Estimating nitrate concentration in the post-denitrification unit of a municipal wastewater treatment plant

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Abstract: Due to stringent environmental regulations, wastewater treatment plants are always challenged to meet new constraints in terms of water pollution prevention. In such an effort, the number of sensors and data available in the plants have increased considerably during the last decades. However, the quality of the collected data and the sensor reliability are often poor mainly due to the hostile environment in which the measurement equipment has to function. In this work, we present the design of an array of soft-sensors to estimate the nitrate concentration in the post-denitrification filter unit of the Viikinmäki wastewater treatment plant in Helsinki (Finland). The developed sensors aim at supporting the existing hardware analysers by providing a reliable back-up system in case of malfunction. After a careful selection of suitable observations and variables to be used for calibrating the estimation models, the experimental results show the accuracy of the developed soft-sensors and their potential for an on-line implementation in the plant’s control system.

Keywords: Water quality monitoring, Soft-sensors, Post-denitrification, Wastewater treatment.

1. INTRODUCTION

Nowadays, wastewater treatment plants (WWTPs) are continuously challenged to satisfy new constraints in terms of quality of the discharged effluent for the compliance with stringent environmental regulations. For such a reason, WWTPs are aiming toward an efficient and safe operation of the plants, leaving behind the old-fashioned idea of poorly monitored plant, to become a modern industry where the collected data are reliable and exploitable for implementing advanced control strategies and, on a higher level, for achieving plant-wide optimization. A major requirement for reaching these objectives relies on real-time supervision on important process indicators related to effluent quality and plant performance. In such a context, soft-sensors are an important technology when online hardware sensors are not available (Kadlec et al., 2009). In addition, soft-sensors can be used to diagnose existing instruments and replace them when unreliable measurements are reported.

This vision has motivated inspiring efforts toward the definition of systematic approaches to data-derived process monitoring and supervision in WWTPs. Especially in the last decade, most of the work has led to the development and application of tools borrowed from chemometrics (Rosen, 2001), multivariate statistical process control (Ordonómez, 2008; Aguado and Rosen, 2008; Lee et al., 2008) and tools for on-line monitoring and supervision of WWTPs (Vanrolleghem and Lee, 2003; Yoo et al., 2008; Baggiani and Marsili-Libelli, 2009; Gilbert et al., 2010). With the increased sensor availability, the need of systems that supply the operators and the plant engineers with decision support information has also increased. In fact, the problem is that even when on-line instrumentation is available, it can not always be relied upon, mainly due to hash environmental conditions in WWTPs. Partial failure in the sensors (e.g., bias, drift, precision degradation, etc.) may result in an erroneous control action and false perception of the performance of the monitored system, sometimes giving rise to less than desirable implications.

In this work, we focus on the nitrate sensors in the post-denitrification filter unit at the Viikinmäki WWTP in Helsinki (Finland). Due to strict treatment requirement of nitrogen compounds, the plant has been updated several times and since 2004, with the introduction of the tertiary filters, a total nitrogen removal level of approximately 90% of yearly average has been achieved. To favor the removal, methanol is dosed with a feedback loop policy according to the nitrate concentration in the filters which is, in turn, measured on-line with analytical instruments. Clearly, the proper functioning of the nitrate sensors is of crucial importance from both an environmental and an economical point of view. On the other hand, the environment where these instruments operate exposes the analysis to a potential malfunction and a back-up is needed to enforce robustness in the control strategy of the unit.
For such a reason, we investigated the possibility to develop a data-derived approach to model the functioning of the post-denitrification process and design an array of soft-sensors that estimate in real-time the nitrate concentration in the filters, starting from other easy-to-measure process variables. Being simplicity one of the main requirements to allow a full-scale implementation of the sensors in the plant’s control system (Kano and Ogawa, 2010), computationally light linear models have been used for the design.

The paper is organized as follows: after a brief description of the investigated unit process (Section 2), the main stages of the sensors’ design are discussed and the development presented and motivated from a process point of view (Section 3). The design is presented in detail, starting from the preliminary preprocessing of the available process measurements where sample and variable selection has been performed (Section 3.1 and 3.2), toward the calibration of the regression models (Section 3.3) and discussion on the results of the sensors performance (Section 4).

2. PROCESS DESCRIPTION

The Viikinmäki WWTP (800000 Population Equivalent) is the largest wastewater treatment plant in Finland; it is built inside a bed rock and treats an average influent flowrate of 250000 m³/d with peaks of 800000 m³/d. The wastewater treatment line of the plant consists of bar screening, grit removal, pre-aeration, primary sedimentation, activated sludge process (divided into 8 treatment lines), secondary sedimentation and a biological post-filtration (post-denitrification). The sludge treatment is achieved with four mesophilic digesters and subsequent dewatering systems. The biogas from the sludge digestion is utilised for electricity and heat production.

The post-denitrification unit receives wastewater from the secondary sedimentation unit and nitrate removal is achieved by means of ten Biostyr™ filters arranged in parallel, Figure 1(a). The influent wastewater is equally distributed to ten filter cells and, before each cell, the incoming flow is split in two separate streams (Fi-QW-1/2) where methanol diluted in water (a constant 10% dilution is used) is added independently to each line, Figure 1(b). Methanol provides a readily biodegradable organic substrate as energy source for the denitrifying bacteria. The diluted methanol flowrate is measured in each line (Fi-QM-1/2) and the overall flowrate to each filter is manipulated by a feedback loop controlling the nitrate concentration in the cell (Fi-NO₃). The nitrate concentration in the cell is measured in real-time using an optical instrument (Nitratax™ plus). Inside the cell, wastewater flows upwards through a floating support media where biomass is attached; the support media fills approximately half of the bed. The biomass attached to the support media tends to clog the cell and periodic backwashes are needed at intervals ranging from 12 to 72 hours according to the head-loss. The cells are usually backwashed one at a time using the effluent wastewater (Fi-QWW) with a counter-current air flow (Fi-QWA). Backwash discharge water is pumped to the beginning of the wastewater treatment line of the plant. The average retention time of the filtering process is 25 minutes. After

Table 1. Process variables

<table>
<thead>
<tr>
<th>TAG</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>I-NO₃-1</td>
<td>Influent Nitrate (sensor 1)</td>
<td>mg/l</td>
</tr>
<tr>
<td>I-NO₃-2</td>
<td>Influent Nitrate (sensor 2)</td>
<td>mg/l</td>
</tr>
<tr>
<td>I-SS-1</td>
<td>Influent Suspended Solids (sensor 1)</td>
<td>mg/l</td>
</tr>
<tr>
<td>I-SS-2</td>
<td>Influent Suspended Solids (sensor 2)</td>
<td>mg/l</td>
</tr>
<tr>
<td>I-O₂</td>
<td>Influent Dissolved Oxygen</td>
<td>mg/l</td>
</tr>
<tr>
<td>I-OP</td>
<td>Influent Phosphate-Phosphorus</td>
<td>mg/l</td>
</tr>
<tr>
<td>I-TP</td>
<td>Influent Total Phosphorus</td>
<td>mg/l</td>
</tr>
<tr>
<td>Fi-QWW</td>
<td>i-th Filter Backwashing water flowrate</td>
<td>m³/s</td>
</tr>
<tr>
<td>Fi-QWA</td>
<td>i-th Filter Backwashing air flowrate</td>
<td>m³/s</td>
</tr>
<tr>
<td>Fi-QW-1</td>
<td>i-th Filter Wastewater flowrate (line 1)</td>
<td>m³/s</td>
</tr>
<tr>
<td>Fi-QW-2</td>
<td>i-th Filter Wastewater flowrate (line 2)</td>
<td>m³/h</td>
</tr>
<tr>
<td>Fi-QM-1</td>
<td>i-th Filter Methanol flowrate (line 1)</td>
<td>m³/h</td>
</tr>
<tr>
<td>Fi-QM-2</td>
<td>i-th Filter Methanol flowrate (line 2)</td>
<td>m³/h</td>
</tr>
<tr>
<td>Fi-P-1</td>
<td>i-th Filter Pressure at the bottom</td>
<td>kPa</td>
</tr>
<tr>
<td>Fi-P-2</td>
<td>i-th Filter Pressure at the top</td>
<td>kPa</td>
</tr>
<tr>
<td>Fi-NO₃</td>
<td>i-th Filter Effluent Nitrate</td>
<td>mg/l</td>
</tr>
<tr>
<td>Fi-HL</td>
<td>i-th Filter Head-Loss</td>
<td>m</td>
</tr>
<tr>
<td>Fi-CR</td>
<td>i-th Filter Clogging rate</td>
<td>%</td>
</tr>
<tr>
<td>Fi-HRU</td>
<td>i-th Filter Hour in use</td>
<td>0 – 1</td>
</tr>
<tr>
<td>Fi-ITW</td>
<td>i-th Filter Intermediate time of backwash</td>
<td>0 – 1</td>
</tr>
<tr>
<td>E-NO₃</td>
<td>Nitrate concentration in the effluent</td>
<td>mg/l</td>
</tr>
<tr>
<td>E-TOC</td>
<td>Total Organic Carbon in the effluent</td>
<td>mg/l</td>
</tr>
<tr>
<td>E-OP</td>
<td>Phosphate-Phosphorus in the effluent</td>
<td>mg/l</td>
</tr>
<tr>
<td>E-TP</td>
<td>Total Phosphorus in the effluent</td>
<td>mg/l</td>
</tr>
<tr>
<td>E-T</td>
<td>Temperature in the effluent</td>
<td>°C</td>
</tr>
</tbody>
</table>

For such a reason, we investigated the possibility to develop a data-derived approach to model the functioning of the post-denitrification process and design an array of soft-sensors that estimate in real-time the nitrate concentration in the filters, starting from other easy-to-measure process variables. Being simplicity one of the main requirements to allow a full-scale implementation of the sensors in the plant’s control system (Kano and Ogawa, 2010), computationally light linear models have been used for the design.

The paper is organized as follows: after a brief description of the investigated unit process (Section 2), the main stages of the sensors’ design are discussed and the development presented and motivated from a process point of view (Section 3). The design is presented in detail, starting from the preliminary preprocessing of the available process measurements where sample and variable selection has been performed (Section 3.1 and 3.2), toward the calibration of the regression models (Section 3.3) and discussion on the results of the sensors performance (Section 4).
filtration, the wastewater treated in the filter is discharged into the effluent channel where streams from Filter 10 to 1 are collected.

The quality of the influent wastewater is monitored online, before division to each of the cells, in terms of dissolved oxygen (I-O2), suspended solids (I-SS-1/2), nitrate (I-NO3-1/2), phosphate (I-P) and total phosphorus (I-TP). As for the effluent, temperature (E-T), total organic carbon (E-TOC), nitrate (E-NO3), phosphate (E-P) and total phosphorus (E-TP) are measured on-line before pumping away the treated wastewater from the discharge channel. Laboratory analyses of daily averaged samples for nutrient (nitrogen and phosphorus compounds), suspended solids and organic compounds in the influent and effluent wastewater, are available twice per week.

3. SOFT-SENSOR DEVELOPMENT

According to the plant’s management, the on-line measurements of nitrate in the filter cells are often disturbed by the frequent backwashes and prone to potential unreliability. One principal problem is vicinity of the analysers to the effluent channel, the effect of backwash in one upstream filter (say Filter 7) propagates to all the following filters downstream (that is, Filter 6 to 1). Moreover, all the instruments are exposed to an aggressive environment. On the other hand, a reliable analysis of these primary variables is mandatory because of the economical and environmental implications due to incorrect dosing of methanol. For such a reason, the main goal of this study is to investigate the possibility to develop an array of soft-sensors (one for each filter) that estimate in real-time the nitrate concentration in the cells. A design based on simple and computationally light regression models is a priority for direct implementation in plant’s control system.

To design the sensors, a set of process measurements from the plant’s data acquisition system has been collected. The data correspond to two years of continuous operations (Jan 1, 2008 - Dec 31, 2009), recorded as hourly averages. The overall number of available process variable relevant to the task is 142: 7 for the influent, 5 for the effluent and 13 × 10 for the filters including nitrate, as summarized in Table 1. Here, the main stages of the design are discussed. Data from the first year have been used for the exploratory analysis (observation and variable selection, Section 3.1 and 3.2) and learning the calibration models (Section 3.3), data from the second year are then used as independent set for testing the models’ performance (Section 4).

3.1 Sample selection

Given the poor quality of the measurements of nitrate concentration in the filters, the first stage of the design consisted of performing a selection of those samples to be used to calibrate the regression models. The task has been approached starting from the consideration that, in normal operating conditions, the filters should operate in ideally identical ways. This implies that the nitrate measurements should be overlapping and any deviation from the prime operational modes is thus to be associated to instrumental deviations and these spurious measurements discarded.

Thus, deviations can be readily detected by analyzing the data matrix $Y = [y_1, y_2, \ldots, y_i, \ldots, y_{10}]$ where $y_i$ denotes a vector of nitrate concentrations $Fi$ for the $i$-th filter. For the sake of clarity, note that $Y$ contains only the $K$ samples that correspond to normal operations; that is, when the filter is not-backwashing and, for each filter, when none of the filters upstream is backwashing. Given the ideal collinearity between variables, such a matrix is expected to be characterized by a very high (ideally, one) and flat correlation matrix and by very low dimensionality (ideally, intrinsic dimensionality is one).

![Fig. 2.](image)

The correlation matrix depicted in Figure 2(a) clearly confirms this for Filter 4 to 8 and shows how this structure is still strong but slightly deteriorated for Filter 2, 3 and 9. On the other hand, Filter 1 and 10 show a behavior strongly different from the other cells, suggesting a potential malfunction of the corresponding instruments. As for the intrinsic dimensionality, a standard Principal Component Analysis PCA (Jolliffe, 2002) has been performed. By PCA, the $K \times I$ matrix $Y$ is factorised into a $K \times S$ score matrix T and a $I \times S$ loading matrix P by the eigenvalue decomposition of the covariance matrix of Y to obtain:

$$Y = TP' + E,$$

with $E$ the $K \times I$ residual matrix; if $S = I$, then $E = 0$ because all sources of variation have been considered. In our case, low residuals are already expected with low values of $S$, and this is particularly true for Filter 4 to 8. For such a reason, to select a number of principal components $S$ for a PCA model that appropriately reconstructs only the main modes of variation in the filters but discards instrumental deviations, the reconstruction error for each filter has been analyzed for a varying number of components.

The reconstruction error has been quantified in terms of Root Mean Squared Error (RMSE); for the $i$-th filter:

$$RMSE_i = \left( \frac{1}{K} \sum_{k=1}^{K} (y_i(k) - \hat{y}_i(k))^2 \right)^{1/2},$$

where $y_i(k)$ and $\hat{y}_i(k)$ denote the measurement at time $k$ and its reconstruction from the PCA model, respectively. In Figure 2(b), the reconstruction error is reported. It is possible to notice how with only two components the signal corresponding to Filter 6 is already very well recovered, thus confirming the intrinsically low-dimensional variability of the process. As for Filter 1 and 10, a higher number of components would be needed to reconstruct the residual variability in the signals (due to measurement anomaly).
For such reasons, a PCA model with $S = 2$ principal components is considered; the model explains 60% of the total variance. On such a model, samples can be selected based on the residuals of the PCA model. To analyse the residuals, two commonly used measures of fit (the squared prediction error $SPE$ and the Hotelling’s $T^2$ or $Q$-statistic) have been considered. $SPE$ measures the distance of an observation $y(k)$ from its reconstruction $\hat{y}(k)$ on the principal component subspace; that is,

$$SPE(k) = \sum_{i=1}^{D} \left( y_i(k) - \hat{y}_i(k) \right)^2 \quad \text{with} \quad D = 10,$$

where $i$ again denotes the original variable in $Y$, hence the filter. $T^2$ measures the (normalized) distance of the projected observation $t(k)$ in $\mathbb{R}^2$ from the origin of the principal component subspace, and it is defined as

$$T^2(k) = t(k)^T \Lambda^{-1} t(k),$$

here $\Lambda^{-1}$ denotes a diagonal matrix with the inverse of the eigenvalues associated with the retained components. An observation that associates with a change in the relationship between variables (i.e., outside the PCA model) will increase the $SPE$, whereas an observation inside the model but distant from its centre will manifest itself with an increase in the $T^2$. The two statistics can be combined into a single index (Raich and Cinar, 1996), the $J$-statistic

$$J(k) = \lambda T^2(k) + (1 - \lambda)SPE(k) \quad \text{with} \quad 0 \leq \lambda \leq 1,$$

which summarises how well an observation at time $k$ globally correlates with the rest of the PCA model. The parameter $\lambda$ controls the contribution from observations inside the principal component subspace (e.g., uncommon operating conditions) over the contribution from observations outside the principal component subspace (e.g., instrumentation drifts and erroneous measurements).

The type of anomalies we are interested in are deviations from the principal modes of variation of the array of filters, this suggests a low value of $\lambda$; in the experiments $\lambda$ was set to be equal to 0.1. In addition, a restrictive threshold $J_0$ on the $J$-statistic has been set to identify only those observations that truly belong to the low-dimensional PCA model; $J_0$ has been selected so that only 10% of the observations are retained (the 10-quantile). Such samples have been used to learn the regression models that estimate the nitrate concentration in the cells.

As an example, Figure 3 displays the results obtained with the sample selection technique presented above. From the diagram, it can be clearly noticed how the method is able to detect and locate the anomaly associated to a malfunction of the sensor of Filter 10 (grey area). The fault is correctly associated with the nearly-constant measurements reported by $F10-NO_3$. For comparison, notice how the measurements are in contrast with the correct analysis reported for Filter 6 by $F6-NO_3$. Before April 26, both measurements correctly represented the similar operation of the corresponding cells. The performance of the sensor was reinstated after the annual instrument maintenance.

3.2 Variable selection

Before proceeding in the design of the sensors, it has been necessary to identify, among all the candidate input variables ($5 + 7 + 12$ for each filter), a small but yet representative subset that truly contributes to a macroscopic characterization of each cell in terms of nitrogen removal.

For each filter, an independent subset of selected variables is to be used as inputs to the regression model that estimates the nitrate concentration, the output. However, given the ideal similarity in the design of the filters, the subset of input variables should be common to all the filters as for those input variables selected from the influent and effluent streams. Conversely, filter-related variables should be individually selected for each cell, according to specific operations. For the purpose, variable selection has been approached starting from the physical understanding of the nutrient removal process. The selection has been further confirmed from the analysis of the correlation coefficients between the key process variables and the individual $F_i-NO_3$. The choice of correlation as measure of dependence is justified by the need of light linear models that can be implemented in the control system without introducing additional computational burden.

In Figure 4 the correlation plots of some representative filters are presented as examples of different dependency behavior of key process variables compared to $F_i-NO_3$. In particular, it can be noticed how the outermost ones (Filter 1 in Figure 4(a), and Filter 10 in Figure 4(d)) show a quite low dependency and seem to differ from the other cells on the grounds of correlation. In fact, most of the inner cells as, for instance Filter 4 in Figure 4(b), and Filter 6 in Figure 4(c), exhibit similar correlation behavior where the dependency on filter variables like, $F_i-QW$ (sum of $F_i-QW-1/2$) and $F_i-QM$ (sum of $F_i-QM-1/2$), is quite high. With regard to the variables in the effluent flow stream, $E-NO_3$ show the strongest correlation, being the correlation coefficient ranging from 0.4 to 0.8. The temperature influence on the denitrification process is seen by the dependence shown with $E-T$, with a correlation ranging between 0.2 and 0.4. Although, the denitrifying bacteria in the filtration process use the biological available phosphorus for their growth, the correlation coefficients of phosphorus compounds are quite low with regard both to the influent ($I-OP$ and $I-TP$) and effluent ($E-OP$ and $E-TP$). This is probably due to the nonlinear dependency between phosphorus and nitrogen compounds. On the other hand, the effect of influent dissolved oxygen $I-O_2$ on
In this section, the estimation performances of the soft-sensors are presented. For the sake of brevity, two examples are discussed as representative of different conditions of the nitrate sensors in the post-denitrification filters. In the first example, it is shown how the soft-sensors can be used as back-up system to conventional analytical equipment and how, as shown in the second example, they can be used to replace out-of-order instruments.

4. RESULTS AND DISCUSSION

In the second example, the complete failure of the nitrate sensor in Filter 9 is experienced during the autumn season with increased influent flowrate, subsequent dilution in the influent nitrate concentration in the filter. This is confirmed by the comparison between the soft-sensor estimation and the plant data for a properly working sensor, as for instance in Filter 6 (Figure 5(c)). Here, the estimation model is fully capable to reconstruct the dynamics in the filter and accurately estimate the output. Considering the similar operational conditions between filters, as reported in terms of incoming flowrate for Filter 6 in Figure 5(a) and Filter 10 in Figure 5(b), it is expected that the behaviour of Filter 10 is correctly represented by the soft-sensor estimates, in Figure 5(d).

Table 2 summarizes the performances of the soft-sensors in prediction for samples that correspond to normal operations: i.e., when the filter is not-backwashing and, for each filter, when none of the filters upstream is backwashing. Results show accuracies of about 0.2 mg/l, which are comparable with the accuracy of the hardware-sensors.

Fig. 4. Example of the measure of dependency for F1-NO3 (a), F4-NO3 (b), F6-NO3 (c) and F10-NO3 (d). Denitrification is quite evident, but again the correlation coefficient range is 0.1-0.5. The same holds for I-NO3 (the calculated average of I-NO3-1/2).

On the attempt of defining parsimonious models, that with only few representative variables are accessible to process experts, for each filter only five inputs (I-NO3, F1-QW, F6-QM, E-NO3 and E-T) are selected for the soft-sensors.

3.3 Regression models

It is well known that many subprocesses within a wastewater treatment plant show a nonlinear behavior, and that nonlinear models might give an answer to their mathematical representation. However, from a wider point of view, which is the operator point of view as well, wastewater treatment processes display a linear behavior in the vicinity of normal operating conditions. Mainly, for this reason a standard Partial Least Square Regression (PLSR) method has been chosen for our prediction purposes.

PLSR (Wold, 1975) is a multivariate algorithm that finds a linear regression model between the variable to be predicted (the output, $y_i$) and the observable variables (the inputs, here $X_i \in \mathbb{R}^d$). The model is constructed through an iterative decomposition of $X_i$ and $y_i$ that aims at maximizing the variance in the input space and the covariance between the input and the output measurements. The PLSR regression model is parameterized by the number of latent variables to be retained for prediction; in our experiments, this parameter has been optimized with a standard resampling method for cross-validation, the Leave-One-Out, LOO (Hastie et al., 2009). It is also worthwhile noticing that, in order to account for the nonlinearities highlighted by the correlation analysis, those input variables associated with the influent (I-NO3) and those specifically related to the filter operation ($F_i\cdot QW, F_i\cdot QM$) have been transformed using a logarithmic function prior to the calibration of the PLSR models (Rosen et al., 2003).
Fig. 6. Nitrate estimations when the filter sensor is properly working (c) and absent (d) with decreasing influent nitrate (a) and temperature (b).

Table 2. Estimation results in prediction

<table>
<thead>
<tr>
<th>Filter</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
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<tbody>
<tr>
<td>RMSE</td>
<td>0.3</td>
<td>0.1</td>
<td>0.1</td>
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</tr>
<tr>
<td></td>
<td>6</td>
<td>7</td>
<td>8</td>
<td>9</td>
<td>10</td>
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<tr>
<td>RMSE</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
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</tr>
</tbody>
</table>

5. CONCLUSION

In this work we presented the results of a feasibility investigation for the development of an array of soft-sensors to estimate the nitrate concentration in a post-denitrification filter unit at the Viikinmäki WWTP.

Based on the experimental results, it appears that simple linear models are able to describe the behavior of the filters even in case of abrupt changes in the operating conditions. A careful selection and pre-processing of the available experimental data is however a key step in the design of the soft-sensors and permits good prediction accuracies and an improvement in the sample selection conditions. A careful selection and pre-processing of the filters even in case of abrupt changes in the operating conditions.

Summarizing, the application of the proposed methodology has demonstrated the potential benefits for the WWTP supervision and monitoring. It has been shown that the compliance with stricter regulations can be effectively enforced through the use of soft-sensors, which can be used as a back-up system to conventional analytical equipment for validating field measurements or replacing out-of-order components.

6. ACKNOWLEDGMENTS

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REFERENCES


