Integration of Set Point Optimization Techniques into Nonlinear MPC for Improving the Operation of WWTPs

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***Abstract*—Optimization and control strategies are necessary to keep wastewater treatment plants (WWTPs) operating in the best possible conditions, maximizing effluent quality with the minimum consumption of energy. In this work, a benchmarking of different hierarchical control structures for WWTPs that combines static and dynamic Real Time Optimization (RTO) and non linear model predictive control (NMPC) is presented. The objective is to evaluate the enhancement of the operation in terms of economics and effluent quality that can be achieved when introducing NMPC technologies in the distinct levels of the multilayer structure. Three multilayer hierarchical structures are evaluated and compared for the N-Removal process considering the short term and long term operation in a rain weather scenario. A reduction in the operation costs of approximately 20% with a satisfactory compromise to Effluent Quality is achieved with the application of these control scheme.**

I. INTRODUCTION

Process control and optimization systems are important for the successful operation of plants. In most of the process industries, the control and decision making tasks are performed following a functional decomposition that executes the appropriated actions at different time scales. The resulting hierarchical architecture is useful to operate the plant effectively, dealing with different environmental and process conditions such as seasonal demand, varying load changes, and energy availability among others issues affecting business and operation strategies. In the multiple layer structure, the highest levels are dedicated to planning and scheduling while the subsequent levels deal with the implementation of optimal operation policies (site-wide and local optimization), supervisory control, regulatory control and data acquisition functions (Skogestad, 2000; Seborg et al., 2004). Planning and scheduling are usually called strategic levels, while optimization and control are tactical or operational levels (Manenti, 2011). A general scheme of the hierarchical structure is presented in Figure 1 (Skogestad, 2000; Araujo et al., 2011), nevertheless the structure can be extended or modified according with the particular operation objectives.

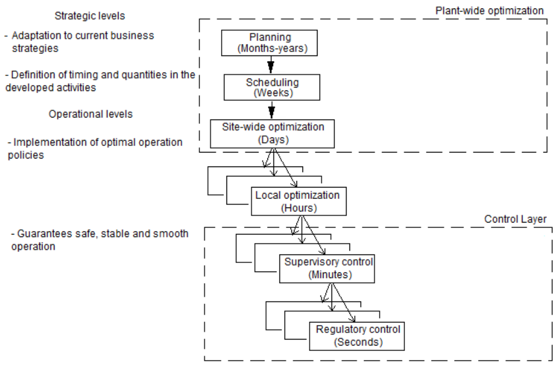

Figure 1. Multiple layer hierarchical structure of process control given by functional decomposition.

This work focuses on the operational levels, specifically on the implementation of optimal operation policies by integrating Real Time Optimization (RTO) and Model Predictive Control (MPC) techniques in Wastewater Treatment Plants. In the literature the optimization and control levels are treated as a two-layer control structure encapsulated within the multiple layer hierarchical architecture (Engell, 2007; Scattolini, 2009).Typically, in industrial applications, a Real Time Optimization (RTO), either stationary, dynamic or both, is performed in the upper layer to provide set-points, constraints and additional information regarding the economically optimal operating point to the control layer. This is possible when enough degrees of freedom are available to be adjusted in the process. The direct control layer carries out the actions to regulate the output variables, maintaining them as close as possible to the optimal set-points in the presence of disturbances. The direct control layer may be comprised by advanced Model Predictive Controllers (MPCs), simple PIDs controllers or a sequence of layers including MPC for supervisory purposes (constrained control) and MPCs or PIDs for regulatory purposes (Tatjewsky, 2008).

The benefits of the Real Time Optimization are demonstrated by its successful implementation in a number of industrial applications leading to significant economical profits (Edgar, 2004). The RTO is recommended when significant changes occurs in the operating conditions affect strongly the plant profitability. In large plants, seasonal and day-to night variations may be sufficient to justify RTO (Darby et al., 2014). Additionally, the temporal decomposition is a solution for complex multi-scale processes to cope with the different dynamics of the state variables or disturbances (Tatjewsky, 2008). The sampling time and optimization horizon are larger in the upper layers dedicated to the slower process dynamics and disturbances. Thus, beyond the functional hierarchical decomposition carrying out specific tasks at different rates, a temporal decomposition with different time scales within one of the functional layers is recommended to achieve the optimal operation.

The dynamical properties of disturbances are crucial in the formulation of the multilayer optimization strategy. The classical static RTO/ MPC structure is compatible with processes facing slow-varying disturbances or processes with disturbances that changes abruptly but rare respect to the controlled process dynamics (Tatjewsky, 2008). If the time scale of disturbances is longer than RTO sampling period, the economic static optimization can be solved reasonable less frequently than the MPC optimization executes, updating the operating point to current conditions. However, in industrial practice is common to find processes where the disturbances dynamic is not slow, in the worst case it may be comparable to the process dynamics. In those cases, the static economic optimization fails producing a significant loss of economic effectiveness (Lawrynczuk et al., 2008). Consequently, it is necessary to compute the optimal set points more often and therefore, the dynamic optimization (D-RTO) using MPCs is an appealing strategy to perform efficiently the economic optimization accounting for disturbances and process dynamics. Furthermore, in the presence of multi-scale disturbances, a combination of stationary RTO and dynamic RTO can be appropriated to optimize the operation of the plant as it is considered in this paper. This optimization strategy is also appropriated to address the problem of multi-scale behaviour in complex processes which exhibits substantial differences between rates of change of faster and slower state variables.

The use of Model Predictive Control (MPC) is justified because it is an advanced control technology widely accepted in the process industry, proven by a considerable number of successful applications reported in literature (Qin and Badgwell, 2003). The MPC deals with the control problem transforming it into an optimization one. The classical objective function is a quadratic index which penalizes the deviations of the states and inputs from the targets; nevertheless it is possible to use different formulations as in Economic Model Predictive Control (EMPC) (Ellis and Christofides, 2014) . The noteworthy advantages of the MPC strategy are the ability to handle multivariable interactions and the possibility of including constraints imposed on inputs, outputs or states directly in the problem formulation to anticipate and prevent future violations (Qin and Badgwell, 2003; Edgar, 2004; Lawrynczuket et al, 2008). The constraints not only represent the admissible range of the inputs and control variables, but also decisions related to production quality, economic efficiency and general operation requirements.

Wastewater treatment plants (WWTPs) are non-productive process subjected to very high economic penalties for off-specification discharges and very high operation costs basically associated with the aeration system and pumping energy. These plants exhibits complex and non-linear dynamics making difficult the control and the optimization tasks. In this type of processes, frequent and significant changes in the inputs affect the process behaviour, the climatic characteristics of the region define seasonal profiles and the influent variations tend to be cyclical, depending on the daily and weekly population activities. Moreover, WWTPs are complex systems with clearly separable slow and fast dynamics due to the non-linear and interacting biological processes occurring in multiple time scales. In that case as mentioned above, a temporal decomposition may be necessary for an adequate distribution of optimization and control tasks (Brdys et al., 2008; Picasso et al., 2010; Scattolini, 2009). Summarizing, all the mentioned above characteristics of the WWTs justify the application of hierarchical control strategies involving RTO and advanced control techniques in order to improve their operation in terms of economics, guarantee water quality and avoid legal sanctions. A solution proposed in this paper is the implementation of multilayer structures comprising static Real Time Optimization (RTO) for the slower process and disturbances dynamics, a MPC dynamic Real Time Optimization (D-RTO) to capture the medium to fast process and disturbances dynamics, and MPC regulatory layer to improve economically the plant performance.

Several works have focused on the integration of Real Time Optimization (RTO) and Model Predictive Control (MPC). Some of these attempts are discussed and reported in Engell (2007) and Tatjewsky (2008). Sequeira et al. (2002) propose the Real Time Evolution (RTE) where the fulfillment of stationary conditions is not necessary. The so-called LP-MPC and QP-MPC two-stage MPC structures, which are frequently used in industry to integrate the low frequency steady-state optimization carried out in the RTO layer and the relatively fast regulatory linear MPC. A RTO is followed by an intermediate MPC layer that calculates the set points for the controlled variables and the manipulated inputs for a lower level MPC that executes the direct control actions (Engell, 2007). In some approaches (Kadam et al., 2002; Zhu et al., 2004; Ochoa et al. , 2010; Wurth et al., 2009), a dynamic real-time optimization (D-RTO) is performed instead of the RTO based on of steady-state models. In Kadam et al. (2002) and Ochoa et al. (2010) an alternative structure consisting of two interconnected NMPCs is employed. The upper level NMPC determines the optimal values for the manipulated and control variables in terms of cost, considering a sampling time that captures the slow process dynamics. In the lower level, the sampling time has to be significantly smaller, and the optimization is performed for the tracking of the reference trajectories given by the upper level.

Some authors go beyond by using one layer approaches for solving the optimization and control problem. Zanin et al., (2000) and Zanin et al., (2002) integrate the steady-state optimization into MPC algorithm. These approaches are applicable in processes with slow dynamics and not computationally complicated models. Another one layer dynamic real time optimization approach is the economically oriented Model Predictive Control (EMPC) which focuses in the optimization of the economic performance of the process over the prediction horizon and at the same time it calculates control actions. The conventional MPC quadratic cost function is replaced by an economic (not necessarily quadratic) cost function is used directly as the cost in MPC (Rawlings and Amrit, 2009; Ochoa et al., 2010; Heidarinejad et al., 2012). In recent work, Ellis and Christofides (2014) propose a two layer approach, consisting of an economic MPC (EMPC) in the upper layer and a conventional MPC in the regulatory layer. The EMPC receives state feedback and time-dependent economic information and computes economically optimal time-varying operating trajectories for the process by optimizing a time-dependent economic cost function over a finite prediction horizon subject to a nonlinear dynamic process model.

Regarding the optimization of the operation of WWTPs, some works propose the use of simple PI control schemes and perform the set point optimization off line (Machado et al., 2009; Araujo et al., 2011; Guerrero et al., 2011). Machado et al. (2009) presented a hierarchical structure of two cascaded PI for optimizing the operation of a nutrient removal WWTP. Araujo et al., (2011) used the steady state version of the process model for the calculation of the optimal fixed set points that allow keeping the variables related to the environmental regulation constraints within their limits , with minimum cost. In Guerrero et al. (2011), a model based set point optimization for influent profiles which are already known is performed considering different control strategies. The objective is to minimize the Overall Cost Index (OCI) and the time period that the Effluent Quality (EQ) index is above the allowed limits.

Advanced control strategies are applied and real time optimization is carried out in Piotrowski et al. (2008) and Brdys et al. (2008). The first presents a hierarchical control structure for DO control with a MIMO robust MPC and other advanced methods in the optimizing layer. In the second, Brdys et al. (2008) an integrated wastewater treatment plant and sewer system is considered. They propose a functional decomposition consisting of supervisory, optimizing and follow-up layers. A temporal decomposition of the optimizing control layer produces three sub-layers for slow, medium and fast dynamics. Robust linear MPC control strategies are applied. This structure allows for significant cost savings while the discharge limits over a long operation period under the full range of disturbances are fulfilled.

Although, the mentioned techniques have been widely and successfully used in different fields of engineering and process industry, the integration of Real Time Optimization (RTO) and MPC technology and its application are still an open field of research, especially in the field of bioprocesses as WWTP

This paper deals with the integration of the Real Time Optimization (RTO) and MPC technology considering non-linear phenomenological models for achieving the optimal operation and constrained multivariable control of Wastewater Treatment Plants (WWTP). The study presents a benchmarking of different hierarchical control structures with the objective of evaluating and comparing different strategies in a systematic way in order to determine if it is worthwhile using them. The criteria for evaluating the advantages of the implementation of the different architectures are the tradeoff between economic benefit, process and control performance and the complexity of the control structure.

The proposed approach is based on the use of non-linear phenomenological models of the process to describe all relevant dynamics and to cover a wide operating range, providing accurate predictions and ensuring the performance and robustness of the control systems (Backx, 2002). As it is well known, although the combination of static RTO and linear MPC has been widely used in industrial applications due to its computational efficiency, it can lead to a substantial loss of economic optimality in WWTPs because of the approximate linear model. In general, the dynamic behaviour of WWTPs is slow enough to cope with non-linear optimization problems despite the required computational effort.

The WWTP process selected as a case study follows the specifications given in the Benchmark Simulation Protocol (BSM1) (Alex et al., 2008) which are widely accepted by the scientific community. Particularly, in this work, the model focuses on the N-Removal process. This is an interesting case study which is quite different from the standard applications of static-RTO/linear-MPC in the petrochemical area (Edgar, 2004).

The paper is organized as follows: section 2 is devoted to the description and mathematical formulation of the proposed hierarchical control strategies integrating RTO and NMPC. The description of the N-Removal process and the performance indices used to test the optimization protocol are presented in section 3. The direct layer NMPC is described in section 4.
In section 5, the formulation of the set point optimization problems with static and dynamic models for the process in study is presented as well as the results for the short term operation period. The results of the long term operation evaluation are presented in section 6 and finally the conclusions of the work are also presented.

II. INTEGRATION OF REAL TIME OPTIMIZATION AND MODEL PREDICTIVE CONTROL

The formulation of the economic optimization problems for the WWTPs within the control structure depends strongly on the dynamical properties of disturbances as well as biological processes dynamics. The inflows to the systems depends on the daily and weekly population activities. A characteristic daily profile exhibits peaks in the morning and valleys in the night. The loads can vary during weekends and holiday seasons and rain and storm events occur with certain frequency, they are abrupt disturbances of different intensity depending on climatic characteristics of the region. It is possible to distinguish faster disturbances affecting the plant in a scale of minutes (Short time horizon variations), medium to fast disturbances in a scale from hours to days (Medium time horizon variations), and, finally, slow disturbances in the scale of days to weeks (Long time horizon variations) as is shown figure 2.

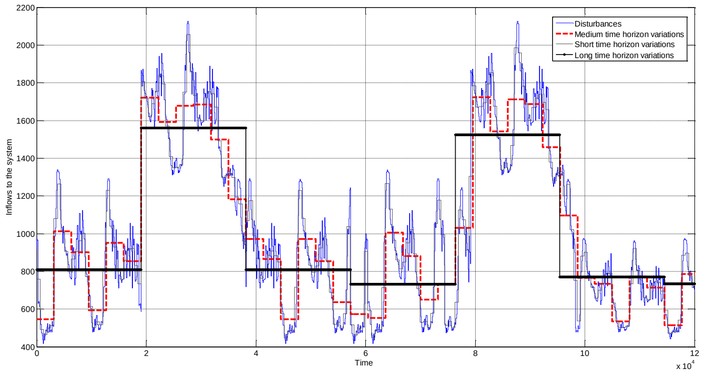

Figure 2. Characteristic paths defined by disturbances behavior in different time scales.

Such characteristics are a determining factor in the formulation of the multilayer control structures for the economic optimization of the WWTP operation. Three multilayer hierarchical structures are proposed, comprising Real Time Optimization (RTO) and direct control tasks at different rates. The RTO level performs the economical optimization of the operating conditions to obtain the best set points for the current influent characteristics. The optimal set points are passed to a nonlinear Model Predictive Controller (NMPC) which actually drives the outputs to those desired values taking into account a set of operation and control constraints. The non-linear prediction model provides a good representation of process dynamics which allows for more effective control actions to deal with large disturbances and an accurate tracking of the optimum as it changes with time.

The full multilayer structure, contemplates the temporal decomposition of the RTO to cope with the multi-scale behavior of disturbances and plant dynamics. The proposed strategy comprises a static Real Time Optimization (RTO) that handles long term objectives and deals with the slower disturbances over a horizon of days to weeks. Long time horizon targets (set points or optimal values of performance indices) are computed to be passed to the subsequent layer which performs a dynamic Real Time Optimization (D-RTO). The D-RTO is carried out to capture the medium to fast dynamics of process and disturbances over a horizon of hours to days providing economically optimum set points to the NMPC control layer. Such structure is described in figure 3.

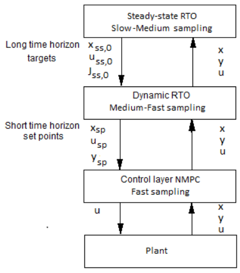

Figure 3. Full hierarchical structure for process control considering the temporal decomposition

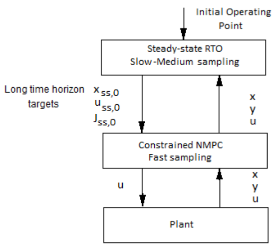

Figure 4. Two layers hierarchical structure Static RTO +NMPC

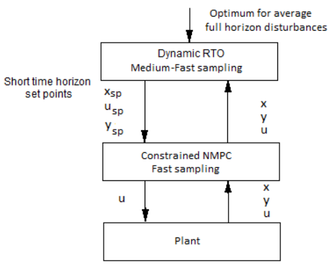

Figure 5. Two layers hierarchical structure Dynamic RTO +NMPC

One drawback of the implementation of multiple layers is the increase of the complexity of the control system. In order to reduce the complexity, two alternative structures as described in figures 4 and 5 are also considered. The intention is to determine if an increase in the number of layers to capture the different plant and disturbances dynamics is economically worthwhile.

Thus, the proposed structures are identified as: full hierarchical structure, Static RTO+NMPC and Dynamic RTO+NMPC structures. The mathematical formulation of these optimization problems are described below.

Direct Control layer:

In the proposed structures, a NMPC is used to obtain, in a fast time scale, the optimal values of the manipulated variables to be applied to the plant in order to achieve proper disturbance rejection and set point tracking. The optimization problem solved by this NMPC each sampling time T_{MPC} subject to a set of constraints is the following:

$$\min_{\mathbf{u}(k+i);0\le i\le H_c-1} J_{MPC}(k)=\min\left(\left\|\mathbf{y}(k+H_p\mid k)-\mathbf{y}_{sp}\right\|_P^2+\sum_{i=1}^{H_p}\left(\left\|\mathbf{y}(k+i\mid k)-\mathbf{y}_{sp}\right\|_Q^2\right)+\sum_{i=0}^{H_c-1}\left(\left\|\mathbf{u}(k+i\mid k)-\mathbf{u}_{sp}\right\|_S^2+\left\|\Delta\mathbf{u}(k+i\mid k)\right\|_R^2\right)\right) \tag{1}$$

s.t.

$$\begin{aligned}
&\mathbf{u}_{\min}<\mathbf{u}(k+i\mid k)<\mathbf{u}_{\max} \quad i=0,\dots,H_c-1\\
&\mathbf{y}_{\min}<\mathbf{y}(k+i\mid k)<\mathbf{y}_{\max} \quad i=1,\dots,H_p\\
&\Delta\mathbf{u}_{\min}<\Delta\mathbf{u}(k+i\mid k)<\Delta\mathbf{u}_{\max} \quad i=0,\dots,H_c-1
\end{aligned} \tag{2}$$

where $\boldsymbol{y}$ is the vector of process outputs, $\boldsymbol{u}$ the vector of manipulated variables, $\boldsymbol{y_{sp}}$ is the set points vector, $\boldsymbol{u_{sp}}$ is the target vector for the manipulated variables, $\boldsymbol{P}$ is the terminal penalty weight matrix, $\boldsymbol{Q}$ is the output weighting matrix, $\boldsymbol{R}$ is the move suppression weighting matrix and $\boldsymbol{S}$ is the input deviations weighting matrix, all of them positive definite H_p and H_c are the prediction and control horizons in this layer. The values of $\boldsymbol{y_{sp}}$ and $\boldsymbol{u_{sp}}$ are fixed goals provided by the optimization strategy together with all required information related to the optimal operating point.

The predictions are obtained using the following nonlinear discrete time prediction model of the process along H_p:

$$\begin{aligned}
&\mathbf{x}(k+1\mid k)=\mathbf{f}(\mathbf{x}(k\mid k),\mathbf{u}(k\mid k),\mathbf{d}(k\mid k))\\
&\mathbf{y}(k\mid k)=\mathbf{g}(\mathbf{x}(k\mid k),\mathbf{u}(k\mid k),\mathbf{d}(k\mid k))
\end{aligned} \tag{3}$$

where $\boldsymbol{x}$ is the vector of measure or estimated states, and $\boldsymbol{d}$ the vector of measured disturbances (which are kept constant along H_p)

Real Time Optimization layer:

<u>Static optimization</u>

In the proposed structure, a stationary RTO is used in the upper layer to achieve long term economic objectives. The optimization is carried out in a medium-to-slow sampling time scale (days-weeks) in order to obtain the optimal targets to be sent to the subsequent layer. Those targets can be: set point values or trajectories, updated constraints limits or the desired goals for the performance indices. The selected time horizon (T_{ss}) defines an operating window where filtered (or average) values of the inputs are considered and the optimized variables impact positively on the process economics.

It is assumed that for the optimal steady-state operation of the process a scalar cost function $J_{ss}: \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}$ can be defined, where n_x and n_u are the number of states and manipulated variables respectively. The optimization problem for the steady state RTO is stated as:

$$\min_{\mathbf{u}_{ss}} J_{ss}\left(\mathbf{x}_{ss},\mathbf{u}_{ss}\right) \tag{4}$$

subject to constraints:

$\mathbf{x}_{ss\min} \le \mathbf{x}_{ss} \le \mathbf{x}_{ss\max}$ (bounds in states)
$\mathbf{u}_{ss\min} \le \mathbf{u}_{ss} \le \mathbf{u}_{ss\max}$ (bounds in manipulated variables)

$$F\left(\mathbf{x}_{ss},\mathbf{u}_{ss},\bar{\mathbf{d}}\right) = 0 \tag{5}$$
$$h\left(\mathbf{x}_{ss},\mathbf{u}_{ss},\bar{\mathbf{d}}\right) \le 0 \tag{6}$$
$$\mathbf{y}_{ss} = g\left(\mathbf{x}_{ss},\mathbf{u}_{ss},\bar{\mathbf{d}}\right) \tag{7}$$

where $\mathbf{x}_{ss} \in \mathbb{R}^{n_x}$ is the vector representing the steady state values of the model used for representing the static process behavior, $\mathbf{u}_{ss} \in \mathbb{R}^{n_u}$ is the vector of the corresponding steady state manipulated variables, $\bar{\mathbf{d}} \in \mathbb{R}^{n_d}$ is the vector of disturbances, their current estimate or measurement, short-prediction, or filtered disturbances, with n_d the number of disturbances, $\mathbf{x}_{ss\min}$ and $\mathbf{x}_{ss\max}$ are the lower and upper bounds for $\mathbf{x}_{ss}$, $\mathbf{u}_{ss\min}$ and $\mathbf{u}_{ss\max}$ are the lower and upper bounds for $\mathbf{u}_{ss}$, F is a function representing the steady state model equations of the process, h is a function representing process constraints and others, and g is a function representing the model output equations.

The problem is solved each T_{ss}, that is the sampling time corresponding to the selected operating window, assuming that steady state is achieved. The results of the optimization problem are the optimal manipulated variables $\mathbf{u}_{\mathbf{ss,o}}$ and the corresponding steady states $\mathbf{x}_{\mathbf{ss,o}}$, which could be sent to the next optimization layer as optimal set points or constraints.

In this work, the static RTO is carried out in a full hierarchical structure to send the optimal value of the cost function $J_{ss,o}$ as targets to the intermediate dynamic RTO layer, as well as, in the Static RTO+NMPC structure to pass optimal set points to the control layer.

Dynamic Optimization :

A non-linear Model Predictive Controller (NMPC) is proposed to obtain the optimal operating to be sent to the control layer. The optimization problem solved by the NMPC each sampling time T_{eco} is the following:

$$\min_{\mathbf{u}(k+i);0\le i\le N_u-1} J_{eco}\left(k\right) = \min\left(J_{eco}\left(\mathbf{y}\left(k+j\,|\,k\right),\mathbf{u}\left(k+i\,|\,k\right)\right) - J_{ss,o}\right) \tag{8}$$
s.t.

$$\mathbf{y}_{\min} \le \mathbf{y}(k+j \mid k) \le \mathbf{y}_{\max} \quad j = 1,\dots,N_y \tag{9}$$
$$\mathbf{u}_{\min} \le \mathbf{u}(k+i \mid k) \le \mathbf{u}_{\max} \quad i = 0,\dots,N_u - 1 \tag{10}$$

where N_y and N_u are the prediction and control horizons respectively.

Note that the prediction and control horizons in this layer (N_y and N_u) are different from those at the control layer (H_p and H_c), due to the different time scales considered.

The function J_{eco} represents the economic costs regarding the medium to fast time scale operation, and it depends on the values of the manipulated variables **u**, disturbances **d** and outputs **y** for the period T_{eco}, where **x** is the vector of measured or estimated states, **u** the manipulated variables vector, and **y** the vector of controlled variables $\boldsymbol{f}$ and $\boldsymbol{g}$ are vector functions that represent the mathematical model or the process (non-linear differential equations), $\hat{\mathbf{y}}$ and $\hat{\mathbf{x}}$ are the predicted outputs and states.

As mentioned, before the objective of this layer is to provide optimal set points $\mathbf{y}_{\mathrm{sp}}$, and the corresponding manipulated variables $\mathbf{u}_{\mathrm{sp}}$, to the direct control layer. The values are taken at the end of the prediction horizon, allowing for the stabilization of the process and assuming a constant set point policy satisfying all variable and process constraints and ensuring that the computed set points are reachable, since the whole control sequence is evaluated.

$$\begin{aligned} \mathbf{y}_{sp} &= \hat{\mathbf{y}}(k+N_y \mid k) \\ \mathbf{u}_{sp} &= \mathbf{u}(k+N_u - 1 \mid k) \end{aligned} \tag{11}$$

When the D-RTO is included in the full hierarchical structure, the value of $J_{ss,o}$ is updated each T_{ss} to consider the optimization of the long term objectives by the upper static RTO. In the Dynamic RTO+NMPC structure, the $J_{ss,o}$ is a fixed value corresponding to the global optimum respect to the inputs average for the whole operation horizon.

Note that, either in the stationary or dynamic RTO, all the information concerning to the optimal operating point is used to update the process information in the subsequent layer. On the other hand, the different time scales considered in the problem make necessary the use of different sampling times for each layer, satisfying the following inequality:

$$T_{MPC} < T_{eco} < T_{ss} \tag{12}$$

The different hierarchical control structures that combining static and dynamic Real Time Optimization (RTO) and Non-linear Model Predictive Control (NMPC) technology are evaluated and compared in a systematic way in order to determine if it is worthwhile using them. The criteria for evaluating the advantages of the implementation of the different architectures are the tradeoff between economic benefit, process performance, and complexity of the control structure. The performance evaluation criteria is the indicated in the BSM1 protocol for WWTPs.

III. N-REMOVAL PROCESS DESCRIPTION AND CONTROL

Process description.

The most important Biological treatment in a WWTP is the nitrogen removal process (N-removal process). The goal is the elimination of nutrients and organic matter in the wastewater to reach the limits imposed by the environmental regulations. The activated sludge process (ASP) is commonly selected for the biological treatment. In the ASP, the organic matter is oxidized and the nitrification is achieved by the biological conversion of ammonium to nitrates in aerobic conditions. The denitrification process, that is the reduction of nitrates to nitrogen gas (N_2), occurs in anoxic conditions.

The typical values of effluent quality requirements imposed to WWTPs are shown in Table 1. The N-Removal process variables are presented in Table 2.

Table 1. Effluent Quality Requirements

Variable	**Bound**
*Total Nitrogen (Nt)***	< 22grN/m^3
Chemical Oxygen Demand ($COD_{,e}$)	<125 grCOD/m^3
Ammonium concentration ($S_{NH,e}$)	<4 grN/m^3
Nitrate concentration ($S_{NO,e}$)	<10 grN/m^3

**Real value 18 grN/m^3

Table 2. N-Removal process variables

Description	**Variable**
Readily biodegradable substrate concentration (gr COD/m3)	S_S
Active heterotrophic biomass concentration (gr COD/m3)	$X_{B,H}$
Active autotrophic biomass concentration (gr COD/m3)	$X_{B,A}$
Dissolved oxygen concentration (gr/m3)	S_O
Nitrate and nitrite concentration (gr N/m3)	S_{NO}
NH4+ + NH3 concentration (gr N/m3)	S_{NH}
Dissolved oxygen concentration (gr/m3)	S_O
Influent flow rate	Q_{in}
Organic matter concentration	$S_{S,in}$
Ammonium compounds concentration	$S_{NH,in}$
Internal recycle flow	Q_a
Oxygen transfer coefficient	KLa
Oxygen saturation concentration	$S_{O,sat}$

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Heterotrophic max. specific growth rate	μ_H
Half saturation coefficient for heterotrophs	K_s
Oxygen saturation coefficient for heterotrophs	$K_{O,H}$
Ammonia saturation coefficient for heterotrophs	K_{NH}
Oxygen saturation coefficient for autotrophs	$K_{O,A}$
Heterotrophic yield	Y_H
Autotrophic yield	Y_A
Nitrogen fraction in biomass	i_{XB}
Anoxic reactor volume	V_1
Aerobic reactors volume	V_2

Process model.

The WWTP process selected as a case study follows the specifications given in the Benchmark Simulation Protocol (BSM1) (Alex et al., 2008) which are widely accepted by the scientific community. However, the model focuses on the N-Removal process. The Benchmark Simulation Model (BSM1) has been widely applied to test control strategies for the Activated Sludge Process (ASP) in wastewater treatment plants. It consists of 5 bioreactors: 2 anoxic and 3 aerobic. In the simplified model considered in this work, only the significant variables of the BSM1 model on a medium time scale are taken into account. The processes with slow variations in time (the growth of autotrophic and heterotrophic microorganisms and hydrolyse processes) are neglected. The BSM1 representation is reduced to one anoxic and one aerated reactor as shown in Figure 5. The volumes of the two tanks are 2000m^3 and 3999m^3, to make them equivalent to total volumes of the anoxic and the aerobic compartments in the BSM1.

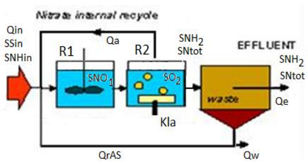

Figure 5.Schematic representation of the plant.

Thus, the biological processes considered in the model are described by the following equations:

$$\rho_{1i} = \mu_H \cdot \left(\frac{S_{Si}}{K_s + S_{Si}}\right) \cdot \left(\frac{S_{Oi}}{K_{O,H} + S_{Oi}}\right) X_{B,H} \quad (13)$$

$$\rho_{2i} = \mu_H \cdot \left(\frac{S_{Si}}{K_s + S_{Si}}\right) \cdot \left(\frac{K_{O,H}}{K_{O,H} + S_{Oi}}\right) \left(\frac{S_{NOi}}{K_{NO} + S_{NOi}}\right) n_g X_{B,H} \quad (14)$$

$$\rho_{3i} = \mu_A \cdot \left(\frac{S_{NHi}}{K_{NH} + S_{NHi}} \right) \cdot \left(\frac{S_{Oi}}{K_{O,A} + S_{Oi}} \right) X_{B,A} \tag{15}$$

where i:1,2. The index 1 refers to the anoxic tank and index 2 to the aerobic.

The differential equations describing the model are:

$$\frac{dS_{NH1}}{dt} = \frac{1}{V_1}\left[Q_{in} \cdot S_{NHin} + Q_a S_{NH2} - (Q_{in} + \cdot Q_a) \cdot S_{NH1}\right] - i_{Xb} \cdot \rho_{11} - i_{Xb} \cdot \rho_{21} - \left(i_{Xb} + \frac{1}{Y_A} \right) \cdot \rho_{31} \tag{16}$$

$$\frac{dS_{NO1}}{dt} = \frac{1}{V_1}\left[Q_a S_{NO2} - (Q_{in} + \cdot Q_a) S_{NO1}\right] - \frac{1-Y_H}{2.86 Y_H} \rho_{21} + \frac{1}{Y_A} \cdot \rho_{31} \tag{17}$$

$$\frac{dS_{S1}}{dt} = \frac{1}{V_1}\left[Q_{in} \cdot S_{Sin} + Q_a S_{S2} - (Q_{in} + \cdot Q_a) S_{S1}\right] - \frac{1}{Y_H} \rho_{11} - \frac{1}{Y_H} \rho_{21} \tag{18}$$

$$\frac{dS_{O1}}{dt} = \frac{1}{V_1}\left[Q_a \cdot S_{O2} - (Q_0 + Q_a) S_{O1}\right] - \left[\frac{1-Y_H}{Y_H} \rho_{11} + \left(\frac{4.57}{Y_A} + 1 \right) \rho_{31} \right] \tag{19}$$

$$\frac{dS_{NH2}}{dt} = \frac{1}{V_2}\left[(Q_{in} + \cdot Q_a) S_{NH1} - (Q_{in} + \cdot Q_a) S_{NH2} \right] - i_{xb} \cdot \rho_{12} - \left(ix_b + \frac{1}{Y_A} \right) \cdot \rho_{32} \tag{20}$$

$$\frac{dS_{NO2}}{dt} = \frac{1}{V_2}\left[(Q_{in} + \cdot Q_a) S_{NO1} - (Q_{in} + \cdot Q_a) S_{NO2}\right] - \frac{1-Y_H}{2.86 Y_H} \rho_{22} + \frac{1}{Y_A} \cdot \rho_{32} \tag{21}$$

$$\frac{dS_{S2}}{dt} = \frac{1}{V_2}\left[(Q_{in} + \cdot Q_a) S_{S1} - (Q_{in} + \cdot Q_a) S_{S2}\right] - \frac{1}{Y_H} \rho_{12} - \frac{1}{Y_H} \rho_{22} \tag{22}$$

$$\frac{dS_{O2}}{dt} = \frac{1}{V_2}\left[(Q_{in} + \cdot Q_a) \cdot S_{O1} - (Q_{in} + \cdot Q_a) \cdot S_{O2}\right] - \left[\frac{1-Y_H}{Y_H} \rho_{12} + \frac{4.57 - Y_A}{Y_A} \rho_{32} \right] + KLa\left(S_{O,sat} - S_{O2}\right) \tag{23}$$

The values of the kinetic and physical parameters are assumed to be the same as for BSM1 (Alex et al., 2008).

Influent profiles.

The different influent profiles of the Benchmark Simulation Model (BSM1) are used to study the effect of the multilayer structure over economics in the plant operation in this study. In this influent strong variations in the flow and concentrations are observed during the rain event and storm events. A long-term influent profile has been prepared. This input profile mixes different zones of the BSM1's rain weather and storm weather influent profiles. The first 10 days are characteristic of dry weather with normal influent flow and periods of reduced loads , a period of heavy rain occurs between the second and third week. The last ten days combine periods of storms with low influent flow.

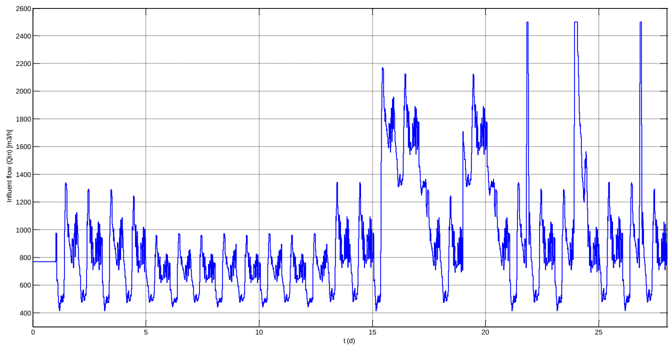

Figure 6. Long term influent flow profile for a 28 days operation horizon

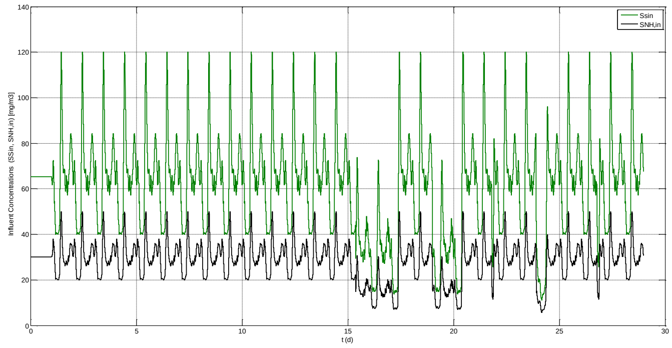

Figure 7. Long term influent concentrations profile for a 28 days operation horizon

For the two layer optimization strategies and for the controller performance evaluation, a portion of the influent profile that concentrates the most significant changes in the inputs (Figure 7) has been selected for simulations and it has been denominated short test influent.

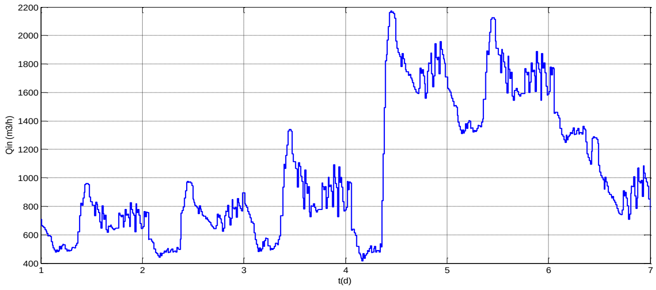

Figure 8. Short test influent profile.

Control problem

For an efficient N-removal in the activated sludge process, the typical controlled variables are the dissolved oxygen concentration in the aerated zone S_{O2} (DO) and the nitrate concentration in the anoxic zone S_{NO1}. The manipulated variables are: the internal recycle flow (Q_a) and the oxygen transfer coefficient (KLa). The disturbances are: the influent flow (Q_{in}), the organic matter concentration, ($S_{S,in}$) and the ammonium concentration ($S_{NH,in}$) in the influent.

The DO concentration in the aerobic zone should be sufficiently high to supply enough oxygen to the microorganisms in the sludge. However, high air flow rates can produce an excess in DO concentration in the aerobic zone that affect negatively the denitrification process through the internal recycle and increases unnecessarily the energy consumption. Hence, the control of the DO concentration is crucial for the satisfactory operation of the activated sludge process. In the denitrification process that takes place in the anoxic zone, the key variable is the nitrate concentration S_{NO1}.

Performance indices.

The performance assessment in BSM1 platform is made at two levels. The first level concerns the local control loops, assessed by ISE (Integral of the Squared Error) criteria. Basically, this serves as a proof that the proposed control strategy has been applied properly. The ISE is a classical index that it is used in process control to evaluate and to compare the control systems performance. In this study, it is desirable not only to minimize other objective functions but also to reduce the ISE. The second level performance assessment is concerned to the effluent quality index and the cost factors for operation given by pumping energy and aeration energy. It provides measures for the effect of the control strategy as such on plant performance (Alex et al., 2008).

The measures used to characterize the effluent quality and energy usage during the N-removal process are the standard performance indices recommended in the BSM1 platform for the evaluation of control strategies applied to WWTPs. The Effluent Quality Index (*EQ*) which integrates the total amount of pollutants for the process with different weights depending on their severity, the Aeration Energy (*AE*) and the Pumping Energy (*PE*) are applied in this work.

The Pumping Energy (*PE*) which represents the energy consumption due to pumping of the internal recycle, is given by:

$$PE = \frac{1}{T}\int_{t_0}^{tf}\left(0.004 \cdot Q_a(t)\right)dt \ \left[{kWh}/{d}\right] \tag{24}$$

The Aeration Energy (AE) is calculated from oxygen transfer coefficient (KLa) according to the following relation:

$$AE = \frac{S_{O,sat}}{T \cdot 1.8 \cdot 1000}\int_{t_0}^{tf}\sum_{k=1}^{k=5} V_k \cdot KLa_k(t)\,dt \ \left[{kWh}/{d}\right] \tag{25}$$

where k is the number of each reactor. It takes into account parameters such as the type of diffuser, bubble size, and depth of submersion.

The overall cost index (OCI) is a measure of the total cost related to energy consumption and sludge treatment. In the reduced N-Removal process describe here, the overall cost includes only the pumping energy and the aeration energy.

$$OCI = (PE + AE)\left[KWh/d\right] \tag{26}$$

The Effluent Quality is averaged over the period of compounds data that have a major influence on the quality of the receiving water:

$$EQ = C_1\int_{t_0}^{tf\,(days)}\begin{bmatrix} 2 \cdot SS_e + COD_e + 30 \cdot Nt \\ +10 \cdot S_{NO,e} + 2 \cdot BOD_e \end{bmatrix} Q_e dt \left[{Kg\ polution}/{d}\right] \tag{27}$$

where:

$$C_1 = \frac{1}{T \cdot 1000}$$

$$BOD_e = 0.25 \cdot \left((1-0.08)\left(X_{B,Ae} + X_{B,He}\right)\right) g/m^3 \tag{28}$$

$$COD_e = \left(S_{Se} + X_{B,Ae} + X_{B,He}\right) g/m^3 \tag{29}$$

$$Nt_e = S_{NOe} + S_{NHe} + i_{XB}\left(X_{B,He} + X_{B,Ae}\right) g/m^3 \tag{30}$$

$$SS_e = 0.75 \cdot \left(X_{S,e} + X_{I,e} + X_{B,H,e} + X_{B,A,e} + X_{P,e}\right) g/m^3 \tag{31}$$

The sub index e refers to the effluent discharge, where $S_{NHe}=S_{NH2}$, $S_{NOe}=S_{NO2}$, $S_{Se}=S_{S2}$. It is supposed that the separation in the settler produces: $X_{B,Ae}=0.0038 \cdot X_{B,A}$ and $X_{B,He}=0.0038 \cdot X_{B,H}$.

In this work, the violation of the constraints over ammonium compounds and total nitrogen discharges to the effluent are quantified by the following indices:

$$dev.NH = \int_{t_0}^{tf}\max\left(\left(S_{NH2} - S_{NH\max}\right), 0\right)dt \ \left[{mg}/{l}\right] \tag{32}$$

$$dev.Ntot = \int_{t_0}^{tf}\max\left(\left(S_{Ntot} - S_{Ntot\max}\right), 0\right)dt \ \left[{mg}/{l}\right] \tag{33}$$

The Integral Square Error (ISE) is a dynamic performance measure commonly used for evaluating control performance. It is calculated respect to the two controlled variables (S_{NO1} and S_{O2}) to evaluate the control performance.

$$ISE_{NO} = \int_{t_0}^{tf}\left(S_{NO1\_SP} - S_{NO1}\right)^2 dt \tag{34}$$

$$ISE_{SO}=\int_{t_0}^{tf}\left(S_{O2\_SP}-S_{O2}\right)^2 dt \quad (35)$$

where S_{NO1_SP} and S_{O2_SP} are the set point values that can be given by the user or an upper layer optimizer system.

In the following sections the proposed hierarchical control structures are compared to the basic NMPC strategy with a fixed set point

IV. Direct control Layer

In this section, details of the NMPC implementation in the direct control layer are presented as well as the evaluation of process performance when applying the basic control strategy in the presence of the disturbances given by the short test influent profile (Figure 7).

The general NMPC formulation for the direct control layer is given in eqs. (1) and (2) is applied here. Recall that the optimization problem solved at each T_{MPC} is:

$$\min_{\mathbf{u}(k+i);0\le i\le H_c-1} J_{MPC}(k)$$

where

$$J_{MPC}(k)=\left\|\mathbf{y}(k+H_p\,|\,k)-\mathbf{y}_{sp}\right\|_P^2+\sum_{i=1}^{H_p}\left(\left\|\mathbf{y}(k+i\,|\,k)-\mathbf{y}_{sp}\right\|_Q^2\right)+\sum_{i=0}^{H_c-1}\left(\left\|\mathbf{u}(k+i\,|\,k)-\mathbf{u}_{sp}\right\|_R^2+\left\|\Delta\mathbf{u}(k+i\,|\,k)\right\|_S^2\right) \quad (1)$$

In the case of the N-Removal process, the specific NMPC variables are:

$$\mathbf{y}=\begin{bmatrix}S_{NO1}\\ S_{O2}\end{bmatrix};\ \ \mathbf{u}=\begin{bmatrix}Q_a\\ KLa\end{bmatrix};\ \mathbf{y}_{sp}=\begin{bmatrix}S_{NO1ss}\\ S_{O2ss}\end{bmatrix};\ \mathbf{u}_{sp}=\begin{bmatrix}Q_{ass}\\ KLa_{ss}\end{bmatrix}$$

$$\mathbf{x}=\begin{bmatrix}S_{NH1} & S_{NO1} & S_{S1} & S_{O1} & S_{NH2} & S_{NO2} & S_{S2} & S_{O2}\end{bmatrix}$$

The bounds and model constraints are given by the process performance specifications, process limitations and treatment objectives. Constraints are imposed over some states and outputs as follows:

$$S_{NH2}(k+j\,|\,k)\le 4\ [mg/l] \qquad 1\le j\le H_p \quad (36)$$
$$N_{tot}(k+j\,|\,k)\le 30\ [mg/l] \qquad 1\le j\le H_p \quad (37)$$
$$0.1\le S_{O2}(k+j\,|\,k)\le 8\ [mg/l] \quad 1\le j\le H_p \quad (38)$$
$$COD(k+j\,|\,k)\le 100\ [mg/l] \qquad 1\le j\le H_p \quad (39)$$
$$BOD(k+j\,|\,k)\le 10\ [mg/l] \qquad 1\le j\le H_p \quad (40)$$
$$0\le KLa\,(k+j\,|\,k)\le 3.5\left[h^{-1}\right] \qquad 0\le j\le H_c-1 \quad (41)$$
$$0\le Q_a(k+j\,|\,k)\le 3850\left[m^3/h\right] \qquad 0\le j\le H_c-1 \quad (42)$$

The bound of N_{tot} in eq. (37) was relaxed after a sensitivity study, because the value indicated in Table 1 was difficult to meet with this simplified model.

Implementation.

The NMPC control performance has been evaluated first considering a fixed set point for tuning purposes. That economical steady state optimum is calculated by solving the steady state problem for the average valued of Q_{in}, $S_{S,in}$ and $S_{NH,in}$ from the BSM1 dry weather influent (Alex et al., 2008). The optimum for ***u:*** ***(****Q_{ass}*, *KLa_{ss}****)*** produces the optimum set points for ***y:*** *(S_{NO1}* and *S_{O2})*. The values of the optimum working point are: Q_{ass}=408 m^3/h, KLa_{ss}=3.87 1/h, S_{NO1ss}=1.67 mg/l and S_{O2ss}=2.38 mg/l.

The NMPC algorithm uses the phenomenological model of the plant described in eqs. (16)-(23) for predictions. The *fmincon* method of Matlab® based on Sequential Quadratic Programming (SQP) is used for the optimization carried out each sampling time (T_{MPC}) to obtain the optimal manipulated variables.

For simplicity a control horizon *Hc*=1 is chosen, the prediction horizon is between *Hp* = 10 and *Hp* = 25, selecting *Hp* = 25 for the tests, and the sampling time is T_{MPC}= 0.0104 d. After the tuning procedure, the selected parameters for the NMPC controller are *Q*=[1 0; 0 1] and *S*=[0.001 0; 0 50].

A sequential optimization technique is used to reduce the impact of the infeasible points in the controller performance. The NMPC law is solved first considering the constraints given by ineqs. (36)-(42), if an infeasible solution is found, the optimization is repeated considering a relaxing factor (*rf*) in the ammonium constraint (NMPC-*rf*).

$$S_{NH2}\left(k+j\,|\,k\right) \le rf \cdot 4\ [mg/l] \qquad 1 \le j \le H_p \tag{43}$$

If the optimization fails at all, the value of the manipulated variables obtained in the previous optimization is used.

The sequential optimization technique was tested with constant and variable relaxing factors. In the simulation of plant response during 7 days with the typical NMPC, following an constant set point 6% of infeasible solutions are observed. It is reduced to 0.5% with a relaxing factor *rf*=2 and none infeasible solution are observed with relaxing factor *rf*=4. Variable relaxing factors introduced noise in the response. Therefore, *rf=4* is selected for the direct control layer NMPC.

V. Optimal Operation Strategies applied to N-Removal Process

In this section is described the implementation of the optimal operation strategies presented in section II particularized to the Activated Sludge Process.

Case 1. Static RTO+NMPC

The first strategy proposed to achieve the optimal operation of the plant is the Static Real Time Optimization (RTO) combined with a NMPC in the direct control layer as described in eqs. (4)-(7). Its application to the N-Removal process is illustrated in Figure 9.

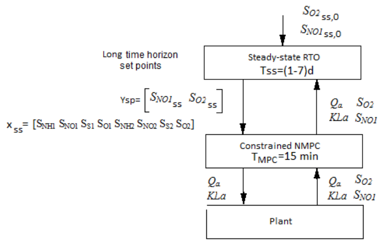

Figure 9. Static RTO + NMPC structure applied to WWTP.

A static RTO is performed in the upper layer to calculate the set points sent to the lower layer considering different economic and performance objectives. Since the plant is under high frequency disturbances it is not possible to achieve a real steady state condition for such variable input profiles. Therefore, it is defined an operating window in a range of time that varies from days to hours (T_{ss}) and the average values of the inputs in that period is considered for approaching the stationary values of the states corresponding to the set points. In the direct control layer, the NMPC receive the optimal set points and compute the control signals for the appropriated set point tracking

Formulation of the Static Optimization problem for the N-removal process

The set point optimization is formulated in the upper layer to find the steady state working point (equilibrium point) that minimizes the energy costs given by the steady state Pumping Energy (PE_{ss}) and Aeration Energy (AE_{ss}) while ensuring the best possible performance of the plant. Therefore, the Effluent Quality (EQ_{ss}) index can be introduced in the objective function and the effluent requirements are introduced as constraints. The decision variables are KLa_{ss} and Q_{ass}, they are used to calculate the S_{NO1} and S_{O2} values in steady state each T_{ss} for the average values of the input variables Q_{in}, $S_{S,in}$ and $S_{NH,in}$ in the horizon given by T_{ss}.

The steady state value of all variables (manipulated, outputs and indexes) is denoted with the sub index *ss*. The optimization problem is stated as:

<u>*Objective function.*</u>

$$\min_{Q_{ass},\mathrm{KLa}_{ss}} J_{ss} \tag{44}$$

where

$$J_{ss} = w_1 \cdot (PE_{ss} + AE_{ss}) + w_2 \cdot EQ_{ss} + w_3 \cdot \alpha_1 + w_4 \cdot \alpha_2 \tag{45}$$

The weights w_i (i:1,..,4) can be modified to evaluate different objectives, and the terms α_1 and α_2 are included in the cost function to represent the fines for discharges which exceed the effluent quality limits.

$$\alpha_1 = \begin{cases} \alpha\left(S_{NH2} - S_{NH2\max}\right) & if \quad S_{NH2} > S_{NH2\max} \\ 0 & if \quad S_{NH2} \le S_{NH2\max} \end{cases} \tag{46}$$

$$\alpha_2 = \begin{cases} \alpha\left(S_{Ntot} - S_{Ntot\max}\right) & if \quad S_{Ntot} > S_{Ntot\max} \\ 0 & if \quad S_{Ntot} \le S_{Ntot\max} \end{cases} \tag{47}$$

The Pumping Energy (PE_{ss}), Aeration Energy (AE_{ss}) and Effluent Quality (EQ_{ss}) in steady state are calculated as:

$$PE_{ss} = 0.004 \cdot Q_{a,ss} \; \left[{}^{kWh}\!/_{d}\right] \tag{48}$$

$$AE_{ss} = \frac{S_{O,sat}}{1.8 \cdot 1000} \cdot V_2 \cdot K_{La,ss} \; \left[{}^{kWh}\!/_{d}\right] \tag{49}$$

$$EQ_{ss} = \frac{1}{1000}\begin{bmatrix} 2 \cdot SS_{ss,e} + COD_{ss,e} + 30 \cdot Nt_{ss} \\ +10 \cdot S_{NOss,e} + 2 \cdot BOD_{ss,e} \end{bmatrix} Q_{ss,e} \left[{}^{Kg}\!/_{d}\right] \tag{50}$$

where $SS_{ss,e}$, $COD_{ss,e}$, $N_{tss,e}$, $S_{NOss,e}$, $BOD_{ss,e}$, are obtained from equations (28)-(31) with steady state values of concentrations.

Process constraints.

The optimization constraints are given by the effluent regulations and process characteristics. They are evaluated in the steady state for the following bounds:

$$S_{NH2,ss} \le 4\,[mg/l] \tag{51}$$

$$S_{Ntot,ss} \le 22\,[mg/l] \tag{52}$$

$$S_{O2,ss} \le 8\,[mg/l] \tag{53}$$

$$S_{O2,ss} \ge 1.5\,[mg/l] \tag{54}$$

$$0 \le KLa_{ss} \le 3.5\,[1/h] \tag{55}$$

$$0 \le Q_{a,ss} \le 3850\;[m^3/h] \tag{56}$$

$$COD_{ss,e} \le 100\,[mg/l] \tag{57}$$

$$BOD_{ss,e} \le 10\,[mg/l] \tag{58}$$

$$EQ_{ss\max} \le EQ_{\max}[\mathrm{K}\,g/\mathrm{d}] \tag{59}$$

The optimisation problem is solved in order to obtain the stationary working point: KLa_{ss}, Qr_{ss}, S_{O2ss} and S_{NO1ss} containing the manipulated variables and oxygen and nitrates set points that optimize the cost function given in eq. (45). The optimal values of the indices OCI_{ss} and EQ_{ss} are passed to the subsequent layer as targets included in $J_{ss,o}$.

Case 2. Dynamic RTO +NMPC

In this scheme, an NMPC in the upper layer computes dynamically, as described in eqs. (8)-(11), the optimal set points that are sent to the immediately lower layer as shown in figure 10.

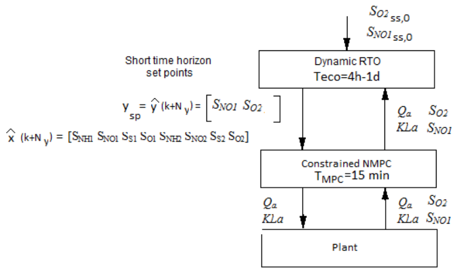

Figure 10.Dynamic RTO + NMPC structure applied to WWTP.

The predictions of the dynamical response of the plant in a time horizon N_y are used to calculate the corresponding performance indices. The problem is stated as the minimization of a cost function J_{eco} with respect to a vector $\boldsymbol{u}$ containing Qr and KLa and the resulting outputs y_{SP} (S_{NO1} and S_{O2}). For obtaining the corresponding optimum set points, the discretized system is simulated with those inputs, and the set points are chosen as:

$$\mathbf{y}_{sp} = \begin{pmatrix} S_{NO1}\left(k+N_y \mid k\right) \\ S_{O2}\left(k+N_y \mid k\right) \end{pmatrix} \tag{11}$$

Formulation of the Dynamic Optimization problem for the N-removal process

<u>Objective function:</u>

The optimization problem for this layer is, at a sampling time k

$$\min_{\mathbf{u}(k+i);0\le i\le N_u-1} J_{eco}(k) \tag{60}$$

where

$$J_{eco}(k) = w_1 \cdot \left(AE\left(\mathbf{u}(k+i \mid k)\right) + PE\left(\mathbf{u}(k+i \mid k)\right)\right) + w_2 \cdot EQ\left(y\left(k+N_y \mid k\right)\right) - J_{ss,o} \tag{61}$$

$$0 \le i \le N_u - 1$$
$$1 \le j \le N_y$$

Note that in this work the control horizon has been selected here as N_u=1, therefore the manipulated variables are kept constant for the rest of the prediction horizon:

$$\mathbf{u}(k+i \mid k) = \mathbf{u}(k \mid k) \quad 1 \le i \le N_y$$

The indexes AE, PE and EQ are calculated discretizing the integrals of (24)-(27), with a discretization time of T_{eco} corresponding to the NMPC of this intermediate layer, and using as starting values the values of the previous sampling time. Then, the values considered in the cost function J_{eco} are the final value of the performance indexes iterating in the following equations N_y times ($0 \le j \le N_y - 1$), that represent the average values in the prediction horizon:

$$PE(k+j+1|k) = PE(k+j|k) + \frac{1}{N_y \cdot T_{eco}} \cdot 0.004 \cdot Q_a(k+j|k) \cdot T_{eco} \left[{kWh}/{d} \right] \quad (62)$$

$$AE(k+j+1|k) = AE(k+j|k) + \frac{1}{N_y \cdot T_{eco}} \cdot \frac{S_{O,sat}}{1.8 \cdot 1000} \cdot V_2 \cdot K_{La}(k+j|k) \cdot T_{eco} \left[{kWh}/{d} \right] \quad (63)$$

$$EQ(k+j+1|k) = EQ(k+j|k) + \frac{1}{N_y \cdot T_{eco}} \cdot \frac{1}{1000} \begin{bmatrix} 2 \cdot SS_e(k+j|k) \\ +COD_e(k+j|k) \\ +30 \cdot Nt_e(k+j|k) \\ +10 \cdot S_{NOe}(k+j|k) \\ +2 \cdot BOD_e(k+j|k) \end{bmatrix} Q_e(k+j+1|k) \cdot T_{eco} \left[{Kg}/{d} \right] \quad (64)$$

where SS_e, COD_e, N_{te}, S_{NOe}, BOD_e, are obtained from equations (28)-(31).

The outputs and states needed for calculation of (60) are obtained using the nonlinear prediction model of the process.

Process constraints.

The optimization constraints are given by the effluent regulations and process characteristics. They are evaluated in the steady state for the following bounds:

$$S_{NH2}(k+j|k) \le 4\ [mg/l] \qquad 1 \le j \le N_y \quad (65)$$

$$N_{tot}(k+j|k) \le 22\ [mg/l] \qquad 1 \le j \le N_y \quad (66)$$

$$0 \le KLa\,(k+j|k) \le 1.5\,[h^{-1}] \qquad 0 \le j \le N_u - 1 \quad (67)$$

$$0 \le Q_a(k+j|k) \le 3850\,[m^3/d] \qquad 0 \le j \le N_u - 1 \quad (68)$$

$$0.1 \le S_{O2}(k+j|k) \le 8\ [mg/l] \quad 1 \le j \le N_y \quad (69)$$

$$COD(k+j|k) \le 100\ [mg/l] \qquad 1 \le j \le N_y \quad (70)$$

$$BOD(k+j|k) \le 10\ [mg/l] \qquad 1 \le j \le N_y \quad (71)$$

$$EQ(k+j|k) \le EQ_{max}\,[Kg/d] \quad 1 \le j \le N_y \quad (72)$$

Preliminary Results

Some preliminary tests to select critical parameters as the cost function weights in the different optimizations and the best sampling for each layer have been carried out using the short influent profile shown in figure 8.

First, a study of the sensitivity of the performance indicators regarding the different optimization objectives has been carried out. The static set point optimization is executed with different weights in the objective function (eq. 44) in order to observe the sensibility of the results to changes in these parameters. The evolution of the performance indices considering the short influent profile as the input to WWTP are shown in table 3. The optimization was carried out each 8 hours ($T_{ss}=8$).

Table 3. Evaluation of the effect of different weights in the objective function with the Static RTO +NMPC strategy (Tss=8)

	w_1=1, w_2=2	w_1=1	w_3=1000, w_4=500	w_2=2 w_3=1000,w_4=500
OCI (EUR/d)	1412.1	1384.6	1759.5	2034.0
PE (Kwh/d)	89.62	90.70	110.13	108.31
AE(Kwh/d)	1322.5	1293.9	1649.4	1925.6
EQ (Kg/d)	7582.8	7739.0	7350.5	7335.8
Desv. NH	2.117	3.55	0.801	0.917
DesvNtot	0.828	1.283	0.749	0.757
ISE_{SO}	0.174	0.344	0.206	0.126
ISE_{NO}	0.336	1.131	0.129	0.350

It can be noticed that accounting only energy costs in the objective function ($w_1=1$, $w_2=0$) leads to operating conditions with the minimun costs and acceptable effluent quality characteristics. The addition of a term ($w_1=1$, $w_2=2$) to penalize the Effluent Quality index (EQ) produce a solution with an slight increase in the costs (OCI) but improved EQ. If only the fines that penalize discharges over allowed limits of S_{NH2} and S_{Ntot} are taken into account for the calculation of the optimal set points ($w_3=1000$, $w_4=500$) an important increase in the overal costs is observed. It rises when considering the fines and the EQ together ($w_2=2$, $w_3=1000$, $w_4=500$). This behaviour evidence a trade off between the objectives related to the energy costs and those related to the effluent quality in the set point optimization.The evolution of the OCI and EQ indices in Figures 11 and 12 respectively illustrates this effect.

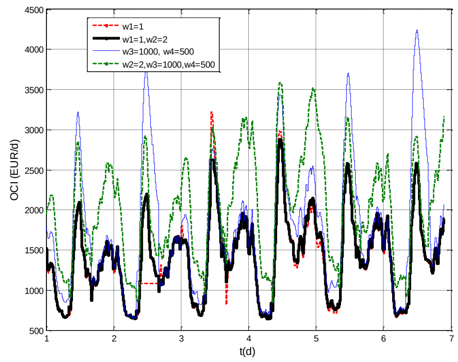

Figure 11. Static RTO +NMPC. OCI index evolution with different weights of the objective function (T_{ss}=8)

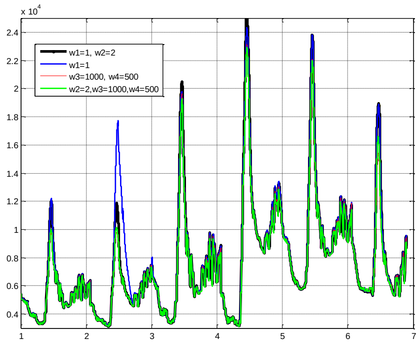

Figure 12. Static RTO +NMPC. EQ index evolution with different weights of the objective function (T_{ss}=8)

The response of the controlled variables y_{SP} (S_{NO1} and S_{O2}) and the evolution of the constrained variables (S_{NH2} and S_{Ntot}) static RTO+ NMPC structure with an objective function with $w_1=1$, $w_2=2$ is shown in figures 13 to 16. A T_{ss}=8h is selected to test the performance of the structure in the presence of continuous set point changes. Good tracking of the direct NMPC is observed in spite of the frequent changes of set point and the strong variations in the loads due to the rain events. It is observed that the concentrations S_{NH2} *and* S_{Ntot} are below the limits most of the simulation time, however, the peaks in the input flow rate produces constraints violations.

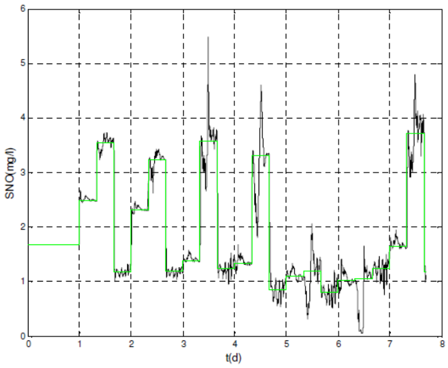

Figure 13. Static RTO +NMPC -Nitrate concentration (S_{NO1}) in the anoxic tank (T_{ss}=8).

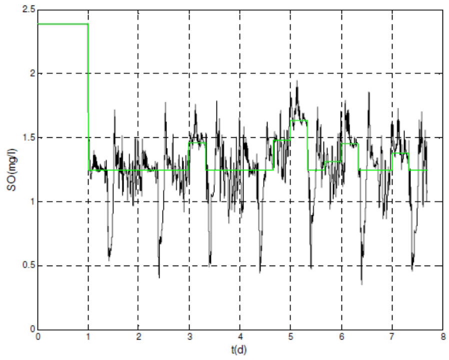

Figure 14. Static RTO +NMPC. Oxygen (S_{O2}), concentration in the aerobic tank (T_{ss}=8).

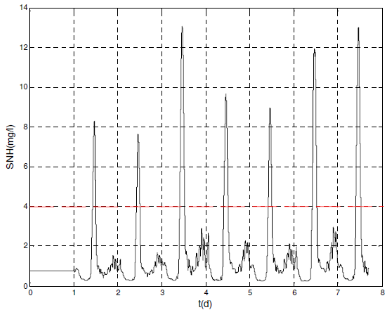

Figure 15. Static RTO +NMPC. Ammonium concentration (S_{NH2}) in the effluent (T_{ss}=8).

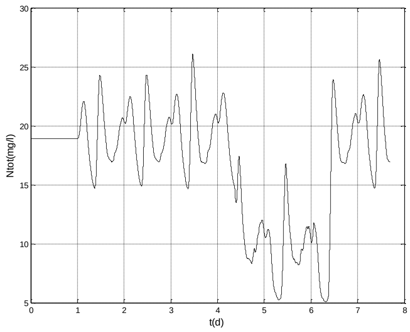

Figure 16. Static RTO +NMPC. Total Nitrogen (S_{Ntot}) in the effluent (T_{ss}=8).

The dynamic RTO + NMPC strategy is evaluated also with weights $w_1=1$, $w_2=2$ in the objective function. In figures 17 and 18 are presented the controlled variables y_{SP} (S_{NO1} and S_{O2}) and the evolution of the constrained variables (S_{NH2} and S_{Ntot}) in figures 19 and 20. An acceptable disturbance rejection and good tracking is observed. The set point changes calculated dynamically are softer than those obtained with the Static RTO but produce a similar impact in the economic, therefore, this strategy seems to be effortless in terms of control movements.

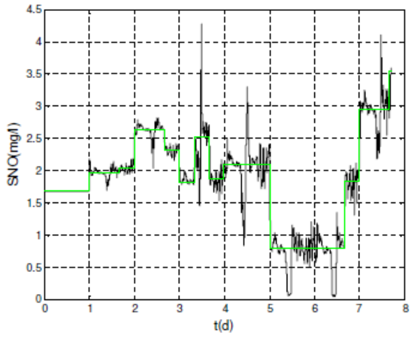

Figure 17. Dynamic RTO +NMPC -Nitrate concentration (S_{NO1}) in the anoxic tank (T_{eco}=8).

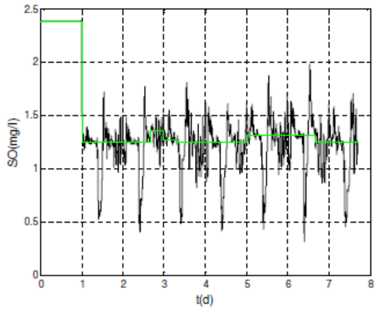

Figure 18. Dynamic RTO +NMPC. Oxygen (S_{O2}), concentration in the aerobic tank (T_{eco} =8).

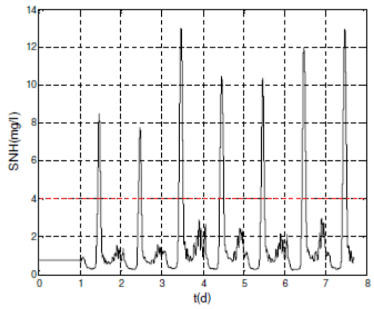

Figure 19. Dynamic RTO +NMPC. Ammonium concentration (S_{NH2}) in the effluent (T_{eco} =8).

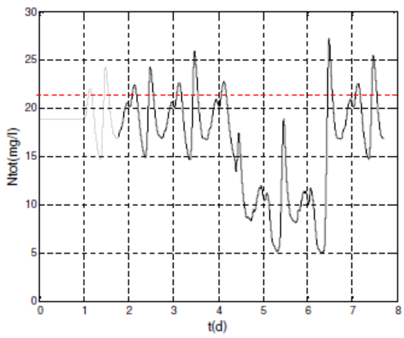

Figure 20. Dynamic RTO +NMPC. Total Nitrogen (S_{Ntot}) in the effluent (T_{eco}=8).

In order to compare the economic efficiency of the proposed strategies, the performance of the plant with the hierarchical strategies is compared with fixed set point operation in terms of the overall cost index, effluent quality and ISE. The evolution of the Overall Cost Index (OCI) in the whole operation horizon (T_{ss}=T_{eco}=8 hours) is presented in Figure 21. The performance indices are reported in Table 4.

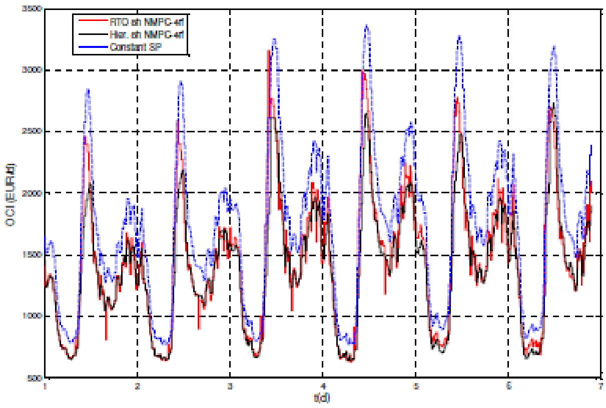

Figure 21. OCI index evolution with hierarchical strategies and constant set point (T_{ss}=T_{eco}=8 hours)

The hierarchical strategies are superior to fixed sep point operation in terms of economics in this particular case study the OCI index. Comparing Static and Dynamic RTO, the last one exhibits the best economic performance. In figure 21 the OCI index corresponding to the Dynamic RTO structure operation is below the others in most of the operation horizon. According to the indices shown in Table 9, a 19.4% saving in the operational cost (OCI) is achieved, mainly related to a significant reduction in the aeration energy. An improvement in the effluent quality (EQ) with hierarchical strategies is observed also. However, the control performance indices (ISE) get worse due to the continuous changes in the set points.

Table 4. Comparison of Performance Indices obtained with the different strategies: constant set point, Static RTO +NMPC and Dynamic RTO +NMPC optimization (T_{eco}=T_{ss}=8h).

	Fixed SP	Static	Dynamic
OCI (EUR/d)	1734.8	1412.1	1397.5
PE (Kwh/d)	84.87	89.62	82.95
AE(Kwh/d)	1649.9	1322.5	1314.6
EQ (Kg/d)	7734.8	7582.8	7680.2
Desv. NH	0.79	2.117	2.619
DesvNtot	0.74	0.828	0.216
ISE_{SO}	0.086	0.174	0.195

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ISE_{NO}	0.078	0.336	0.283

Another important aspect in the implementation of the hierarchical structure is the selection of the frequency to update the set points. The performance of the hierarchical structures considering different sampling times (T_{ss} and T_{eco}) is evaluated, the results are presented in table 5.

Table 5. Performance indices for different optimization sampling times (Topt) with the Static RTO +NMPC strategy

	Static RTO			Dynamic RTO			
	1d	8h	4h	1d	8h	6h	4h
OCI (EUR/d)	1402.6	1412.1	1428.5	1420.1	1397.5	1435.3	1401.1
PE (Kwh/d)	96.69	89.62	87.01	89.45	82.95	120.48	89.2
AE(Kwh/d)	1305.9	1322.5	1341.5	1330.6	1314.6	1314.8	1312.1
EQ (Kg/d)	7662.5	7582.8	7657.0	7515.3	7680.2	7574.2	7596.6
Desv. NH	2.669	2.117	2.462	2.781	2.619	2.048	2.179
DesvNtot	1.120	0.828	0.702	0.245	0.216	0.679	0.683

According to the information presented in table 6. In the time horizon considered (1d-4h) the sampling time variations seems to have a low effect over the Overall Costs. It is possible that the process is slow enough to satisfy the steady state assumption in the static RTO, even with T_{ss}=4h. The dynamic RTO with T_{eco}=8h is the best option in terms of economy. Computationally, performing RTO each 4h is inefficient.

In the next section, a more interesting scenario for the application of the hierarchical multilayer structures to the N-Removal is presented. The long term scenario, with a long horizon influent profile exhibiting seasonal variations, rain and storm events is studied.According to the results of the preliminary tests, w_1=1 and w_2=2 as well as T_{eco}=8h are selected for the dynamical optimization in the dynamic RTO+NMPC and the full hierarchical estructure.

VI. FULL HIERARCHICAL CONTROL STRUCTURE AND LONG TERM PERFORMANCE EVALUATION

A long-term influent profile (Figures 6 and 7) has been prepared to study the effect of the proposed multilayer structures over economics in the plant operation.

Formulation of the Full Hierarchical Optimization problem for the N-removal process

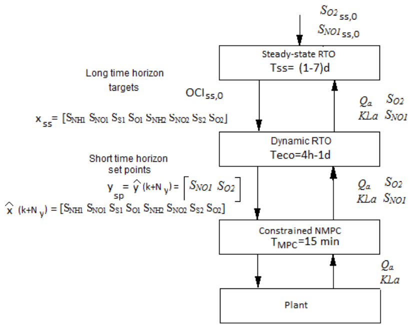

Figure 22.Full hierarchical structure applied to WWTP.

The full hierarchical strategy implemented to the N-Removal process is represented in Figure22. In the upper layer, the static RTO described in eqs. (44)-(59) is performed to update the process working point regarding long time horizon disturbances. The weights for the objective function given in eq. (44) are w_1=1, $w2$=0, $w3$=0, $w4$=0. The sampling time is T_{ss}=3d, it correspond to the different seasons in the influent profile. The optimization is carried out to obtain the optimum steady state operating point in T_{ss} and, in this particular implementation the optimal OCI value is passed as a target to the Dynamic RTO in the subsequent layer.

In a second layer, the dynamic RTO described in eqs. (60)-(72) is carried out to capture the medium to fast dynamics, considering the OCI target received from the upper layer each T_{eco}. The weights for the objective function (eq. 61) are w_1=1, $w2$=0 and T_{eco}=8h. In the direct control NMPC is used to track those set points and to reject the faster disturbances.

In Table 7, the performance indices for all the proposed strategies: Static RTO +NMPC, Dynamic RTO +NMPC and full hierarchical structure are compared in terms of economic performance and effluent quality. All the proposed hierarchical strategies produce a reduction of the overall cost index (OCI) with respect to the constant set point operation, in particular, the combination dynamic RTO with NMPC decreases de the OCI in 19%. Consequently, an slightly loss in the effluent quality is observed, the EQ increase around 4.7% and the ammonium discharges increase also. Nevertheless, these results demonstrates that Real Time Optimization can be useful for improving the economic operation of WWTPs with minimum losses in product quality.

Regarding the temporal decomposition, both dynamical and static RTO were effective to capture the slow and fast dynamics of disturbances in their corresponding time horizon .The static RTO exhibits the best economic performance (19% reduction in OCI) with respect to the other set point optimization strategies. However, the full hierarchical structure offers the best compromise between economy and effluent quality, with the second best OCI (17.2%) but the best EQ and ammonium discharges. In this particular case, it is possible to think that the benefits achieved do not compensate the increase of complexity of the control system. However, in the model of the WWTP used in this work the slow dynamics are simplified.
The good results obtained indicate that the full hierarchical structure can be a potential solution for the control WWTPs when exhibiting their whole dynamics.

The responses and control signal of the plant applying the full hierarchical strategy are shown in Figures 22 to 28.

Table 6. Evaluation of the performance of the multilayer hierarchical strategies.

	Full structure	Static RTO	Dynamic RTO	Constant SP
OCI (EUR/d)	1432.9	1405.0	1438.2	1729.0
PE (Kwh/d)	94.39	72.67	104.65	72.01
AE(Kwh/d)	1338.6	1332.3	1333.4	1657.0
EQ (Kg/d)	7102.9	7197.9	7139.8	6870.7
DesvNH4	12.23	16.25	13.37	5.95
DesvNtot	5.50	6.78	6.01	5.92
ISESO	1.01	1.38	1.16	0.63
ISENO	0.94	1.40	0.89	0.79

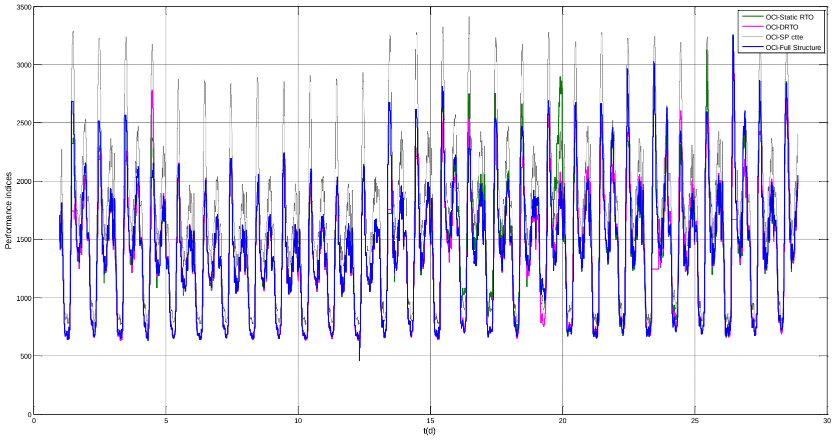

Figure 23. OCI index evolution with hierarchical strategies and constant set point in the long term scenario (Tss=3d/Teco=8 hours).

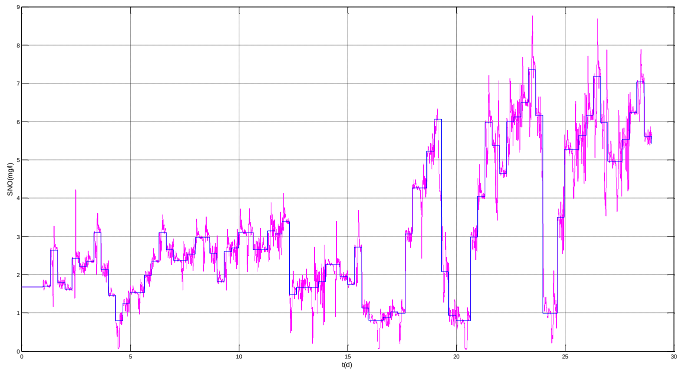

Figure 24.Full Hierarchical Structure. Nitrate concentration (SNO1) in the anoxic tank.

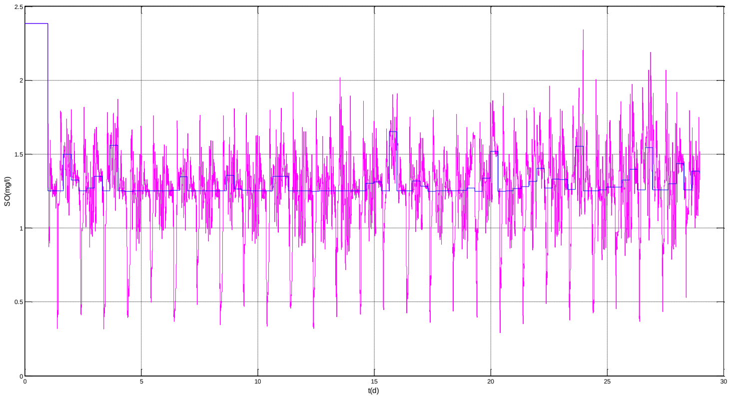

Figure 25. Full Hierarchical Structure. Oxygen (SO2), concentration in the aerobic tank.

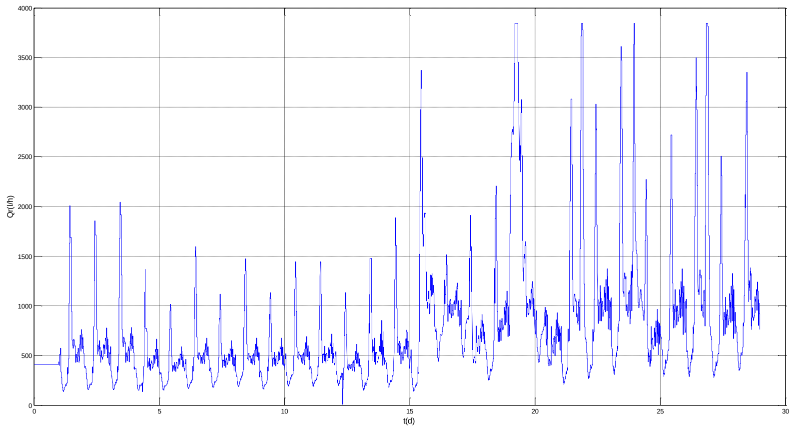

Figure 26. Full Hierarchical Structure. Control signal. Internal recycle flow (Qa)

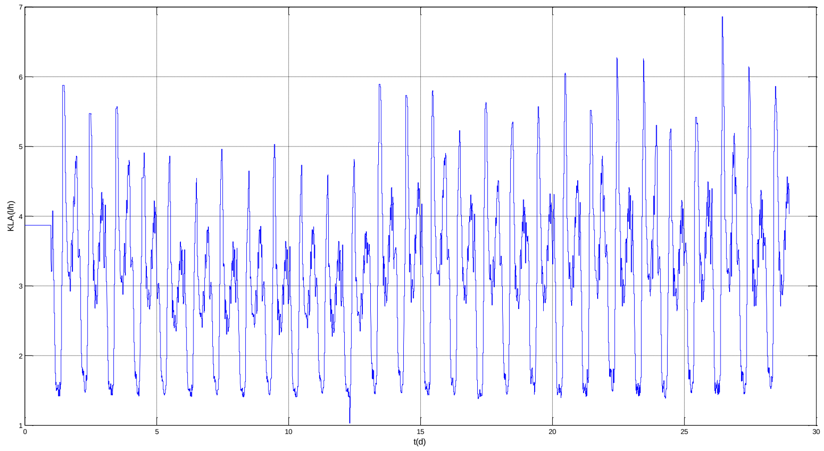

Figure 27. Full Hierarchical Structure. Control signal for the oxygen transfer coefficient (KLa)

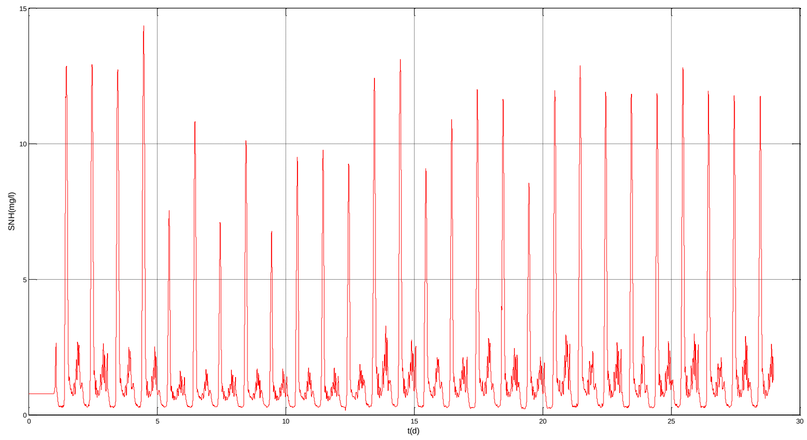

Figure 28. Full Hierarchical Structure. Ammonium concentration (SNH2) in the effluent.

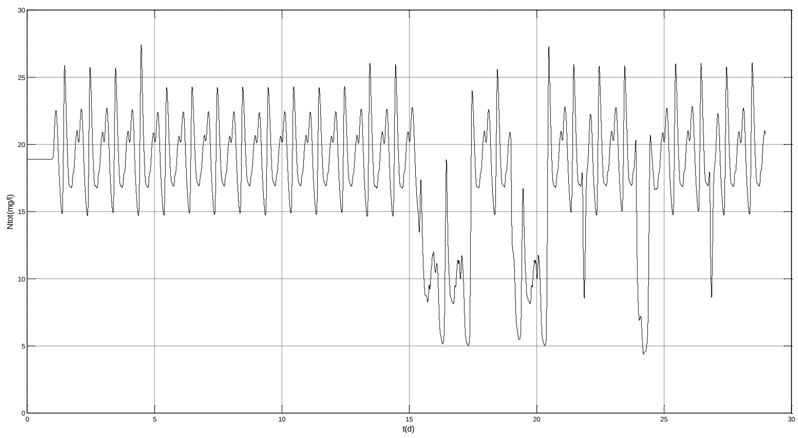

Figure 29. Full Hierarchical Structure. Total Nitrogen (SNtot) in the effluent.

This study demonstrate the advantages of the implementation of Real Time Optimization Strategies integrating NMPCs in hierarchical control structures for improving the operation of WWTPs. This strategies update the process operation conditions to optimal values, in agreement to the disturbances in the influent, even though, those occurs in different time scales. In this particular case, the implementation of hierarchical strategies allows for energy savings in the WWTPs while attaining the desired product quality. The non linear prediction model provides a good representation of the process behavior and constraints with a reasonable computational effort. The regulatory NMPC achieves an excellent disturbance rejection and an accurate tracking of the set point trajectories at the same time as it ensures the satisfaction of the process constraints.

VII. CONCLUSION

In this paper, a benchmarking of different hierarchical control strategies applied to the N-Removal process in a WWTP is presented. The strategies drive the plant to the economically optimal operating condition in spite of strong disturbances in the influent and they capture the multi-scale dynamics of disturbances. Their performances have been compared in different operating scenarios and conditions in order to demonstrate the advantages that the implementation of these advanced control strategies can produce in terms of economy and process performance.

A NMPC has been implemented in the direct control layer exhibiting an excellent performance in the presence of strong disturbances with different time scales. The integration of the regulatory NMPC to the Static or Dynamic set point optimization layers have been satisfactory, exhibiting fast response and accurate set point tracking as well as appropriately accommodating the process constraints in the control algorithm. In the dynamic RTO the NMPC provides a good representation of the dynamic response of the plant to provide cost-efficient set points with no modeling mismatch with respect to the regulatory layer.

The application of the proposed hierarchical control strategies produces a reduction of approximately 20% in the operational costs together with a satisfactory compromise with regard to Effluent Quality in the short term operation scenario as well as in the case of the long term operation scenario where seasonal variations affect the optimization results. In this case study, the dynamical RTO in the upper layer combined with a NMPC in the regulatory layer is the best option in terms of economy, effluent quality and complexity of the structure.

ACKNOWLEDGMENTS

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