioreactor

- PO₄-P
- NO₃-N
- TSS
- TTF

There were a large number of on-line process parameters available and acoustic data were gathered from sensors (piezoelectric accelerometers from Kistler) installed on BR1, BR5 and the MBR. The number of samples that had both process data and acoustic spectra varied between 28-42 samples. For more details on equipment, exact number of samples, specification of which on-line parameters that were measured in the different process positions etc., see (Nilsson et al., 2017).

5.3 Modelling results

Soft sensor models were developed for all manually analyzed parameters. Before calculating the models, data were split into a calibration set for the calculation of each model, and a validation set for external validation of the model. The first 1/6 and last 1/6 of the data were selected as validation set, and the rest was used as calibration set. All data, except for the acoustic data, were centered and scaled to unit variance before modelling.

5.3.1 Training of models

PLS models were calculated for the data in the calibration set. To improve the models, x-variables that did not contribute to the models were excluded. The decision of which x-variables to exclude was based on each variable's VIP-value, which reflects the extent to which the variable explains X and correlates to Y. The main results of the model training are shown in Table 5. For more detailed information, see (Nilsson et al., 2017).

To evaluate the models and select the best model for each parameter, cross-validation was used to estimate the predictive power of the models. The cross-validation was made with seven cross validation groups. The first 1/7 of the observations formed the first group, the second 1/7 of the observations formed the second group and so on. Response permutation testing was then used to decrease the risk of selecting models that were overfitted to the calibration data, i.e. that were describing noise.

5.3.2 External validation of models

The best model for each parameter in each sampling point was then externally validated with the data in the validation dataset. Out of 26 soft sensors, 4 models had a relRMSEP of less than 15 % (NH₄-N in untreated water based on process data, COD in the first bioreactor based on acoustic data, NH₄-N in the last bioreactor based on process data and TSS in the membrane bioreactor based on process data). 12 models had a $\text{relRMSEP}_{\text{true}}$ of less than 15 %, out of which 6 models had a $\text{relRMSEP}_{\text{true}}$ of less than 10 % (NO₃-N in untreated water based on process data, COD, TSS and NO₃-N in the first bioreactor based on acoustic data, NH₄-N in the last bioreactor based on process data and TSS in the membrane bioreactor based on process data). The main results from the validation of the models are shown in Table 6. For more elaborate and detailed information, see (Nilsson et al., 2017).

Table 5. Properties of the best PLS-model for each parameter RMSE_{cv} – prediction error for cross validation.

	Parameter	RMSE _{cv}
IN	tot-P	1.28
	tot-N	11.8
	COD	132
	TSS	77
	PO ₄ -P	0.45
	NO ₃ -N	0.17
	NH ₄ -N	4
	COD _f	49
BR1	tot-P	9.9
	tot-N	27.1
	logCOD	690
	TSS	289
	PO ₄ -P	0.08
	NO ₃ -N	0.3
	NH ₄ -N	0.23
	COD _f	8.8
BR5	NO ₃ -N	1
	NH ₄ -N	0.37
BR6	TSS	367
	NO ₃ -N	1.11
	NH ₄ -N	0.559
MBR	TSS	336
	PO ₄ -P	0.08
	NO ₃ -N	0.98
	TTF	2.37
	TTF _{norm}	1.88

Table 6. Results from the external validation, $\text{relRMSEP}_{\text{true}}$ - relative RMSEP adjusted for measurement error and sampling error.

	Parameter	$\text{relRMSEP}_{\text{true}}$
IN	tot-P	16.8
	tot-N	15.9
	COD	22.2
	TSS	27.1
	PO ₄ -P	18.0
	NO ₃ -N	0
	NH ₄ -N	13.7
	COD _f	10.5
BR1	tot-P	14.4
	tot-N	25.2
	logCOD	9.5
	TSS	0
	PO ₄ -P	65.8
	NO ₃ -N	0
BR5	NH ₄ -N	12.9
	COD _f	23.5
	NO ₃ -N	34.9
	NH ₄ -N	31.4
BR6	TSS	0
	NO ₃ -N	37.8
	NH ₄ -N	7.9
MBR	TSS	0
	PO ₄ -P	13.8
	NO ₃ -N	21.0
	TTF	119.3
	TTF _{norm}	137.6

5.4 Discussion and conclusions

Since the composition of the incoming wastewater varies greatly between seasons and different weather conditions, more sampling campaigns should be done. Preferably, they should be spread out over at least one year to generate data that is representable enough to draw more extensive

conclusions about the suitability of soft sensors as a possible method to generate online data for wastewater treatment.

The amount of rainfall varied considerably during the sampling campaign, which significantly affected the composition of the wastewater. This increased the risk that the range of wastewater composition in the external validation set was not covered by the calibration set, which results in that the external validation indicates that the predictive ability of the models is lower than it would have been if the validation set would have been representative for the calibration set.

A number of soft sensors showed a relatively good predictive ability, which indicated that soft sensors have the potential to provide WWTPs with online process values relevant for process monitoring and control.

For the majority of the parameters, the soft sensors that were based on acoustic data had comparable or better performance than corresponding models based process data. This brought the authors to the conclusion that data from acoustic sensors can be used as input variables for soft sensors at WWTPs.

The soft sensors could probably be further improved by calibrating them with data generated during a longer period of time, which could reduce the prediction errors and as expand the validity domains of the models, and/or by improving the acoustic data by optimizing the calculation of the acoustic spectra and the signal processing or by using other types of accelerometers. This further strengthened the conclusion that soft sensors is a promising approach for WWTPs.

6 Soft sensors for acoustic monitoring of an SBR and low phosphorus concentration in MBR effluent

This section is based on work presented in the conference presentation "Experiences from using acoustic soft sensors in wastewater treatment – results from pilot studies" (Åmand et. al, 2017).

6.1 Aim

The aim of the two pilot studies in this section was to test the use of acoustic soft sensors in real case wastewater treatment processes. Soft sensors were developed for two applications: (1) Predicting phosphate ($\text{PO}_4\text{-P}$) concentrations in the effluent from a membrane bioreactor (MBR) and (2) Process monitoring of an advanced sequencing batch reactor (SBR) with continuous inflow (ICEASTM, Sanitaire, Xylem Inc.).

6.2 Generation of data

6.2.1 Soft sensor for phosphate in MBR effluent

The phosphate concentration in the MBR-effluent at Hammarby Sjöstadswerk is normally very constant and low, which lead to the conclusion that the phosphate concentration range was too

limited for model development. Instead, a batch calibration test was conducted by adding different amounts of phosphoric acid to the effluent to simulate phosphorous concentration variations between 0.07 and 22.2 mg/L. The phosphorous containing effluent was run in an acoustic rig (Figure 5) with a constriction equipped with an acoustic sensor (4396 Bruel & Kjaer accelerometer). Data from the accelerometer were acquired with a data acquisition module (NI PCI-4461). Spectral frequency range was 0 to 102.4 kHz, using 2048 frequency bins.

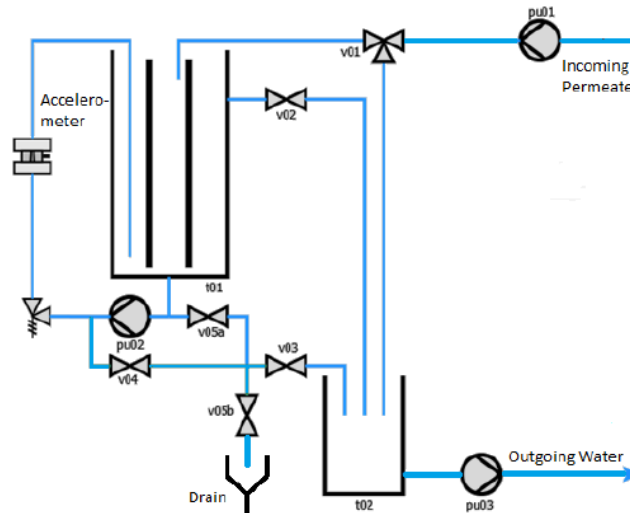
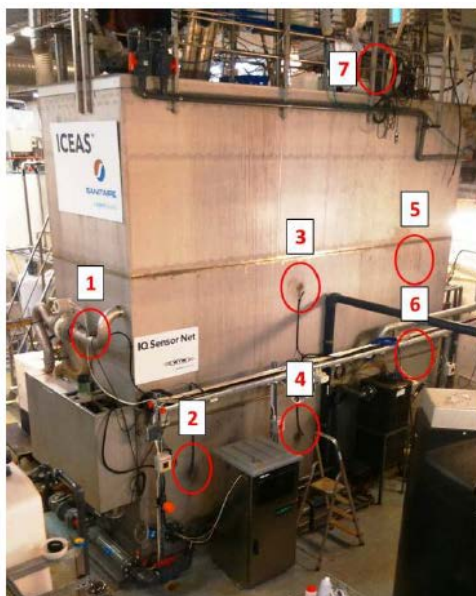


Figure 5. Schematic outline of the acoustic rig used for phosphorous measurements in the MBR effluent.

6.2.2 Process monitoring in a continuous SBR

On-line instruments monitored the influent flow rate, influent TSS, water temperature, pH, oxidation-reduction potential, water level in tank, suspended solids, ammonia, phosphate, dissolved oxygen and air flow rate in the SBR. In addition, the process tanks were equipped with seven acoustic sensors (Kistler Type 8714B100M5, see Figure 6 for sensor positioning). Data from the accelerometers were acquired with two NI cDAQ 9181 chassis. The frequency range was 0 to 25.6 kHz for the spectra, using 1024 frequency bins.



No	Position	Description
1	TT	Effluent transfer tank
2	MRZWAS	Main reaction zone, waste sludge outtake
3	MRZH	Main reaction zone, high position
4	MRZL	Main reaction zone, low position
5	PRZH	Pre reaction zone, high position
6	PRZL	Pre reaction zone, low position
7	MT	Influent mixing tank

Figure 6. Positioning of accelerometers on the SBR process tanks. The water flows through the mixing, pre reaction, main reaction and transfer tanks in this order.

6.3 Modelling results

6.3.1 Soft sensor for phosphate in MBR effluent

Observations with phosphate concentrations > 10 mg/L were excluded and a PLS model was built on the remaining 33 data points. The PLS model had four principal components, $R^2Y = 0.99$, $Q^2 = 0.90$ and $RMSEE = 0.25$. The observed versus predicted phosphate concentrations are shown in Figure 7. The intention was to have the system running continuously and to use the soft sensor in the monitoring and control of the MBR process after the end of the project.

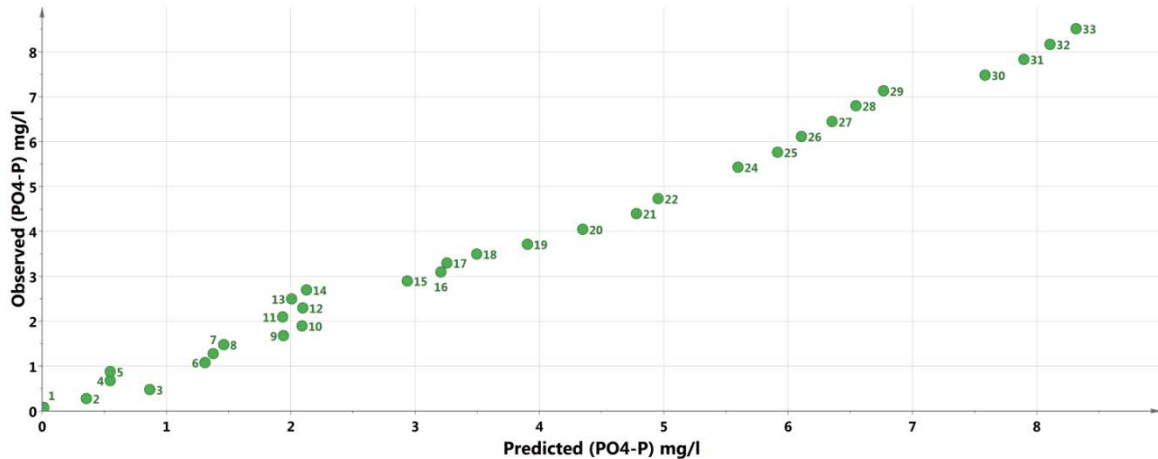


Figure 7. Observed phosphate concentrations (mg/L) in MBR permeate versus Predicted phosphate concentrations (mg/L) from the PLS model.

6.3.2 Process monitoring in a continuous SBR

All major process noises were captured in the PCA models, including pumping, aeration, decanting of floating sludge and mixing. The best PLS models were those capturing the influent flow rate ($R^2Y = 0.94$) and TSS in incoming water ($R^2Y = 0.84$) to the SBR (Figure 8) and air flow rate in the main reaction zone (not shown). Floating sludge was when necessary removed from the main reaction zone through decanting, leading to a reduced variance in the first principal component score value (t_1) of the PCA representing the mixing tank (Figure 9). A principal component is a condensate of the original (measured) parameters, and a score value is the principal component value for an observation (Martens and Naes, 1989)

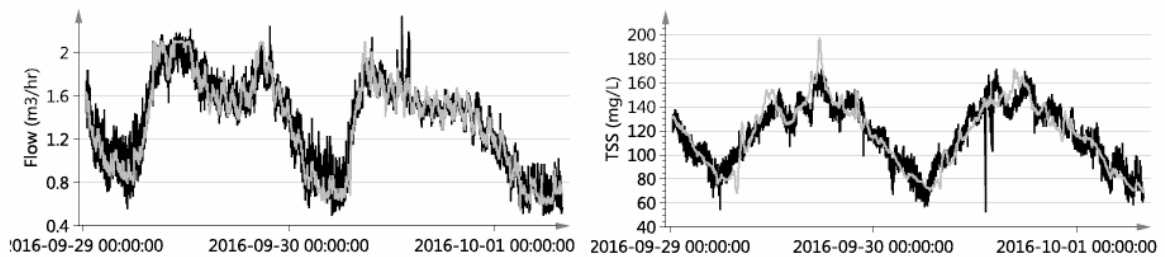


Figure 8. Acoustic soft sensors for influent flow rate and influent TSS in SBR mixing tank (measured values in grey, predicted values in black). Both models consisted of four principal components.

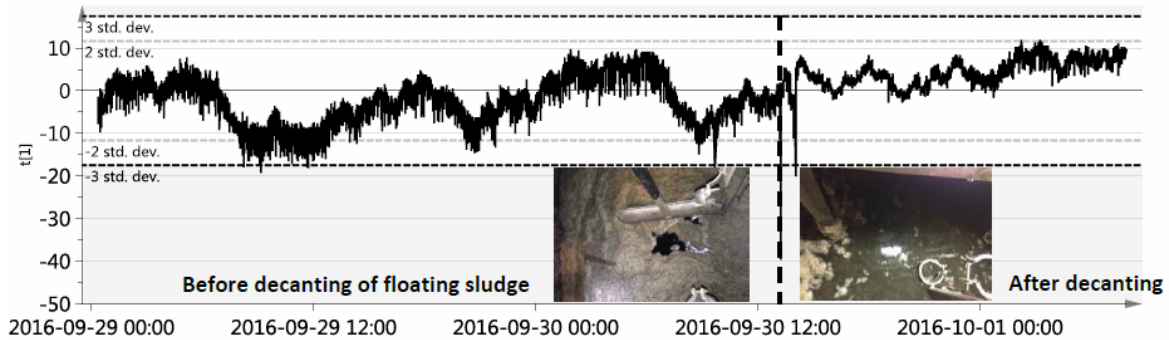


Figure 9. The variance of the score for the first principal component (t_1) in the mixing tank PCA model is reduced after floating sludge is removed from the main reaction zone. The phenomenon occurs after all three recorded occasions.

6.4 Discussion and conclusions

Results showed that modelling spectral data from acoustic sensors could predict effluent phosphate concentrations including variations by measuring fluid vibrations in the effluent of an MBR. A second trial with a higher water temperature indicated that the soft sensor developed was temperature sensitive, leading to the conclusion that the effect of temperature would need to be further investigated before implementing the method for continuous use.

Process variations and process noise could be modelled with the acoustic sensors installed on the SBR process tank. The models experienced some problems with robustness over time and noise disturbances, and the authors suggested incorporating data from an acoustic sensor measuring background sounds in the surroundings to improve the model robustness.

7 Overall conclusions and discussion

To create soft sensor models for wastewater properties is not an easy task. The considerable seasonal and daily changes in load and composition are major challenges. Nevertheless, a number of the soft sensors that have been developed showed a relatively good predictive ability, which indicates **that soft sensors have the potential to provide WWTPs with online process values** relevant for process monitoring and control.

For the majority of the parameters for which both acoustic and process data were available as input data, the soft sensors that were based on acoustic data had comparable or better performance than corresponding models based process data. This demonstrates that data from **acoustic sensors** in many cases preferably could be used as input data to soft sensor models for WWTPs, either alone or together with online process data.

A number of possibilities for further improvement of the soft sensors were identified:

- All studies mentioned in this report agreed on that more data should have been used for calibration and validation of the models. To calibrate reliable models, **a significant amount of data is needed**, and the data collection should preferably to be spread out over the year.
- If the models are to be used during specific conditions such as flooding, thawing etc., data also have to be collected specifically during such conditions. Separate models might have to be used for different seasons and different conditions.

- Furthermore, the relationships between the different parameters might change as changes in the sewer network are introduced in form of for example new industries, new living habits or climate changes. The validity of the models must therefore be checked regularly, preferably also with automatic model diagnostics tools, to signal when the models have to be **re-calibrated**.
- For soft sensor models that describe properties of wastewater that has passed one or more treatment steps, changes in the operation of the previous treatment process(es) will probably also make re-calibration of the models necessary.
- To give the **validation** of the soft sensors credibility, more efforts have to be made on generating data for external validation.
- When data from previous process steps were used in the models, those data were lagged. The **lagging** of data is an approximation, and a more complex lagging principle might be necessary to create a more accurate lagging and thus better soft sensor models.
- The soft sensors based on acoustic data can probably be improved by further developing the **calculation of the acoustic spectra**, optimizing the **signal processing** and/or by testing other types of accelerometers

The potential for model improvements further strengthens the conclusion that soft sensors is a promising approach for WWTPs.

It is important that the **online sensors** that are used by the models are **well maintained**, e.g. good cleaning and calibration routines are necessary.

When evaluating the performance of the soft sensors, their accuracy should be compared with the accuracy of commercially available online sensors, which in many cases is far from perfect. In many cases, there are no online sensors available. Furthermore, data from laboratory analyzes are also associated with uncertainties. The samples might not be representative, which introduces a sampling error, and the results from laboratory analyzes are not very accurate, which introduces a measurement error. Furthermore, the samples are most often not analyzed immediately after collection, which introduces an effect of storage since storage time, conditions and handling can affect the composition of the samples.

8 Outlook

Wastewater treatment plants have a need for efficient sensors to measure complex properties of process streams online. That need will increase as plants move from a “treat water” paradigm to a broader “resource recovery” paradigm. Throughout this shift, some process steps will be intensified, thus processing conditions or geometry of process units will be changed yielding shorter retention time that could require tighter measurements and control of relevant species or properties of the fluids to be processed. More extreme weather conditions can lead to greater fluctuations in flow and composition of incoming water and adequate online monitoring and control will be important to make it possible to adapt the processes to the new requirements this will bring. In addition, future stricter effluent regulations are also a further driver for better online process data.

From the sensor and connectivity side of the work presented in this report, sensors themselves are becoming cheaper and the wireless data transmission capacity is increasing while the cost goes down. In addition, the possibility to have heavier signal processing and more complex data

processing models in a board directly connected to the sensor is increasing, making it possible to use more sensors at lower cost and with easier installation. When utilizing vibrations sensors to predict properties of or species in wastewater streams, we need both good signal processing of the vibration signals and good prediction models. Improved signal processing should be utilized to extract more features that are relevant before estimating the prediction models. Note that saving raw time-series data from a vibration-acoustic sensor is not an option since it yields 16 GB/day. Signal processing is therefore a necessity to lower the amount of data to store. There are examples in the literature that are more feasible to implement today with the ever-increasing computing power than when they were introduced. Similarly, there has been a development of frameworks and types prediction models that could be tested, and there are examples from literature that indicate a possibility for improvement of the final prediction quality (Björk and Danielsson, 2002).

Concluding our outlook, it is our opinion that soft sensors based on vibration-acoustic sensors as well as soft sensors based on regular process sensors can be successful in the long run in waste water treatment. Further work will be needed to take advantage of the rapid development in information technology.

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IVL Swedish Environmental Research Institute Ltd.
P.O. Box 210 60 // S-100 31 Stockholm // Sweden
Phone +46-(0)10-7886500 // Fax +46-(0)10-7886590 // www.ivl.se