IEEE Access
Multidisciplinary ⁝ Rapid Review ⁝ Open Access Journal

Received July 31, 2019, accepted October 23, 2019, date of publication October 31, 2019, date of current version November 13, 2019.

Digital Object Identifier 10.1109/ACCESS.2019.2950852

LSTM-Based Wastewater Treatment Plants Operation Strategies for Effluent Quality Improvement

IVAN PISA[1,2], IGNACIO SANTÍN[2], ANTONI MORELL[1], JOSE LOPEZ VICARIO[1], AND RAMON VILANOVA[2], (Member, IEEE)

[1]Wireless Information Networking Group, Escola d'Enginyeria, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain
[2]Advanced Systems for Automation and Control Group, Escola d'Enginyeria, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Corresponding author: Ivan Pisa (ivan.pisa@uab.cat)

This work was supported in part by the Catalan Government under Project 2017 SGR 1202 and Project 2017 SGR 1670, in part by the La Secretaria d'Universitats i Recerca del Departament d'Empresa i Coneixement de la Generalitat de Catalunya i del Fons Social Europeu under FI Grant, in part by the Spanish Government under Project TEC2017- 84321-C4-4-R and Project DPI2016-77271-R, and in part by the European Regional Development Funds of the European Union.

ABSTRACT Wastewater Treatment Plants (WWTPs) are facilities devoted to managing and reducing the pollutant concentrations present in the urban residual waters. Some of them consist in nitrogen and phosphorus derived products which are harmful for the environment. Consequently, certain constraints are applied to pollutant concentrations in order to make sure that treated waters comply with the established regulations. In that sense, efforts have been applied to the development of control strategies that help in the pollutant reduction tasks. Furthermore, the appearance of Artificial Neural Networks (ANNs) has encouraged the adoption of predictive control strategies. In such a fashion, this work is mainly focused on the adoption and development of them to actuate over the pollutant concentrations only when predictions of effluents determine that violations will be produced. In that manner, the overall WWTP's operational costs can be reduced. Predictions are generated by means of an ANN-based Soft-Sensor which adopts Long-Short Term Memory cells to predict effluent pollutant levels. These are the ammonium ($S_{NH,e}$) and the total nitrogen ($S_{Ntot,e}$) which are predicted considering influent parameters such as the ammonium concentration at the entrance of the WWTP reactor tanks ($S_{NH,po}$), the reactors' input flow rate (Q_{po}), the WWTP recirculation rate (Q_a) and the environmental temperature (T_{as}). Moreover, this work presents a new multi-objective control scenario which consists in a unique control structure performing the reduction of $S_{NH,e}$ and $S_{Ntot,e}$ concentrations simultaneously. Performance of this new control approach is contrasted with other strategies to determine the improvement provided by the ANN-based Soft-Sensor as well as by the fact of being controlling two pollutants at the same time. Results show that some brief and small violations are still produced. Nevertheless, an improvement in the WWTPs performance w.r.t. the most common control strategies around 96.58% and 98.31% is achieved for $S_{NH,e}$ and $S_{Ntot,e}$, respectively.

INDEX TERMS Artificial neural networks, BSM2 framework, industrial control, violation reduction, water pollution.

I. INTRODUCTION

The pollutant reduction process of urban residual waters is performed at Wastewater Treatment Plants (WWTPs) which are facilities devoted to treating the incoming waters and return them to its natural cycle. Their main aim is to reduce the concentration levels of phosphorus, nitrogen derived components, biochemical oxygen demand and total suspended solids to assure that they are harmless to the environment and aquatic life where treated waters are spilled. For that reason, some regulations, like the European Directive 91/271 [1], are applied to these facilities to

The associate editor coordinating the review of this manuscript and approving it for publication was Gilberto Pastorello.

assure that pollutant parameters are maintained below certain limits.

These pollutant reduction processes are carried out by means of highly complex and non-linear biological and biochemical processes which are described by the Activated Sludge Models (ASMs): the Activated Sludge Models No.1 (ASM1), No.2 (ASM2), No.2d (ASM2d) and No.3 (ASM3), all of them developed by the International Water Association (IWA). ASM1 consists in a mathematical model showing the reduction of nitrogen derived pollutants [2]. Besides, it has been extended with the development of Activated Sludge Models No.2 and 2d (ASM2 & ASM2d), where the former models the phosphorus pollutant reduction and the latter improves the denitrification process. ASM1 has also been extended with Activated Sludge Model No.3 (ASM3), a new tool of the next generation of Activated Sludge Models [3].

In this context, control strategies have been designed and deployed at WWTPs to try to maintain the pollutant levels under the limits established by the regulations. However, there are a lot of WWTPs architectures depending on their purpose. For that reason, the well-known Benchmark Simulation Model No.1 and No.2 (BSM1 and BSM2) have arisen as frameworks where the evaluation of the control strategies performance is done. Those simulation models have been designed and implemented to offer a standardised WWTP architecture which allows for generalisation, easy comparison and replication of results. Therefore, they define their own simulation protocols and regulations [4].

From the control point of view, BSM1 and BSM2 implement a default control strategy based on Proportional Integral (PI) controllers [5] which maintain the dissolved oxygen concentration (S_O) of certain reactor tanks at the set-point of $2\,mg/L$ by means of modifying the oxygen transfer coefficient (K_La) [6]. More complex control strategies such as the Model Predictive Control (MPC) and Fuzzy Logic have also been adopted in the literature. For instance, the adoption of an MPC controller is proposed in [7], where the authors propose the deployment of MPCs with and without Feed Forward over BSM1 framework in order to assure that pollutant concentrations are upheld the regulation limits. Another control approach consists in the development of hierarchical control strategies like the one proposed by Nopens *et al.* [8]. They implement a hierarchical closed-loop (CL) control based on PI controllers that will modify the S_O parameter of the BSM2 tanks in order to maintain the ammonium concentration of the fifth tank ($S_{NH,5}$) at a given set-point of $1.5\,mg/L$.

Artificial Neural Networks (ANNs) have been applied in certain works as predictive tools able to learn and generate mathematical models of highly non-linear relations such as in the ASMs [9]. Moreover, ANNs have also been considered for control purposes, where they are in charge of forecasting or predicting some parameters to feed a control strategy. In that sense, *Foscoliano et.al* propose the adoption of recurrent neural networks (RNNs) to predict the WWTP's nutrient concentrations and then, feed an MPC strategy to assure that concentrations are under the established limits [10]. Another approach consists in the adoption of Adaptive Fuzzy Neural Networks (ANNs + Fuzzy Logic). For instance in [11] and [12], this approach has been adopted to track the optimal set-points of the dissolved oxygen ($S_{O,5}$) ($2\,mg/L$) at the fifth tank and nitrate nitrogen ($S_{NO,2}$) ($1\,mg/L$) at the second one. Furthermore, in [13] two Multilayer Perceptron (MLP) neural networks are adopted to predict both, the ammonium ($S_{NH,e}$) and total nitrogen concentrations ($S_{Ntot,e}$) in the effluent, and determine whenever a violation of their limits is likely to occur. When a violation of the pollutant limits is detected, a hierarchical control strategy based on the implementation of MPC and Fuzzy Logic controllers is activated automatically. However, the prediction performed by the MLP corresponds to the effluent's maximum value observed in a day, i.e., the time dependence among influent and effluent is not considered. Furthermore, ANNs have been also adopted as the main tool to fix certain set-points of the WWTP control strategies. For instance, in [14], three different neural networks with feedback input are considered in the optimal set-point design of an MPC controller. Among the different parameters under control, these networks are focused on tracking the S_O and $S_{NH,5}$ set-points adopted by the controllers.

In such a context, this work is based on the development and deployment of an improved predictive control approach able to control more than one pollutant concentration at the same time. It consists mainly of two parts: the predictive and the control. The predictive part consists of an ANN-based Soft-Sensor which is in charge of predicting the pollutant concentrations. These are obtained by means of Long Short Term Memory (LSTM) cells which are ANNs able to model highly non-linear and complex systems [15] like WWTPs. Besides, these networks have been considered to perform predictions due to their ability in modelling sequences since they take into account the high time correlation between WWTP's data [16] [17, Chapter 10]. In terms of the control part, predictions will determine when and which control actuations have to be applied. These actuations are focused on reducing the pollutant concentrations and consequently their violations. For instance, violations of $S_{NH,e}$ and $S_{Ntot,e}$, since the former is toxic for the aquatic life and the latter is a limiting nutrient that causes eutrophication [18], [19]. Phosphorus is not considered in this work since it is based on BSM2 which only implements ASM1 models.

Results of the proposed control approach will be compared with BSM2 default control strategies and also with the ones adopted in [13]. An improvement of the performance is expected since predictive control strategies are able to actuate in advance for the case of BSM2 default control strategy. In terms of the hierarchical control presented in [13], an improvement is also expected as a consequence of taking into account LSTM cells. Moreover, this work proposes to control both pollutant variables at the same time by means of a new control approach where two predictive control strategies based on MPC and Mamdani Fuzzy Logic controllers are considered. Therefore, the reduction of $S_{NH,e}$ and $S_{Ntot,e}$

TABLE 1. State-of-art review.

Control Strategies	Objectives	Reference
PI	Default PI to maintain $S_{O,4}$ at a set-point of $2\,mg/L$	Jeppsson [6]
	Hierarchical PI to maintain the $S_{O,4}$ and $S_{NH,e}$ at the set-points of $2\,mg/L$ and $1\,mg/L$, respectively. Improves [6]	Nopens [8]
MPC	MPC controller with feed-forward action and non-linear MPC with penalty function to maintain the effluent concentrations below their quality limits	Shen [7]
ANN + Fuzzy Logic	ANN + Fuzzy Logic adopted to trace the $S_{O,5}$ and $S_{NO,2}$ previously computed set-points of $2\,mg/L$ and $1\,mg/L$, respectively.	Qiao [11], Han [12]
ANN + MPC	ANN + MPC to design the MPC optimal set-points to be tracked. They correspond to the S_O and $S_{NH,5}$ set-points	Sadeghassadi [14]
ANN + MPC + Fuzzy Logic	ANN + MPC + Fuzzy Logic to reduce the $S_{NH,e}$ and $S_{Ntot,e}$ levels when violations are predicted. Predictions are performed considering the maximum concentration levels observed in a day. These values will determine which control strategy, either the MPC, or the Fuzzy Logic, has to be applied. Each concentration is controlled separately, i.e., the actuation over a concentration can increase the other	Santín [13]
LSTM + MPC + Fuzzy Logic	The control strategy adopted in this work. It is based on the adoption of LSTMs to determine which control strategy has to be applied to avoid violations of $S_{NH,e}$ and $S_{Ntot,e}$. Here, predictions are performed considering WWTP influent data without losing their time-correlation (time dependance). Besides, the concentrations of interest are controlled simultaneously, so the actuation over a concentration does not penalize the other one.	This work

concentrations is performed simultaneously. In that sense, Tab. 1 summarises the different control strategies applied in the WWTP facilities as well as the main contribution of this work w.r.t. the reviewed ones.

It is important to notice that in this work, the ANN-based soft-sensor providing predictions will not only be used to predict the full plant output concentration, but also to determine when they will generate a violation over the prescribed limits. In that sense, the application of this soft-sensor will help in the reduction of the WWTP operational costs since they will only be increased when a violation is detected. Thus, no extra action is needed when the effluents are below the limits. This ANN-based Soft-Sensor has been previously designed in [20]. In there, the soft-sensor was able to predict the effluent concentrations but, the pollutant peaks were not correctly predicted since the imbalance data problem in the training process was not addressed. This was solved in [21], where the soft-sensor was improved and calibrated by means of data preprocessing techniques which circumvent the problem of imbalanced data. However, in both cases it was neither deployed in BSM2 framework nor tested with control strategies. Consequently, this paper is an extension of [20] and [21]. Here the performance of the ANN-based soft-sensor is evaluated by considering the interaction with control strategies in a BSM2 environment. As shown, the ANN needs to be retrained considering the actuations of control strategies since they are counterproductive.

It is also important to put into place the work contribution from the WWTP operation point of view. One of the appealing aspects of the proposal, in addition to the performance improvement that it may provide with respect to existing approaches, is that it can be understood as an additional decision layer that can improve existing operation. Therefore, it does not ask for changes in instrumentation nor in already existing control equipment (either software and/or hardware). This soft-sensor based layer takes measurements already existing because of usual control-loops and builds up operation decisions on the basis of the (not)predicted effluent limit violation. Therefore, the potential improvement will come not just because reducing the number of effluent limit violations but also from the ease of deployment. For instance, the adoption of such a soft-sensor allows us to dissociate the predictions of pollutant concentrations from the WWTP architecture since it only requires input and output data of the processes to model.

The outline of this paper is as follows. Next section is devoted to presenting the BSM2 framework which this work is based on. Next, the adopted ANN-based soft-sensor predicting the effluent concentrations is described. Later, results are presented in terms of the percentage of violations and also in terms of the effluent and costs index. Finally, Section V concludes the paper.

II. BENCHMARK SIMULATION MODEL NO.2

The purpose of this work is to analyse the improvement of a WWTP when an Artificial Neural Network-based Soft-Sensor (ANN-based Soft-Sensor) is applied as a predictive mechanism feeding predictive control strategies. For that reason, it will be implemented and deployed in a well-known WWTP benchmark scenario, the BSM2, which describes and models a standard biological WWTP [22], [23].

As a WWTP simulator, BSM2 implements a simulation protocol which takes into account a whole year of influent data. These data represent different types of weather: dry, rainy and stormy. Besides, influent data not only gives information about the weather, but also about the nutrients present in it. However, BSM2 has to be calibrated before being able to simulate the real behaviour of a WWTP facility. This calibration is in charge of leading BSM2 to a steady-state by means of simulating a 200-days constant influent with no noise measurements. Once calibrated, it is able to simulate the WWTP behaviour. To do so, 609 days of influent showing rainy episodes as well as variations in the environmental temperatures is adopted. From these 609 days simulation, only

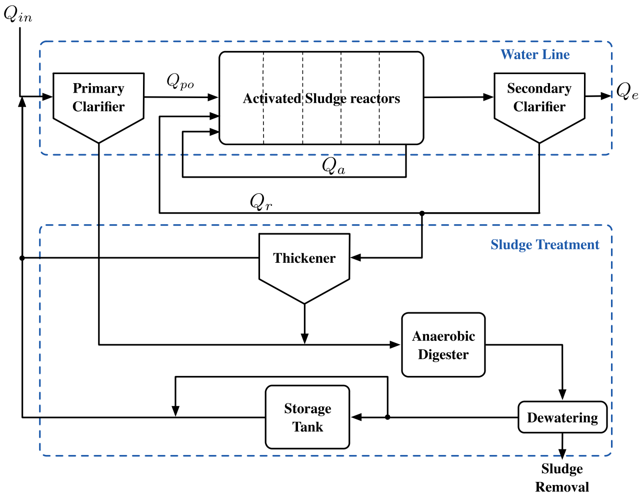


FIGURE 1. BSM2 layout modelling the architecture of a wastewater treatment plant.

TABLE 2. BSM2 flow rates.

Flow	Description
Q_{in} (m^3/day)	Influent flow rate
Q_{po} (m^3/day)	Primary clarifier's overflow rate
Q_a (m^3/day)	Internal Recirculation flow rate
Q_r (m^3/day)	Sludge's internal recycle flow rate
Q_e (m^3/day)	WWTP's effluent flow rate

TABLE 3. BSM2 effluent quality limits.

Variable	Value
$S_{Ntot,e}$	$< 18\,mg/L$
COD	$< 100\,mg/L$
$S_{NH,e}$	$< 4\,mg/L$
TSS	$< 30\,mg/L$
BOD_5	$< 10\,mg/L$

results of 365 days (from day 245 to day 609) are considered for WWTP performance computation [6], [23].

A. BSM2 LAYOUT

BSM2 defines the WWTP's water line, where the pollutant reduction tasks are performed, and the sludge treatment where the WWTP's sludge is managed. The water line consists of a set of five reactor tanks (Activated Sludge reactors), the first two are anoxic (they present a lack of dissolved oxygen) whilst the remaining three are aerobic (they are working under aerated conditions). The processes performed in the water line are defined by ASM1 model [2], therefore, we will focus on those related with the nitrogen and its derived reduction processes. They correspond to nitrification and denitrification, where the former oxides the ammonium ions into nitrate, and the latter transforms the nitrate into nitrogen and gaseous products [24]. The sludge treatment part consists of the different modules devoted to treating the sludge adopted in the pollutant reduction process. These modules correspond to: the primary and secondary clarifiers, which are in charge of the sedimentation process defined by the Tákacks model [25]; the Anaerobic Digester, where sediments obtained from the clarifiers will be treated to process the organic material and transform it in sludges; the Dewatering module, which will remove the excess of sludges; and the Storage Tank, which will store an amount of sludge to be reused in the water line [23].

The layout considered in the BSM2 scenario can be observed in Fig. 1 where the water line and the sludge treatment modules are differentiated. Besides, BSM2 has been designed to manage an average flow rate of 20648.36 m^3/day. The anoxic tanks support a maximum volume of 1500 m^3 whereas the aerated ones support 3000 m^3. This yields to an average retention time of 14 hours [6], [23]. In other words, the incoming water will remain 14 hours in the WWTP plant. Tab. 2 shows the different flow rates considered in the BSM2 layout, where Q_a corresponds to the quantity of aerated flow going from the last reactor tank to the first anoxic one and Q_r corresponds to the sludge's internal recycle flow which moves some sludges from the second clarifier to the first reactor tank. Furthermore, the rest of BSM2 model parameters as well as the processes involved in the pollutant reduction process are defined in [23].

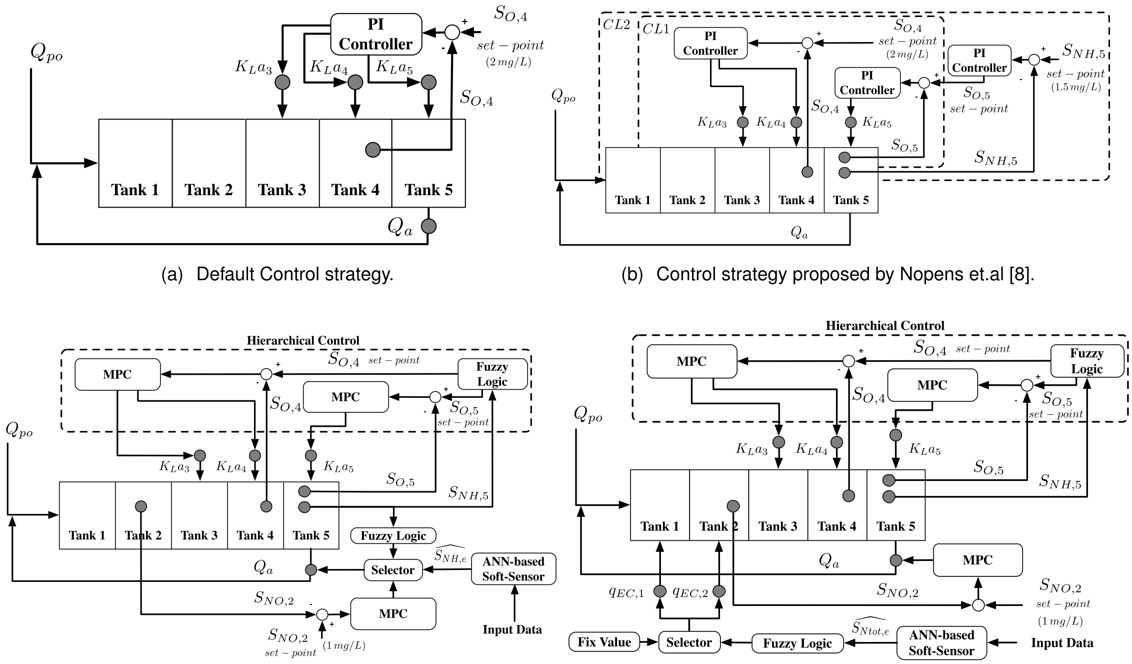
B. BSM2 REGULATIONS

BSM2 does not only implement its own simulation protocol and WWTP model, but also its own regulations. This is motivated by the fact that it has been designed as a general framework scenario whose aim is to offer generality, easy comparison and replication of results among different control strategies [4].

In that sense, BSM2 limits correspond to the ones shown in Tab. 3, where the pollutant limits for the Chemical Oxygen Demand (COD), the Biochemical Oxygen Demand (BOD_5), the Total Suspended Solids (TSS) and the ammonium $S_{NH,e}$ and total nitrogen concentrations $S_{Ntot,e}$ are defined. Although those are very similar to the ones adopted in the European Directive 91/271 [1] for WWTPs, BSM2 limits are more restrictive due to the fact that a violation is performed whenever the limits are exceeded. In this case, the two most important limits to take into account are those derived from the nitrogen ($S_{NH,e}$ and $S_{Ntot,e}$) because they are the most difficult to tackle. Besides, violations of COD, BOD_5 and TSS are well treated and managed by usual control and operational strategies [6], [8], [13]. On the other hand, phosphorus pollutant derived components cannot be addressed by BSM2 framework since it is based on ASM1 models. Therefore, BSM2 regulations do not consider any kind of violations related to phosphorus components. If these pollutants have to be considered, BSM2 has to be redefined to follow Activated Sludge Models 2 and 2d [3].

C. CONTROL STRATEGIES

Since BSM2 implements its own protocol and regulations, it is usually adopted as a benchmark where control strategies are compared and tested in terms of the reduction of pollutant



(a) Default Control strategy.

(b) Control strategy proposed by Nopens et.al [8].

(c) Control Strategy adopted to reduce the $S_{NH,e}$ violations.

(d) Control Strategy adopted to reduce the $S_{Ntot,e}$ violations.

FIGURE 2. **Control Strategies. Notice that Default control strategy and the one proposed by Nopens *et al.* [8] consider the application of conventional PI controllers. Their main difference consists in the fact that Nopens et.al propose a hierarchical control structure instead of a unique PI. Finally, the control strategies adopting the ANN-based Soft-Sensor are differentiated in the manner they use the soft-sensor itself. The strategy reducing the $S_{NH,e}$ violations applies the soft-sensor to decide if the Mamdani Fuzzy or the MPC will be applied in the manipulation of Q_a. The strategy reducing $S_{Ntot,e}$ considers the soft-sensor to determine the amount of carbon that will be added to the first and second WWTP's reactor tanks.**

violations and WWTP's operational costs. In our case, four different control strategies will be considered, two of them adopt predictive control strategies based on the hierarchical control of [13] whereas the two remaining consist in the BSM2 default control strategies [6], [8], which are based on the application of Proportional Integral controllers (PI) [5].

The first considered control strategy corresponds to the BSM2 default control (DS) defined in [6]. It is in charge of managing the S_O present at the fourth tank by means of manipulating the oxygen transfer coefficient (K_La) of the three aerated tanks (see Fig. 2). In addition, the control strategies presented by Nopens *et al.* [8] have also been considered. They are based on the application of PI controllers in the S_O control loop to maintain the dissolved oxygen of the fourth and fifth tanks at the given set-points of $2\,mg/L$. In this case, the first approach (closed loop control (CL)) corresponds to a modification of the default control strategy shown in [6].

The two predictive control approaches are based on the implementation of a hierarchical control and a predictive control structure based on the predictions performed by an Artificial Neural Network-based Soft-Sensor (ANN-based Soft-Sensor). It will predict the effluent concentrations, $S_{NH,e}$ and $S_{Ntot,e}$, and feed a selector which will determine the control strategy to apply. Both approaches have a common part which corresponds to the hierarchical control presented in [13]. Its main aim is to maintain the dissolved oxygen of tanks 4 and 5 ($S_{O,4}$ and $S_{O,5}$) at the given set-point of $2\,mg/L$ and $1\,mg/L$, respectively. The predictive control structure in charge of reducing ammonium violations implements an MPC and a Mamdani Fuzzy Logic to maintain the $S_{NO,2}$ concentration at $1\ mg/L$. To achieve this, Q_a is manipulated taking into account the predictions performed by the ANN-based Soft-Sensor. It will determine if the MPC or the Mamdani Fuzzy is applied (see Fig. 2c). On the other hand, the control structure reducing $S_{Ntot,e}$ violations considers the ANN-based Soft-Sensor's predictions to decide when extra carbon has to be added to tanks 1 and 2 or if a fixed value will be added instead [13]. Moreover, an additional MPC + Mamdani Fuzzy Logic is considered to track and maintain the $S_{NO,2}$ at the given set-point ($1\ mg/L$) manipulating the Q_a (see Fig. 2d).

D. PERFORMANCE METRICS

BSM2 performance is computed adopting three different metrics devoted to evaluating the effects of the control strategies on BSM2. They can be divided into two main groups: (i) economical metrics and (ii) behaviour metrics.

Economical metrics are those which inform about the cost that the implemented control strategy will spend on the pollutant reduction process. In the case of this work, the metric showing this corresponds to the Overall Cost Index (OCI). It computes the overall costs of the WWTP plant as the sum of the different consumed energies:

$$OCI = AE + PE + 3 \cdot SP + 3 \cdot EC + ME - 6 \cdot MP + HE_{net} \tag{1}$$

where AE corresponds to the aeration energy, PE to the pumping energy, ME to the mixing energy and HE_{net} to the heating energy of anoxic tanks' sludge. SP is defined as the sludge production for disposal, EC corresponds to the amount of consumed external carbon and finally, MP is defined as the energy provided by the methane produced in the anaerobic digesters. This energy is subtracted from the OCI since it corresponds to a benefit from the economical point of view. Further details on how to compute the different parameters involved in the OCI computation are shown in [6], [13].

It has to be stressed that OCI is an aggregated measure that has no monetary units. The specific costs will be dependent on the WWTP location as energy regulations, for example, vary from one country to another. Also, in the specific case of using an external source for carbon addition to help denitrification, costs may be affected. Many external carbon sources are derived from fossil fuel based raw materials [26]. Significant price fluctuations in the methanol, ethanol, and acetic acid markets can have a huge impact on the prices of these carbon sources.

On the other hand, the metrics devoted to computing the plant performance in terms of its behaviour are: (i) the percentage of time that effluents are violated w.r.t. the WWTP operational time, and (ii) the Effluent Quality Index (EQI). The first metric corresponds to the amount of time that $S_{NH,e}$ and $S_{Ntot,e}$ pollutant levels are above the BSM2 limits, 4 mg/L and 18 mg/L, respectively. Besides, this metric has been complemented providing information about the number of violations that have been produced during the simulation time. Their maximum level, their average (μ) and standard deviation (σ) are also considered. Finally, EQI corresponds to an aggregated metric measuring the quality of the effluent [23]. It is computed as the average of the effluent pollutant levels over the observation period:

$$EQI = \frac{1}{1000 \cdot T} \int_{t=245days}^{t=609days} (2 \cdot TSS(t) + COD(t) + 30 \cdot S_{NKj}(t) + 10 \cdot S_{NO}(t) + 2 \cdot BOD_5(t)) \cdot Q(t) \cdot dt \tag{2}$$

where TSS is the Total Suspended Solids, COD is the Chemical Oxygen Demand, S_{NKj} corresponds to the Total Kjeldahl Nitrogen, S_{NO} is the nitrate nitrogen concentration, BOD_5 is the Biochemical Oxygen Demand and $Q(t)$ is the flow rate over time [13], [23].

III. VIOLATION REMOVAL PROCESS BASED ON ARTIFICIAL NEURAL NETWORKS

The adoption of an ANN-based Soft-Sensor seeks the improvement of the WWTP's performance by means of enhancing the predictions adopted by the control scenarios. Thus, the reduction of the number of violations as well as the improvement of WWTP's EQI and OCI metrics are sought. Since the concentrations of interest can be treated as time-series showing a high correlation over time, the application of LSTMs for prediction purposes is highly advisable [17].

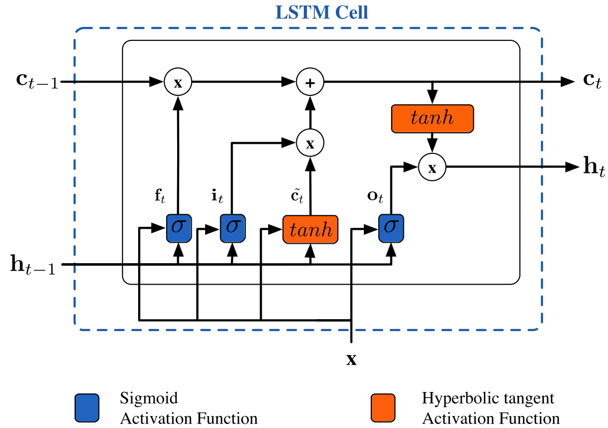


FIGURE 3. LSTM Cell. Input gate (i_t) modifies the LSTM cell state, update gate ($\tilde{c}_t$) determines the new cell state candidates, forget gate (f_t) resets the cell's memory and output gate (o_t) determines the output candidates. x, h and c are the inputs, outputs and state of the LSTM cell, respectively. Further details in [17, Section 10.10].

A. LONG-SHORT TERM MEMORY CELLS

LSTM cells are a type of Gated Neural Networks [17, Section 10.10] which have arisen as a solution that alleviates the RNNs [17, Chapter 10] well-known problem of Vanishing and Exploding gradients [27]. Besides, LSTMs have been considered as the main predictive approach because of their capacity in modelling time-series and time-dependant parameters such as the WWTP's influent and effluent values. This is motivated by the fact that they implement memory cells able to not only take into account the current input, but also the previously observed dynamic [17, Section 10.10]. Fig. 3 shows the main architecture of a LSTM cell. For the sake of brevity, we do not provide specific details (the interested reader is referred to [17, Section 10.10]).

In this work we consider Back Propagation Through Time algorithm, which updates the weights and biases of the LSTM gates toward the reverse of the cost function's gradient [17, Chapter 6]. Moreover, L2 penalty regularisation technique is adopted since ANNs are suitable to present overfitting [17, Chapter 7]. Overfitting is committed whenever the learned model does not fit new input data, achieving good performance only with training data. One common approach to reduce overfitting is to limit the capacity of "specialization" of the network by means of regularization techniques [17, Chapter 7]. For instance, L2 adds extra penalties to the ANN's weights in order to reduce the learning capacity of the network.

B. ANN-BASED SOFT-SENSOR

Concerning the ANN-based Soft-Sensor architecture, it implements two main blocks (see Fig. 4): the Data

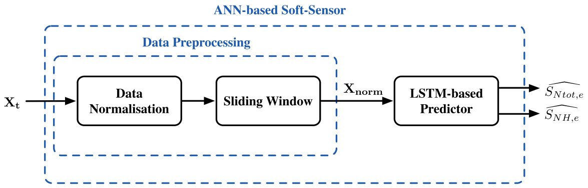


FIGURE 4. ANN-based Soft-Sensor block diagram.

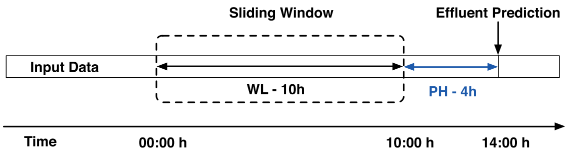


FIGURE 5. Implemented sliding window in the ANN-based soft-sensor.

Preprocessing block devoted to preprocessing the input data, and the LSTM-based Predictor block which implements a LSTM neural network to predict effluent concentrations.

The preprocessing carried out consists of the normalisation of data towards zero-mean and unity variance in order to address the heterogeneity of measurements [28]. This module also considers the implementation of a sliding window to organise the time-dependent measurements, which are sampled every 15 minutes. In such a context, the sliding window has been designed to gather 10h of input data (window length - WL) and perform predictions of the effluent concentrations that will flow out the plant in 4h (prediction horizon - PH) (see Fig. 5). These times have been selected according to their relationship with the prediction performance. The more input data, the better prediction performance. However, the control strategies have an actuation time that has to be also considered. In that sense, 4 hours of prediction horizon is enough for control strategies to completely reduce a pollutant peak. Besides, 10h of input data allows the ANN-based Soft-Sensor to get enough information of the influent that has entered in the WWTP. For instance, to determine if a rainy or stormy episode is being produced. Furthermore, the WL and PH can be changed, but they are chosen taking into account the WWTP's retention time (approximately 14h), i.e., the sum of PH with WL equals to this time.

The ANN-based Soft-Sensor's LSTM-based Predictor is built with two LSTM cells which are stacked, i.e., the output of the first LSTM cell acts as the input to the second one. Besides, each cell gate is formed by an ANN with 50 hidden neurons. The whole structure has been trained in order to find the 31851 model parameters (weights and biases) which offer the best prediction performance. The model hyperparameters have been computed by means of a grid search where the number of cells and neurons per cell are also determined. Then, the performance of the model has been computed by means of a K-Fold strategy as we describe next. First, 15% of the dataset is saved for testing. With the remaining 85%, we split the data into K (K = 5 in our case) sequences (thus keeping temporal order). Then K training processes

TABLE 4. ANN-based soft-sensor's input and output data.

Influent Concentrations & Rates	
$S_{NH,po}$ (mg/L)	Ammonium in the primary clarifier's output
Q_{po} (m^3/d)	Primary clarifier's overflow rate
Plant Variables & Rates	
T_{as} $(°C)$	Environmental Temperature
Q_a (m^3/d)	Internal Recirculation flow rate
Output Data	
$S_{Ntot,e}$ (mg/L)	Total Nitrogen concentration in the effluent
$S_{NH,e}$ (mg/L)	Ammonium concentration in the effluent

are executed. At each execution, K-1 subsets are considered for training (with about 70% of the data) and one subset for validation (with about 15% of the data). Validation data is used to better adjust the learning rate and L2 penalties previously obtained (in our case both equal to $1 \cdot 10^{-3}$). Finally, the test dataset is used to compute the performance of the ANN-based Soft-Sensor.

In a real environment, data considered in the training process will consist of online measurements which are values that can be obtained at the same WWTP plant without the necessity of laboratory analyses. In other words, the ANN-based Soft-Sensor will take measurements of nutrient's concentrations that can be directly obtained from available sensors with a sampling time of 15 minutes. Then, predictions will be performed adopting these data as inputs. Besides, it is worth mentioning that the ANN-based Soft-Sensor can find missing data in a real WWTP due to sensor malfunction. In that case, an additional imputation layer should be considered. However, this work is based on a simulated environment, BSM2, and thus the management of missing data is out of the scope of the paper. Therefore, measurements here refer to BSM2 generated data, which are adopted by the soft-sensor as its inputs, whereas predictions refer to the output of such soft-sensor. In this case, generated data consist in 609 days of influent and effluent measurements sampled every 15 minutes. Thus, the total amount of data consist in 58464 samples which are obtained when BSM2's default influent dynamics showing episodes of dry, rainy and stormy weathers are simulated. As a consequence, the considered hydrochemical parameters have been analysed by processes already implemented in the BSM2 environment. In this case, effluent measurements correspond to ammonium, $S_{NH,e}$, and total nitrogen, $S_{Ntot,e}$. Tab. 4 shows the ANN-based Soft-Sensor's input and output data.

Q_{po} and $S_{NH,po}$ are considered due to their effects in the final pollutant concentrations ($S_{NH,e}$ and $S_{Ntot,e}$): (i) $S_{NH,po}$ has an important effect in the nitrification process yielding to an increment of the ammonium's concentration in the effluent and (ii) Q_{po} determines the amount of water entering in the first reactor tank. T_{as} is considered due to its influence in the nitrification and denitrification processes, and hence the final value of $S_{Ntot,e}$ [2]. Finally, Q_a is considered in the $S_{Ntot,e}$ violation removal strategy since it increases the amount of sludge and dissolved oxygen in the anoxic tanks. However, it is not taken into account in the $S_{NH,e}$ control strategy because this strategy modifies Q_a to reduce the amount of ammonium. Further details on the soft-sensor's implementation and its training and calibration processes can be found in [21]. There, the ANN-based Soft-Sensor has been trained considering data coming from three different levels of control. The objective there was to test its feasibility and performance when predicting WWTP effluent products. Results showed that the soft-sensor is able to generate highly accurate predictions of ammonium and total nitrogen four hours in advance indistinctly of the control. Besides, the lowest Root Mean Squared Error (RMSE) equals to 0.12 mg/L and 0.40 mg/L for $S_{NH,e}$ and $S_{Ntot,e}$ predictions, respectively, when the sensor is trained with the high-level control strategy data.

C. CONTROL SCENARIOS

As it has been previously stated, the ANN-based Soft-Sensor is able to perform predictions taking into account the time-correlation. Consequently, the improvement achieved due to these predictions will be computed and tested by means of four different predictive control scenarios:

- Default Scenario (DS): Non-predictive control scenario which corresponds to the default control strategy adopted in [6] (Fig. 2). It does not consider the ANN-based Soft-Sensor. Here, a PI controller is in charge of controlling the oxygen transfer coefficient of each aerated tank. The amount of carbon added to the first tank ($q_{EC,1}$) is maintained fix at a constant flow rate of 2 m^3/day.
- Hierarchical Scenario (HS): Non-predictive control scenario which corresponds to the control strategies adopted in [8] (Fig. 2b). It does not consider the ANN-based Soft-Sensor. The amount of carbon added to the first tank ($q_{EC,1}$) is maintained fix at a constant flow rate of 1 m^3/day.
- ANN-based Soft-Sensor $S_{NH,e}$ reduction scenario (ASS-NHRS): Predictive control scenario (Fig. 2c) which is focused on reducing the ammonium violations varying the Q_a. It adopts the MPC control strategy defined in [13] and the ANN-based Soft-Sensor. In this case, carbon is only added when the control strategy actuates over the pollutant under control, therefore, costs derived from the addition of external carbon are directly related with the performance of the control strategy. ANN-based Soft-Sensor's input variables are $S_{NH,p}$, Q_{po} and T_{as}. The product between $S_{NH,p}$ and Q_{po} is considered due to its appearance in the mass-balance equations shown in [2]. The soft-sensor has been calibrated to detect violations whenever $\gamma_{S_{NH,e}}$ exceeds 4 mg/L.
- ANN-based Soft-Sensor $S_{Ntot,e}$ reduction scenario (ASS-NTRS): Predictive control scenario (Fig. 2d) which is focused on reducing the total nitrogen violations. It adopts the correspondent control strategy defined in [13] as well as the soft-sensor. In this case, external carbon is only added to tanks 1, 2 and 5 when the control strategy actuates over the pollutant under control. Consequently, costs derived from the addition of external carbon are directly related with the performance of the control strategy. The more violations detected, the more external carbon required, and so, it is important to minimise false detection. Considered ANN-based Soft-Sensor's has an equivalent structure to the one considered in ASS-NHRS, however, it adopts a new input, the recirculation flow rate (Q_a). The soft-sensor has been calibrated to detect violations whenever $\gamma_{S_{Ntot,e}}$ exceeds 17 mg/L. Thus, more violations will be detected at the expense of allowing false positives.

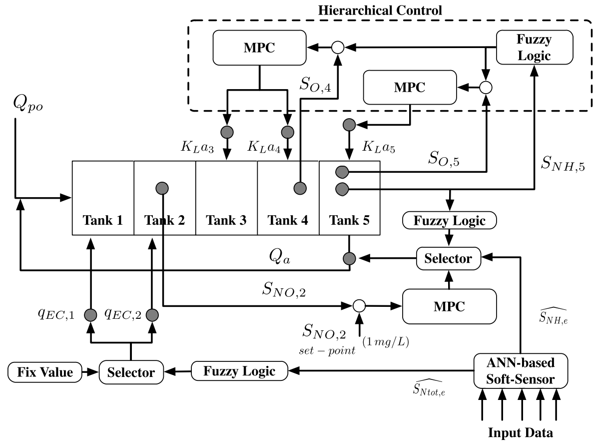


FIGURE 6. ASS-PRS control scenario. Notice that predictive element corresponds to the ANN-based Soft-Sensor which is predicting $S_{NH,e}$ and $S_{Ntot,e}$ at the same time.

Notwithstanding, the predictive control scenarios, ASS-NHRS and ASS-NTRS, are devoted to controlling and actuating over a unique pollutant parameter, either $S_{NH,e}$ or $S_{Ntot,e}$. Thus, effluent quality and overall costs are improved w.r.t. default control strategies since the concentrations of the pollutant under control are reduced. Despite this, violations of the non-controlled pollutants are sometimes increased degrading the EQI and OCI parameters. For instance, $S_{Ntot,e}$ concentration is increased when the $S_{NH,e}$ control actuation is applied. Since $S_{NH,e}$ is reduced varying the Q_a, the amounts of sludges and dissolved oxygen are increased in the anoxic tank, raising the concentrations of nitrates and total nitrogen [13]. This example shows that some actuations controlling a unique pollutant concentration are counterproductive for the others. For that reason, a WWTP has to be observed as a whole system where control actuations have to be applied simultaneously, i.e., $S_{NH,e}$ and $S_{Ntot,e}$ control actuations have to be applied together. Following this point, we have proposed the ANN-based Soft-Sensor pollutant reduction scenario (ASS-PRS), which unifies the ASS-NHRS and ASS-NTRS control strategies. Here, the two control strategies, one per pollutant, will be actuating at the same time with the objective of reducing effluent peaks for $S_{NH,e}$ and $S_{Ntot,e}$. Predictions performed with the ANN-based Soft-Sensor will determine when the control strategies based on MPC and Mamdani Fuzzy Logic have to be applied (see Fig. 6). In that manner, when the actuation over a pollutant increases the concentrations of the other, the control strategy will automatically reduce its concentration in order to avoid the limit violation.

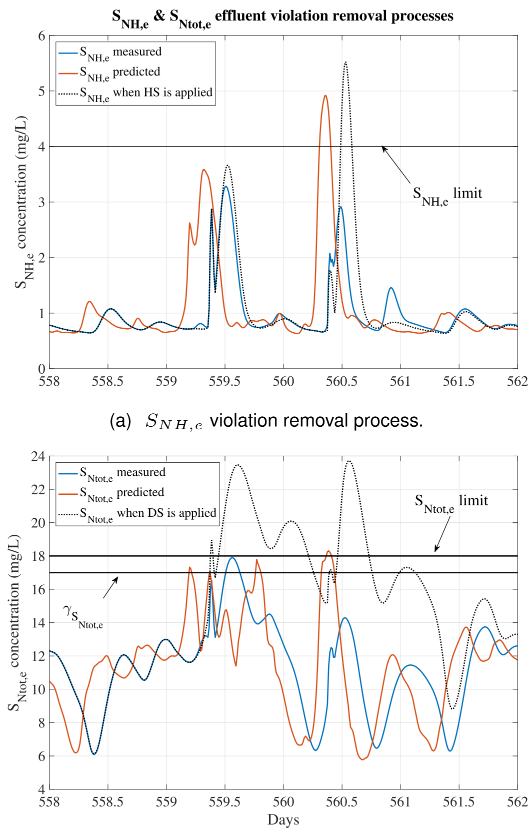
Notice that in this new control scenario, the Q_a parameter is acting as an input of the ANN-based Soft-Sensor at the same time it is modified by the $S_{NH,e}$ control strategy. For that reason, the ANN-based Soft-Sensor has to be trained twice. The first training is performed to obtain the model hyperparameters which will correctly predict the $S_{NH,e}$ concentrations. $S_{Ntot,e}$ concentrations will also be correctly predicted with the exception of that moments where a peak of ammonium is detected. At this point, the control strategy acting over $S_{NH,e}$ will change the Q_a parameters and therefore, predictions of $S_{Ntot,e}$ will be degraded since the network predicting them has not been trained considering these changes: LSTMs predicting $S_{Ntot,e}$ are trained with DS' Q_a measurements. Once a whole year simulation of ASS-PRS scenario is performed, LSTMs predicting $S_{Ntot,e}$ are retrained considering the new Q_a measurements. Thus, information about the actuations devoted to reducing the $S_{NH,e}$ violations is provided in the second retraining process.

IV. RESULTS

A. WWTP PERFORMANCE WITH SEPARATED CONTROL STRATEGIES

WWTP's performance is computed for the four different predictive control scenarios to determine the improvement achieved with the adoption of the ANN-based Soft-Sensor. Results are shown in Tab. 5, where the different stated criteria are computed: EQI, OCI, $S_{Ntot,e}$'s and $S_{NH,e}$'s violations. They show that WWTP's performance depends on the variable under control, i.e., if the control structure is proposed to remove violations of $S_{NH,e}$ or $S_{Ntot,e}$. Results show that both structures are able to totally remove the concentrations they are in charge of at the expense of allowing violations of the non-controlled pollutants.

Focusing on ASS-NHRS, one can observe that a total removal of $S_{NH,e}$ violations is achieved whereas the violations of total nitrogen have increased 1.57 percentage points w.r.t. DS control strategy. This effect is motivated by the fact that whenever a violation of ammonium is predicted, the control strategy modifies the Q_a flow rate increasing the amount of sludge and dissolved oxygen in the anoxic tanks and therefore, worsening the nitrates concentrations. Consequently, this increases the levels and violations of total nitrogen. It is also observed that OCI is reduced a 37.2% since the control strategy is only applied when a violation is detected whereas DS and HS strategies are applied all the time. ASS-NHRS is also able to improve the effluent quality index (EQI) reducing it a 3.30% w.r.t. DS motivated by the reduction of ammonium violations. Fig. 7 shows the detection and reduction of a future $S_{NH,e}$ violation. In this case and for the rest of the paper, figures correspond to the evolution of concentrations in real time. Consequently, measured concentrations show an offset around four hours w.r.t. predicted



(a) $S_{NH,e}$ violation removal process.

(b) $S_{Ntot,e}$ violation removal process.

FIGURE 7. Both concentrations, when DS and HS scenarios are applied, are present to show that if no prediction is performed, $S_{NH,e}$ and $S_{Ntot,e}$ would incur into violations.

ones because predictions of concentrations are given four hours in advance. For instance in Fig. 7, the pollutant peak predicted at day 560.3 corresponds to the peak measured at day 560.6 approximately.

In terms of ASS-NTRS, one can observe that in this case the violations of $S_{Ntot,e}$ are completely removed. However, the $S_{NH,e}$'s limit is violated a 0.14% of the WWTP's operational time. This percentage represents a reduction of violations equivalent to 0.27 and 0.09 percentage points w.r.t. DS and HS, respectively. Since both pollutant products are reduced, the EQI measurement is also improved a 6.14%, a 2.94% and a 0.37% w.r.t. DS, ASS-NHRS and HS, respectively. Moreover, the OCI is increased a 9.38% w.r.t. ASS-NHRS control strategy as it is shown in Tab. 5. This is because whenever a violation is predicted, the control strategy adds external carbon to the first, second and fifth reactor tanks. Moreover, if OCI is compared with DS and HS, it is observed that it has been reduced a 30.70% and a 18.69%, respectively, motivated by the fact that DS an HS are continuously adding carbon at a flow rate of 2 and 1 m^3/day whilst ASS-NTRS does not. Finally, an example of a $S_{Ntot,e}$ violation removal process is shown in Fig. 7b where a violation occurs at day 559.4 if predictive control is not adopted. In this case, the ANN-based Soft-Sensor is able to predict

TABLE 5. WWTP's performance - DS, HS, ASS-NHRS and ASS-NTRS comparison.

Strategy	EQI	OCI	$S_{Ntot,e}$'s violation [% of time]	$S_{NH,e}$'s violation [% of time]
DS [6]	5577.97	9447.24	1.18	0.41
HS [8]	5274	8052	N/A	0.23
ASS-NHRS	5394.11	5932.83	2.75	0
ASS-NTRS	5235.31	6547.21	0	0.14

TABLE 6. Number of violations, average of violation levels and standard deviation. Maximum violations, μ and σ are measured in mg/L.

$S_{Ntot,e}$ violations				
Strategy	Num.	Maximum	μ	σ
DS [6]	29	21.69	18.95	0.84
HS [8]		N/A		
ASS-NHRS	49	23.47	19.62	1.31
ASS-NTRS		-		
$S_{NH,e}$ violations				
Strategy	Num.	Maximum	μ	σ
DS [6]	11	8.36	5.49	1.34
HS [8]	4	6.16	5.63	0.56
ASS-NHRS		-		
ASS-NTRS	4	5.46	4.98	0.62

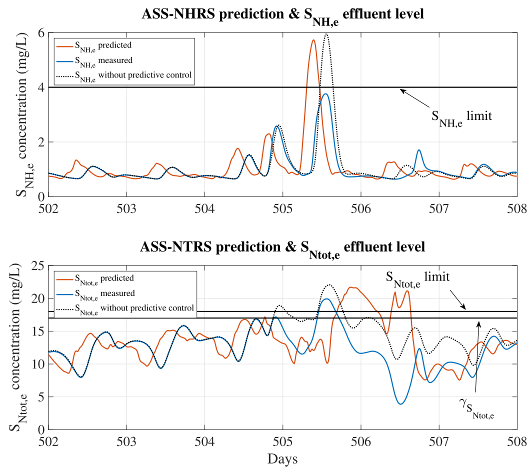


FIGURE 8. $S_{NH,e}$ **violation detected and reduced at day 505.4, thus Q_a will be modified to reduce the effluent peak at day 505.6. Consequently, $S_{Ntot,e}$ is badly predicted since the variations of Q_a have not been considered in the ANN-based Soft-Sensor training process.**

it at day 559.2, thus, the control strategy actuates achieving the reductions of $S_{Ntot,e}$ levels in the effluent avoiding the violation.

In both cases (ASS-NHRS and ASS-NTRS) the same effect is observable in terms of the number of violations, their average and their standard deviation (see Tab. 6). For instance, there are not $S_{Ntot,e}$ violations in ASS-NTRS scenario. However, they have been increased in the case of ASS-NHRS. In the case of $S_{NH,e}$, they have been reduced from 11 in the case of DS scenario to 0 and 4 in the case of ASS-NHRS and ASS-NTRS, respectively. Furthermore, their maximum level has been significantly reduced from 8.36 (DS scenario) to 5.46 (ASS-NTRS). As a summary, the adoption of the ANN-based Soft-Sensor entails the improvement of the control strategies performance in terms of the percentage of time that concentrations under control are violated, the amount of violations and their maximum levels.

B. WWTP PERFORMANCE WITH JOINT CONTROL STRATEGIES

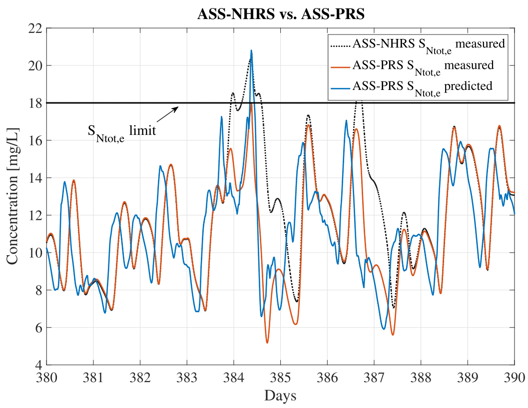
Until this point all the scenarios compared with DS and HS correspond to scenarios where the control strategy is focused on reducing a unique pollutant concentration. However, this does not represent a real scenario where the main aim is to avoid both types of violations ($S_{NH,e}$ and $S_{Ntot,e}$). For that reason, the WWTP performance has also been computed when a more realistic scenario is considered. It corresponds to ASS-PRS, where the efforts are focused on reducing $S_{NH,e}$ and $S_{Ntot,e}$ pollutants at the same time. In such a context, one has to specially consider those parameters (Q_a) that act as inputs of the ANN-based Soft-Sensor and as a manipulated parameter in the violations removal process.

First, performance is computed without retraining the ANN-based Soft-Sensor, i.e., without taking into account the Q_a modifications performed in the $S_{NH,e}$ violations removal process. Results in Tab. 7 show that a reduction of the number of violations is achieved, however, they are not completely removed w.r.t. DS: (i) $S_{Ntot,e}$ violations are reduced 1.1 percentage points, which represent violations during the 0.08% of the WWTP's operational time, and (ii) $S_{NH,e}$ violations are reduced 0.396 percentage points, which are equal to violations during 0.014% of the operational time. Violations cannot be completely removed because when varying Q_a, the levels of nitrate in the anoxic tanks are increased. This is translated into a trade-off between the ammonium reduction and the levels of total nitrogen: when violations of $S_{NH,e}$ are reduced, the levels of total nitrogen are increased and consequently the probability of observing $S_{Ntot,e}$ violations (see Fig. 8). Besides, the ANN-based Soft-Sensor predicting $S_{Ntot,e}$ has not been trained considering these Q_a variations. Consequently, predictions of total nitrogen are not so accurate in those points where a violation of $S_{NH,e}$ is predicted.

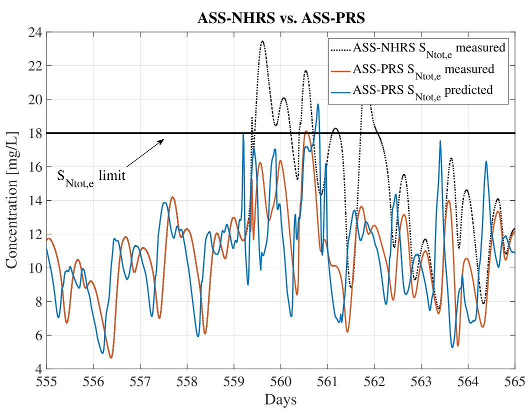
To solve this, the soft-sensor is retrained when a whole year simulation is achieved. Results in Tab. 7 show that the number of $S_{Ntot,e}$ violations is reduced a 75% when the ANN-based Soft-Sensor is retrained. $S_{NH,e}$ predictions do not vary since no action is performed on the considered input variables. In terms of EQI and OCI, the former is decreased a 0.34% whereas the latter is increased a 0.57% w.r.t. the situation where the soft-sensor is not retrained. Finally, if the performance of ASS-PRS is computed in terms of the percentage of operational time that an effluent is violated, an improvement

TABLE 7. WWTP's performance-DS and ASS-PRS comparison.

Strategy	EQI	OCI	$S_{Ntot,e}$'s violation [% of time]	$S_{NH,e}$'s violation [% of time]
DS [6]	5577.97	9447.24	1.18	0.41
HS [8]	5274	8052	N/A	0.23
ASS-PRS	5236.72	6633.73	0.08	0.014
ASS-PRS retrained	5218.76	6671.99	0.02	0.014



(a) $S_{Ntot,e}$ violation removal process from days 380 to 390.



(b) $S_{Ntot,e}$ violation removal process from days 555 to 565.

FIGURE 9. Comparative between violations produced in ASS-NHRS and ASS-PRS scenarios.

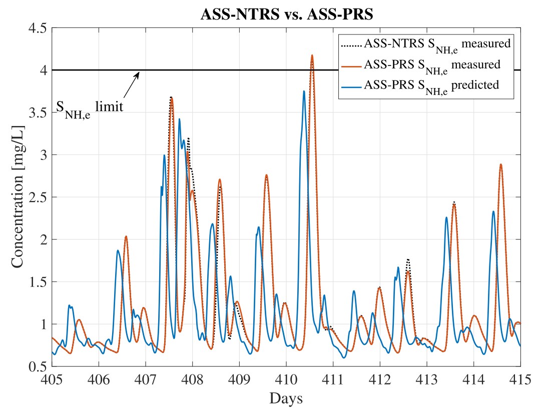


FIGURE 10. Comparative between violations produced in ASS-NTRS and ASS-PRS scenarios. Only the days, where $S_{NH,e}$ violations of ASS-PRS are produced, are shown.

TABLE 8. Number of violations, average of violation levels and standard deviation. Maximum violations, μ and σ are measured in mg/L.

$S_{Ntot,e}$ violations				
Strategy	Num.	Maximum	μ	σ
DS [6]	29	21.69	18.95	0.84
HS [8]		N/A		
ASS-PRS	2	19.92	19.17	1.06
ASS-PRS retrained	2	18.12	18.06	0.08
$S_{NH,e}$ violations				
Strategy	Num.	Maximum	μ	σ
DS [6]	11	8.36	5.49	1.34
HS [8]	4	6.16	5.63	0.56
ASS-PRS	1	4.13	4.13	-
ASS-PRS retrained	1	4.13	4.13	-

of 98.31% in the reduction of $S_{Ntot,e}$ and a 96.58% for $S_{NH,e}$ w.r.t. DS scenario is achieved. This corresponds to a 99.27% for $S_{Ntot,e}$ and 90% for $S_{NH,e}$ in terms of ASS-NHRS and ASS-NTRS, respectively.

Moreover, it is worth noting that, although the complete avoidance of violations is not achieved, they represent a low percentage of the operational time. For instance, a unique violation of $S_{NH,e}$, which equals to a 0.014% of the operational time, is produced at day 410.5. $S_{Ntot,e}$ is violated two times, at days 384.4 and 560.5, which only represents a 0.02% of the WWTP's operational time. In such a context, Fig. 9a, Fig. 9b and Fig. 10 show the differences between the violations that occurred in ASS-NTRS, ASS-NHRS and ASS-PRS. In Figs. 9a and 9b, it is observed that violations performed in ASS-PRS scenario are much lower than those produced in ASS-NHRS. These reach $S_{Ntot,e}$ values of 18 mg/L and 18.12 mg/L at days 384.4 and 560.5, respectively.

On the other hand, Fig. 10 compares the $S_{NH,e}$ violation obtained in ASS-PRS with the same violation performed in the ASS-NTRS scenario. In this case, both violations are produced because the level of ammonium reaches 4.177 mg/L. Both are produced by the actuation performed over $S_{Ntot,e}$ at day 410.5, where a violation of total nitrogen is predicted and reduced. This is clearly shown in Tab. 8, where the amount of violations has not changed from ASS-PRS to ASS-PRS retrained. The improvement here is shown in the average of violations and their maximum. For instance, ASS-PRS $S_{Ntot,e}$'s maximum violation equals to 19.92 mg/L while in ASS-PRS retrained it has been reduced until 18.12 mg/L. Moreover, the average of violations (μ) is also improved. It has been reduced from 19.17 mg/L (ASS-PRS) to 18.06 mg/L (ASS-PRS retrained).

As a summary, the application of ASS-PRS scenario entails the reduction of the % of time that effluent concentrations are exceeding the BSM2 limits. Effluent violations are reduced between 0.216 and 0.396 percentage points for $S_{NH,e}$ and between 1.1 and 1.16 percentage points in the case of $S_{Ntot,e}$. The reduction of pollutant concentrations and the avoidance of violations also help in the improvement of the EQI metric: the lower the pollutant concentrations, the better the EQI. For instance, the ASS-PRS retrained scenario is the one showing the lowest pollutant concentrations and consequently the lowest EQI, 5218.76. In terms of OCI, ASS-PRS scenario only adds external carbon when an effluent limit violation is predicted. Therefore, this is translated into an improvement (reduction) of the WWTP's OCI w.r.t. DS and HS control scenarios where its maximum improvement equals to a 29.78% w.r.t. DS.

V. CONCLUSION

In this paper, the deployment of an ANN-based Soft-Sensor has been tested with predictive control strategies whose main aim is to reduce the $S_{NH,e}$ and $S_{Ntot,e}$ violations. In that sense, the ANN-based Soft-Sensor is in charge of predicting the effluent concentrations that will be adopted by a hierarchical control strategy in order to actuate in advanced and avoid possible violations. Besides, performance of the control strategies has been compared with BSM2 default control. Results show that the application of the ANN-based Soft-Sensor improves the default control in terms of EQI, OCI and number of violations. For instance, control strategies devoted to reducing $S_{NH,e}$ violations are able to completely reduce them whereas BSM2 default control shows violations equivalent to the 0.41% of the WWTP operational time.

On the other hand, the application of the ANN-based Soft-Sensor in a control strategy devoted to reducing $S_{NH,e}$ and $S_{Ntot,e}$ violations at the same time is also addressed in this work. For that purpose, predictive control strategies have been modified to be able to act together. Results emphasize the importance of ANN-based Soft-Sensor's input data. In our case, the recirculation flow (Q_a) acts as an input of the ANN-based Soft-Sensor when predicting $S_{Ntot,e}$ as well as it is one of the variables modified by the control strategy reducing the $S_{NH,e}$ violations. Therefore, Q_a modifications have to be considered in the ANN-based Soft-Sensor training process in order to avoid a degradation of predictions' accuracy.

Then, it is shown that the modified predictive control approach improves the control performance w.r.t. BSM2 default control approaches achieving the reduction of the percentage of time that effluent limits are violated. When comparing the performance of our approach, one can observe that it is able to reduce $S_{NH,e}$ violations around a 90% w.r.t the control strategy focused on reducing $S_{Ntot,e}$ (ASS-NTRS). Furthermore, the percentage of time that effluent limits are violated is reduced 1.1 percentage points in the case of $S_{Ntot,e}$ and approximately 0.325 percentage points in the case of $S_{NH,e}$, both w.r.t. BSM2's default control strategies. Finally, it is important to notice that some considerations have to be adopted when translating our approach into real environments. For instance, filters are usually applied, which attenuate the noise signal. In addition, the controller parameters should be adjusted after an analysis of the sensor signals.

ABBREVIATION AND SYMBOLS

ANN	Artificial Neural Network
ASM	Activated Sludge Model
ASM1	Activated Sludge Model No.1
ASM2	Activated Sludge Model No.2
ASM2d	Activated Sludge Model No.2d
ASM3	Activated Sludge Model No.3
ASS-NHRS	ANN-based Soft-Sensor $S_{NH,e}$ reduction scenario
ASS-NTRS	ANN-based Soft-Sensor $S_{Ntot,e}$ reduction scenario
ASS-PRS	ANN-based Soft-Sensor pollutant reduction scenario
BOD_5	Biochemical Oxygen Demand (mg/L)
BSM1	Benchmark Simulation Model No.1
BSM2	Benchmark Simulation Model No.2
CL	Default control strategy loop adopted in [8]
COD	Chemical Oxygen Demand
DS	Default Scenario
EQI	Effluent Quality Index
HS	Hierarchical Control Scenario
IWA	International Water Association
$K_La\,x$	Oxygen Transfer Coefficient for tank x (d^{-1})
LSTM	Long-Short Term Memory
MLP	Multilayer Perceptron
MPC	Model Predictive Control
OCI	Overall Cost Index
PH	Prediction Horizon
PI	Proportional Integral Controller
$q_{EC,x}$	External carbon flow rate at tank x (m^3/d)
Q_a	Internal recirculation flow rate (m^3/d)
Q_e	Effluent flow rate (m^3/d)
Q_{in}	Influent flow rate (m^3/d)
Q_{po}	Primary Clarifier's flow rate (m^3/d)
Q_r	Sludge internal recycle flow rate (m^3/d)
RMSE	Root Mean Squared Error (mg/L)
RNN	Recurrent Neural Network
S_{NH}	Ammonium Concentration (mg/L)
$S_{NH,e}$	Ammonium Concentration in the effluent (mg/L)
$S_{NH,5}$	Ammonium Concentration at the fifth reactor tank (mg/L)
S_{NKj}	Total Kjeldahl Nitrogen Concentration (mg/L)
$S_{NO,x}$	Nitrate Nitrogen Concentration at tank x (mg/L)
S_{Ntot}	Total Nitrogen Concentration (mg/L)
$S_{Ntot,e}$	Total Nitrogen Concentration in the effluent (mg/L)

$S_{O,x}$	Dissolved Oxygen Concentrations at tank x (mg/L)
T_{as}	Environment Temperature $(°C)$
TSS	Total Suspended Solids (mg/L)
WL	Window Length
WWTP	Wastewater Treatment Plant
$\gamma_{S_{NH,e}}$	$S_{NH,e}$ threshold (mg/L)
$\gamma_{S_{Ntot,e}}$	$S_{Ntot,e}$ threshold (mg/L)

REFERENCES

[1] *Council Directive 91/271/EEC of 21 May 1991 Concerning Urban Waste Water Treatment*, Eur. Commission, Brussels, Belgium, 1991.

[2] M. Henze, L. Grady, Jr., W. Gujer, G. V. R. Marais, and T. Matsuo, ''Activated sludge model no. 1,'' IAWPRC Sci., London, U.K., Tech. Rep. 1, Jan. 1987.

[3] M. Henze, W. Gujer, T. Mino, and M. C. van Loosdrecht, *Activated sludge models ASM1, ASM2, ASM2d ASM3*. London, U.K.: IWA, 2000.

[4] D. Vrecko, E. Volcke, U. Jeppsson, and K. Gernaey, ''Evaluation criteria description and example for BSM2,'' Task Group Benchmarking Control Strategies Wastewater Treatment Plants, Int. Water Assoc., London, U.K., Tech. Rep. 23, 2007.

[5] R. Vilanova and A. Visioli, *PID Control in the Third Millennium: Lessons Learned and New Approaches*. London, U.K.: Springer, 2012.

[6] U. Jeppsson, M.-N. Pons, I. Nopens, J. Alex, J. Copp, K. Gernaey, C. Rosen, J.-P. Steyer, and P. Vanrolleghem, ''Benchmark simulation model no 2: General protocol and exploratory case studies,'' *Water Sci. Technol.*, vol. 56, no. 8, pp. 67–78, Oct. 2007.

[7] W. Shen, X. Chen, and J. P. Corriou, ''Application of model predictive control to the BSM1 benchmark of wastewater treatment process,'' *Comput. Chem. Eng.*, vol. 32, no. 12, pp. 2849–2856, Dec. 2008.

[8] I. Nopens, L. Benedetti, U. Jeppsson, M.-N. Pons, J. Alex, J. B. Copp, K. V. Gernaey, C. Rosen, J.-P. Steyer, and P. A. Vanrolleghem, ''Benchmark simulation model no 2: Finalisation of plant layout and default control strategy,'' *Water Sci. Technol.*, vol. 62, no. 9, pp. 1967–1974, 2010.

[9] H.-S. Ou, C.-H. Wei, H.-Z. Wu, C.-H. Mo, and B.-Y. He, ''Sequential dynamic artificial neural network modeling of a full-scale coking wastewater treatment plant with fluidized bed reactors,'' *Environ. Sci. Pollut. Res.*, vol. 22, no. 20, pp. 15910–15919, 2015.

[10] C. Foscoliano, S. Del Vigo, M. Mulas, and S. Tronci, ''Predictive control of an activated sludge process for long term operation,'' *Chem. Eng. J.*, vol. 304, pp. 1031–1044, Nov. 2016.

[11] J.-F. Qiao, Y. Hou, L. Zhang, and H.-G. Han, ''Adaptive fuzzy neural network control of wastewater treatment process with multiobjective operation,'' *Neurocomputing*, vol. 275, pp. 383–393, Jan. 2018.

[12] H.-G. Han, L. Zhang, H.-X. Liu, and J.-F. Qiao, ''Multiobjective design of fuzzy neural network controller for wastewater treatment process,'' *Appl. Soft Comput.*, vol. 67, pp. 467–478, Jun. 2018.

[13] I. Santín, C. Pedret, R. Vilanova, and M. Meneses, ''Advanced decision control system for effluent violations removal in wastewater treatment plants,'' *Control Eng. Pract.*, vol. 49, no. 2, pp. 60–75, Apr. 2016.

[14] M. Sadeghassadi, C. J. Macnab, B. Gopaluni, and D. Westwick, ''Application of neural networks for optimal-setpoint design and MPC control in biological wastewater treatment,'' *Comput. Chem. Eng.*, vol. 115, pp. 150–160, Jul. 2018.

[15] Z. Y. Wan, P. Vlachas, P. Koumoutsakos, and T. Sapsis, ''Data-assisted reduced-order modeling of extreme events in complex dynamical systems,'' *PLoS ONE*, vol. 13, no. 5, 2018, Art. no. e0197704.

[16] K. Greff, R. K. Srivastava, J. Koutnìk, B. R. Steunebrink, and J. Schmidhuber, ''LSTM: A search space odyssey,'' *IEEE Trans. Neural Netw. Learn. Syst.*, vol. 28, no. 10, pp. 2222–2232, Oct. 2017.

[17] I. Goodfellow, Y. Bengio, and A. Courville, *Deep Learning*. Cambridge, MA, USA: MIT Press, 2016.

[18] R. Vilanova, I. Santín, and C. Pedret, ''Control y operación de estaciones depuradoras de aguas residuales: Modelado y simulación,'' *Revista Iberoamericana de Autom. e Inform. Ind.*, vol. 14, no. 3, pp. 217–233, 2017.

[19] Y. Lorenzo-Toja and I. Vázquez-Rowe, M. J. Amores, M. Termes-Rifé, D. Marín-Navarro, M. T. Moreira, and G. Feijoo, ''Benchmarking wastewater treatment plants under an eco-efficiency perspective,'' *Sci. Total Environ.*, vols. 566–567, pp. 468–479, Oct. 2016.

[20] I. Pisa, I. Santín, J. L. Vicario, A. Morell, and R. Vilanova, ''A recurrent neural network for wastewater treatment plant effuents' prediction,'' in *Proc. Actas 39th Jornadas Autom.*, Badajoz, Spain, Sep. 2018, pp. 621–628. [Online]. Available: http://eii.unex.es/ja2018/actas/JA2018_148.pdf

[21] I. Pisa, I. Santín, J. L. Vicario, A. Morell, and R. Vilanova, ''ANN-based soft sensor to predict effluent violations in wastewater treatment plants,'' *Sensors*, vol. 19, no. 6, p. 1280, 2019.

[22] J. B. Copp, *The COSTSimulation Benchmark: Description and Simulator Manual(a product of COST Action 624 & COST Action 682)*. Luxembourg, U.K.: Office for Official Publications of the European Union, 2002.

[23] K. V. Gernaey, U. Jeppsson, P. A. Vanrolleghem, and J. B. Copp *Benchmarking of Control Strategies for Wastewater Treatment Plants*. London, U.K.: IWA, 2014.

[24] P. Y. Yang and Z. Zhang, ''Nitrification and denitrification in the wastewater treatment system,'' in *Proc. UNESCO—Univ. Tsukuba Int. Seminar Traditional Technol. Environ. Conservation Sustain. Develop. Asian–Pacific Region*, Tsukuba, Japan, Dec. 1995, pp. 145–158.

[25] I. Takács, G. G. Patry, and D. Nolasco, ''A dynamic model of the clarification-thickening process,'' *Water Res.*, vol. 25, no. 10, pp. 1263–1271, 1991.

[26] *Wastewater Treatment Fact Sheet: External Carbon Sources for Nitrogen Removal*, document EPA 832-F-13-016, United States Environmental Protection Agency. Office of Wastewater Management, Aug. 2013.

[27] Y. Bengio, P. Simard, and P. Frasconi, ''Learning long-term dependencies with gradient descent is difficult,'' *IEEE Trans. Neural Netw.*, vol. 5, no. 2, pp. 157–166, Mar. 1994.

[28] S. Garcia, J. Luengo, and F. Herrera, *Data Preprocessing in Data Mining*. New York, NY, USA: Springer, 2015.

IVAN PISA was born in Barcelona, Spain, in 1994. He received the B.Sc. degree in telecommunications systems engineering and the M.Sc. degree in telecommunications engineering from the Universitat Autònoma de Barcelona, Spain, in 2016 and 2018, respectively, where he is currently pursuing the Ph.D. degree in electrical and telecommunications engineering with the Wireless Information Networking (WIN) Group and Advanced Control Systems and Automation (ASAC) Group.

From 2016 to 2018, he was a Research Assistant with the WIN Group. His research interests include machine learning, the IoT, Industry 4.0, and data analytics. In May 2019, he has received the Best Academic Record Award from the Spanish Official College of Telecommunications Engineers (Colegio Oficial de Ingenieros de Telecomunicación-COIT).

IGNACIO SANTÍN was born in Barcelona, Spain, in 1980. He received the B.Sc. degree in electronic engineering, in 2006, the M.Sc. degree in environmental studies (specialized in environmental technology), and the Ph.D. degree in wastewater treatment control, in 2015.

He was involved in the water control of Barcelona sewer systems, and management and improvement of processes, until 2011.

ANTONI MORELL received the M.Sc. degree in electrical and electronics engineering and the Ph.D. degree from the Universitat Politècnica de Catalunya (UPC), Barcelona, in 2002 and 2008, respectively.

He was with the Signal Theory and Communications Department, UPC, from 2002 to 2005, holding a Spanish Government FPU Grant to pursue the Ph.D. degree. He joined the Universitat Autònoma de Barcelona, in 2005, where he is currently an Associate Professor. He has expertise in optimization techniques applied to communications and the IoT/WSN, publishing over articles in recognized international journals and over 50 articles including conference proceedings. His current research interests include the IoT solutions and deep learning applications to e-health and industry 4.0.

JOSE LOPEZ VICARIO received the degree in electrical engineering and the Ph.D. degree *(cum laude)* from the Universitat Politècnica de Catalunya (UPC), Barcelona, in 2002 and 2006, respectively, and the M.B.A. degree from the IESE Business School, Universidad de Navarra.

He is an Associate Professor with the UAB. He has a wide expertise on wireless communications and the IoT/WSN, publishing 32 articles in recognized international journals, over 50 articles in conferences and supervising five Ph.D. thesis (over three in progress). He has received the 2005/06 best Ph.D. prize in information technologies and communications by the UPC. He holds the advanced research accreditation issued by Catalan Government.

RAMON VILANOVA (M'06) was born in Lleida, Spain, in 1968. He received the master's and Ph.D. degrees from the Universitat Autònoma de Barcelona (UAB), in 1991 and 1996, respectively.

He is currently a Lecturer with the School of Engineering, UAB, where develops educational task teaching subjects of signals and systems, automatic control and technology of automated systems. He is the author of several book chapters and has more than 100 publications in international congresses/journals. His research interests include methods of tuning of PID regulators, systems with uncertainty, analysis of control systems with several degrees of freedom, application to environmental systems, and the development of methodologies for the design of machine-man interfaces. He is a member of the IFAC.