Simultaneous Synthesis, Design and Control of Processes Using Model Predictive Control

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Abstract: This work presents the simultaneous synthesis, design and control of an activated sludge process using a Multivariable Model-based Predictive Controller (MPC). The process synthesis and design are carried out simultaneously with the MPC tuning to obtain the most economical plant which satisfies the controllability indices that measure the control performance ($H\infty$ and l1 norms of different sensitivity functions of the system). The mathematical formulation results into a mixed-integer optimization problem with non-linear constraints that is solved using a real coded genetic algorithm. The solutions reflects the effect of applying different bounds over the controllability norms. The results are encouraging for the development of integrated design approaches with advanced control schemes which usually results in complex optimization problems difficult to solve with conventional techniques.

Keywords: Process Design, Controllability indices, Model Based Predictive Control, Genetic Algorithms.

1. INTRODUCTION

The fact that the incorporation of controllability issues at the early stage of process design improves the dynamical behaviour of the plants have motivated the development of different methodologies to deal with the simultaneous process and control system design as Kookos and Perkins (2001), Revollar et al. (2004), Sakizlis et al (2004), Francisco et al. (2005) and more recently Tlacuahuac-Flores and Biegler (2007) and Tlacuahuac-Flores and Biegler (2008).

The simultaneous process and control system design leads to a non linear optimization problem where economic objectives, operability specifications and control performance are considered. The most comprehensive applications contemplate, also, the process synthesis or the control structure selection resulting into a mixed-integer-non-linear optimization problem (MINLP). The controllability analysis might require the evaluation of dynamic performance indices, which translates the problem into a mixed-integer-dynamical optimization (MIDO).

Even thought, the contribution in the field of integrated design is considerable, most of the approaches use conventional PID controllers. Only few works (Sakizlis et al., 2003; Sakizlis et al., 2004; Francisco and Vega, 2006) have been addressed to the application, in the integrated design, of advanced control techniques as Model-Based Predictive Controllers (MPC). The reason is that the advanced control schemes involve solving an optimization problem on-line, leading to a drastic increase in the complexity of the design framework (Sakizlis, et al, 2003; Sakizlis, et al, 2004).

Model based predictive control (MPC or MBPC) makes use of a process model to calculate the optimal control law. The MPC have been mainly accepted due to its natural way of incorporating operating constraints in multivariable process and the successful results in industrial applications (Maciejowsky, 2002; Qin and Badgwell, 2003). The shortcomings of conventional control schemes can be overcome by pursuing an advanced model-based predictive control (MPC) scheme (Sakizlis et al, 2003).

There are several strategies to deal with automatic tuning of MPC based on optimization of dynamical performance index (Ali et al., 1993; Francisco et al, 2005; Li and Du, 2002) but its evaluation requires time-consuming dynamical simulations which is an important drawback of these methodologies. Vega et al (2007) proposed the use of frequency domain methods as controllability indexes to speed up the MPC automatic tuning procedure by solving a mixed sensitivity problem with constraints. It avoids dynamical simulations but the use of linearized models, caused some problems of stability and robustness in the presence of nonlinearities and load disturbances on the process.

The aim of this work is to perform the integrated synthesis and design of a process using model-based predictive controllers (MPC) that will be tuned automatically using the strategy proposed by Vega et al (2007). The activated sludge process of the Manresa's plant was selected to apply the integrated design methodology as has been done in previous work using a conventional PI control technique (Revollar, et al., 2004, Revollar, et al., 2005). Francisco and Vega (2006) applied advanced control techniques for the integrated design of the mentioned plant, but the structure selection was not taken into account in the problem formulation.

The main difficulty for solving the problem is the existence of continuous process and MPC variables, integers for the prediction and control horizon and binary variables for the structural decisions, which leads to a complex mixed integer non linear optimization problem. Therefore, it is necessary the use of advanced algorithms that handle both, continuous and discrete decisions, to lead the optimization to economically optimal processes operating in an efficient dynamic mode around the nominal working point.

Several deterministic mathematical programming optimization techniques have been used for solving the simultaneous design and control problem (Sweiger and Floudas, 1997; Kookos and Perkins, 2001, Sakizlis et al, 2003; Sakizlis et al, 2004) but complex formulations and a considerable computational effort are required for its implementation. On the other hand, stochastic optimization methods as genetic algorithms have been a good alternative for solving such difficult problems with a minimum effort for its implementation. A genetic algorithm has been proposed for the solution of this non linear mixed integer optimization problem.

The paper is organized containing, first, the description of the MPC and the controllability metrics used for the automatic tuning in the integrated design procedure, the formulation of the optimization problem and the description of the process and in section 3. The analysis of the results is presented in section 4. Finally, conclusions and different projections of this work are included.

2. MPC FORMULATION AND CONTROLLABILITY METRICS

The basic MPC formulation consists of the on-line calculation of the future control actions by solving the following optimization problem subject to constraints on inputs, predicted outputs and changes in manipulated variables.

$$\min_{\Delta\hat{u}} V(k) = \sum_{i=Hw}^{Hp} \left\| \hat{y}(k+i\mid k) - r(k+i\mid k) \right\|_{Wy}^2 + \sum_{i=0}^{Hc-1} \left\| \Delta\hat{u}(k+i\mid k) \right\|_{Wu}^2 \qquad (1)$$

where k denotes the current sampling point, $\hat{y}(k+i\mid k)$ is the predicted output vector at time *k+i*, depending of measurements up to time *k*, $r(k+i\mid k)$ is the reference trajectory, $\Delta\hat{u}$ are the changes in the manipulated variables, *Hp* is the upper prediction horizon, *Hw* is the lower prediction horizon, *Hc* is the control horizon, *Wu* and *Wy* are positive definite matrices representing the weights of the change of control variables and the weights of the set-point tracking errors respectively. In this work the matrices *Wy* and *Wu* are diagonal but not time dependent, so the error vector $\hat{y}(k+i\mid k) - r(k+i\mid k)$ is penalized at every point in the prediction horizon and the changes in the control signal $\Delta\hat{u}(k+i\mid k)$ are penalized at every point in the control horizon.

The problem (1) is a Quadratic Programming (QP) problem that gives a sequence of control moves $\Delta\hat{u}(k+i\mid k)$. The first component of this sequence is applied to the system in time *k+1*, and the optimization problem (1) is repeated at the next sampling time (receding horizon strategy).

The MPC prediction model used in this paper is a linear discrete state space model of the plant obtained by linearizing the first-principles nonlinear model of the process Maciejowsky (2002):

$$\begin{cases} x(k+1) = Ax(k) + Bu(k) + B_d d(k) \\ y(k) = Cx(k) \end{cases} \qquad (2)$$

where *x(k)* is the state vector, *u(k)* is the input vector and *d(k)* the disturbance vector. Matrices ***A***, ***B***, ***Bd*** and ***C*** are of adequate dimensions. For this model the prediction is:

$$\hat{y}(k+i|k) = C\hat{x}(k+i|k) = C\left[A^i x(k) + \sum_{j=1}^{i} A^{j-1} Bu(k+i-j|k)\right] \qquad (3)$$

One reason for choosing state space models is that a significant part of the recent research literature on MPC shows contributions based on this type of models. Connections between the standard linear quadratic regulator (LQR) theory and unconstrained MPC when the horizons approach infinity could be another reason for that.

When the MPC controller is linear and unconstrained, it can be represented with a transfer function KMPC. The corresponding transfer function is:

$$u = \begin{pmatrix} K_1 & K_2 & K_3 \end{pmatrix} \cdot \begin{pmatrix} r \\ y \\ d \end{pmatrix} = K_1 r + K_2 y + K_3 d \qquad (4)$$

where Ki are the transfer functions between the control signal and the different inputs (r,y,d) which depend on the control system tuning parameters (Wu, Hp, Hw and Hc). Particularly, in our MPC formulation $K_2 = -K_1$ (Maciejowsky, 2002), then, control law can be stated as:

$$u = K_1(r - y) + K_3 d \qquad (5)$$

Consequently, taking into account control law and the transfer function of the open loop system, the closed loop response can be obtained from

$$y = \frac{GK_1}{1+GK_1} r + \frac{1}{1+GK_1}\tilde{d} \qquad (6)$$

where $\tilde{d}$ are the filtered disturbances

$$\tilde{d} = \left(GK_3 + G_d\right) d \qquad (7)$$

In order to state the automatic tuning problem, is necessary to define: The Sensitivity function *S(s)* between the load disturbances (*d*) and the outputs (*y*) and the Control Sensitivity transfer function *M(s)* between the load disturbances (*d*) and the control signals (*u*) when the reference is zero .

$$S(s) = \frac{y(s)}{d(s)} = \frac{k_3 G + G_d}{1 + GK_1} \quad (8)$$

$$M(s) = \frac{u(s)}{d(s)} = \frac{K_3 - K_1 G_d}{1 + GK_1} \quad (9)$$

For solving the MPC optimization problem, MPC Toolbox of MATLAB has been used, with some specific modifications (Maciejowsky, 2002) implementing an extended state space representation.

Regarding to the controllability indices, some norm based metrics were considered. The first controllability index considered in this work is:

$$\|N\|_\infty = \max_w |N(jw)| \quad (10)$$

where N is a mixed sensitivity index that takes into account both disturbance rejection and control effort objectives. The function N is defined as:

$$N = \begin{pmatrix} Wp \cdot S \\ Wesf \cdot s \cdot M \end{pmatrix} \quad (11)$$

Wesf(s) is chosen to penalize control efforts adequately, and *Wp(s)* is chosen based on the spectra of disturbances to ensure proper disturbance rejection. *Wp(s)* and *Wesf (s)* are suitable weights for optimization. The selection of *Wp(s)* is explained below, and the weight *Wesf(s)* is selected to complete the H∞ mixed sensitivity problem and allows for the significance of control efforts. Note that control efforts rather than magnitudes of control are included in the objective function by considering the derivative of the transfer function *M(s)*.

In order to ensure disturbance rejection we need (considering normalized disturbances):

$$|S(jw)| \cdot |d(w)| < 1 \quad (12)$$

in the disturbances frequency range where *S(jw)* is the frequency response of the sensitivity function, and *d(w)* is the disturbance spectra. By choosing a weight *Wp(s)* satisfying

$$20 \cdot \log |Wp(jw)|^{-1} < 20 \cdot \log |d(w)|^{-1} \quad (13)$$

disturbance rejection can be assured imposing the following constraint in the optimization tuning procedure:

$$\|Wp \cdot S\|_\infty < 1 \quad (14)$$

A typical choice for the weight *Wp(s)* is a rational function with one zero and one pole. *B* is the weight gain for high frequencies, *a* is the gain for low frequencies and w_b represents the required bandwidth for the closed loop system. The parameter *a* is very small to impose integral action to the system but avoiding numerical problems.

$$Wp(s) = \frac{\frac{s}{B} + w_b}{s + w_b a} \quad (15)$$

The maximum value of the manipulated variables (for the worst case of disturbances) can be constrained to be less than u_{max}, by means of the *l1* norm and the following condition:

$$\|M\|_1 < u_{\max} \quad (16)$$

3. PROCESS DESCRIPTION AND PROBLEM FORMULATION

The activated sludge process was selected to study the simultaneous synthesis and control system design methodology. A simple model (Moreno et al., 1992) was selected, to avoid the excessive complexity of models like the ASM1 developed by the IAWPRC.

Moreno et al. (1992) model is based on the wastewater treatment process of the Manresa plant (Spain). It is founded in the classical Monod and Maynard-Smith model. It is assumed that the reactions take place in only one perfectly-mixed tank. However, in this work two possible structural alternatives consisting in one or two aeration tanks are considered.

The activated sludge process corresponds to the secondary wastewater treatment stage. In the aeration tanks or bioreactors, the activity of a mixture of microorganisms is used to reduce the substrate concentration in the water. The dissolved oxygen required is provided by a set of aeration turbines. Water coming out of each reactor goes to the settler, where the clean water is separated from the activated sludge that is recycled to both bioreactors. The control of this process aims to keep the substrate at the output (s_1 or s_2) below a legal value despite the large variations on the incoming substrate concentration (*si*) using the recycling flows qr_1 and qr_2 as manipulated variables (Moreno et al, 2002). The frequency and magnitude of the disturbances at the *si* input make the control of the plant a difficult task. The set of disturbances used for evaluate the control performance while tuning the MPC has been determined by COST 624 program Copp (2002).

3.1. Mathematical Optimization Problem

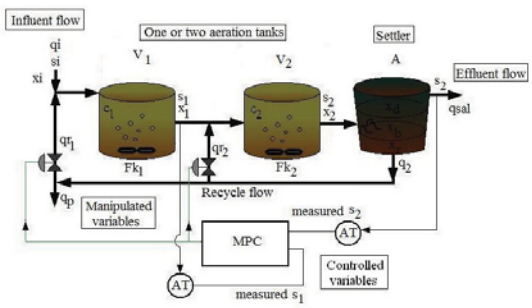

Fig. 1. Activated sludge process superstructure

The simultaneous synthesis, design and control of the activated sludge process pretend to obtain the most economical plant that satisfies the desired control performance. A cost function is defined to measure the economical issues while a predictive controller is tuned to achieve the desired closed loop behaviour according to the controllability norms described in section 2.

The two possible structural alternatives proposed for the plant are represented in a superstructure shown in figure 1. The model equations take the appropriated values for each structural alternative according to the binary y_1.

The mathematical formulation results into a mixed-integer-non-linear optimization problem where the objective is to minimize a cost function considering as decision variables: the structure (y_1), dimensions and controller parameters. Some constraints based in process model are set to find dimensions and initial working point, together with constraints over the norms used to measure the controllability of the plant with the actual controller parameters.

The cost function is:

$$f = p_1 \cdot (v_1 + v_2)^2 + p_2 \cdot A^2 + p_3 \cdot Fk_1^2 + p_3 \cdot Fk_2^2 + p_4 \cdot q_2^2 \qquad (11)$$

where v_1, v_2 are the reactor volumes and A is the cross-sectional area of the settler, Fk_1 and Fk_2 are the aeration factors for each reactor and q_2 is the overall recycle flow. The first three terms are associated to the construction cost that is proportional to the volume of the reactors and the area of the settler. The terms proportional to Fk_1, Fk_2 represent the aeration turbines costs, and the term proportional to q_2 represents pumping costs (purge and recycling).

Logical conditions must be imposed to guarantee the mathematical coherence of the model for any possible structure: if the second reactor does not exist: $y_1=0 \Rightarrow v_2=0$, $x_1=x_2$, $s_1=s_2$, $c_1=c_2$, $Fk_2=0$, $qr_2=0$, if the second reactor exist, then, $y_1=1$ and all the variables take values within their ranges.

The constraints imposed over mass balances in aeration tanks and the settler, are used to define the plant dimensions and the initial stationary working point.

$$\left| v_1 \frac{dx_1}{dt} \right| = \left| \mu_{\max} Y \frac{s_1 x_1}{(K_s + s_1)} v_1 - K_d \frac{x_1^2}{s_1} v_1 - K_c x_1 v_1 + q_{12}(xir_1 - x_1) \right| \le \varepsilon \qquad (17)$$

$$\left| v_1 \frac{ds_1}{dt} \right| = \left| -\mu_{\max} \frac{s_1 x_1}{(K_s + s_1)} v_1 + f_{kd} K_d \frac{x_1^2}{s_1} v_1 + f_{kd} K_c x_1 v_1 + q_{12}(sir_1 - s_1) \right| \le \varepsilon \qquad (18)$$

$$\left| v_1 \frac{dc_1}{dt} \right| = \left| K_{la} Fk_1 (c_s - c_1) v_1 - K_{01} \mu_{\max} \frac{s_1 x_1}{(K_s + s_1)} v_1 - q_{12} c_1 \right| \le \varepsilon \qquad (19)$$

$$\left| v_2 \frac{dx_2}{dt} \right| = \left| \mu_{\max} Y \frac{s_2 x_2}{(K_s + s_2)} v_2 - K_d \frac{x_2^2}{s_2} v_2 - K_c x_2 v_2 + q_{22}(xir_2 - x_2) \right| \le \varepsilon \qquad (20)$$

$$\left| v_2 \frac{ds_2}{dt} \right| = \left| -\mu_{\max} \frac{s_2 x_2}{(K_s + s_2)} v_2 + f_{kd} K_d \frac{x_2^2}{s_2} v_2 + f_{kd} K_c x_2 v_2 + q_{22}(sir_2 - s_2) \right| \le \varepsilon \qquad (21)$$

$$\left| v_2 \frac{dc_2}{dt} \right| = \left| K_{la} Fk_2 (c_s - c_2) v_2 - K_{01} \mu_{\max} \frac{s_2 x_2}{(K_s + s_2)} v_2 - q_{22} c_2 + W_1 \right| \le \varepsilon \qquad (22)$$

$$\left| AL_d \frac{dx_d}{dt} \right| = \left| q_{sal} x_b - q_{sal} x_d - A \cdot nnr \cdot x_d \exp(aar \cdot x_d) \right| \le \varepsilon \qquad (23)$$

$$\left| AL_b \frac{dx_b}{dt} \right| = \left| \begin{matrix} q_{22} x_2 - q_{22} x_b + A \cdot nnr \cdot x_d \exp(aar \cdot x_d) \\ -A \cdot nnr \cdot x_b \exp(aar \cdot x_b) \end{matrix} \right| \le \varepsilon \qquad (24)$$

$$\left| AL_r \frac{dx_r}{dt} \right| = \left| q_2 x_b - q_2 x_r + A \cdot nnr \cdot x_b \exp(aar \cdot x_b) \right| \le \varepsilon \qquad (25)$$

If the second reactor does not exist ($y_1=0$), the values of the variables given by the logical conditions mentioned above, annul the equations (20) and (21), a $W_1 = q_{22} \cdot c_2$ term is used to cancel equation (22).

The operation constraints for the activated sludge process are:

Residence times:

$$2.5 \le \frac{v_1}{q_{12}} \le 8 \qquad (26)$$

$$2.5 \le \frac{v_2 + (1 - y_1) \cdot W_2}{q_{22}} \le 6 \qquad (27)$$

where W_2 annul de constraint for $y_1=0$.

Mass loads in the aeration tanks:

$$0.001 \le \frac{q_i s_i + qr_1 s_2}{v_1 x_1} \le 0.12 \qquad (28)$$

$$0.001 \le \frac{q_{12} s_1 + qr_2 s_2 - (1 - y_1) W_3}{v_2 x_2} \le 0.12 \qquad (29)$$

where W_3 annul de constraint for $y_1=0$.

Sludge age in the settler:

$$2 \le \frac{v_1 x_1 + v_2 x_2 + AL_r x_r}{q_p x_r 24} \le 10 \qquad (30)$$

Limits in hydraulic capacity:

$$\frac{q_{22}}{A} \le 1.5 \qquad (31)$$

Limits in the relationship between the input, recycled and purge flow rates:

$$0.03 \le \frac{q_p}{q_2} \le 0.3 \qquad (32)$$

$$0.05 \le \frac{q_2}{q_i} \le 0.9 \qquad (33)$$

The controllability constraints are the limits over the norms described in section 2 where the transfer functions are referred to s_2 as the output, si y qi as the disturbances, and recycling flows qr_1, qr_2 as control variables. The parameter $u_{\max}$ is an upper bound for the magnitude of control variables. These constraints: $\|N\|_\infty < 1$, $\|Wp \cdot S\|_\infty < 1$, $\|M\|_1 < u_{\max}$ ensure a satisfactory control performance with the tuned MPC.

The main difficulties when solving this problem is the existence of continuous, integer and binary variables and the evaluation of controllability norms that implies the linearization of the process model for each possible solution. GA are particularly suitable, due to its robustness and the straightforward method to compute the objective function and constraints avoiding gradient evaluation.

4. RESULTS

For solving the problem using genetic algorithms (Gen and Cheng, 2000), a fixed length real coded chromosome is defined, containing the continuous normalized process variables, the controller parameters (Wu, Hp, Hc) and a binary variable to set the structure of the plant: [x_1, x_2, S_{sal}, xd xb xr qr_1 qr_2 qp Fk_1 Fk_2 v_1 v_2 A Wu Hp Hc y_1].

The location of the variables in the chromosome is important for the objective function and constraints evaluation procedure.

The genetic algorithm starts by generating randomly a population of possible solutions, that contains the same quantity of individuals for the two structural alternatives ($y_1=0$ and $y_1=1$). Each solution is manipulated to fulfil the logical conditions mentioned in section 3.1, according to the actual value of y_1. The new candidate solutions are manipulated also, according to the logical conditions. The population in the succeeding generation consists of 50% of the best individuals from the previous generation and 50% of the individuals generated by crossover.

The problem is solved using a population size of 200 individuals and 300 maximum iterations. Roulette selection and arithmetic crossover were used. The mutation rate decreases with generations from 0.1 to 0.02 and the crossover probability used is 85%. A penalization strategy is applied to deal with constraints. The genetic algorithm was run 10 times for each case study, giving optimal feasible solutions for each run with an average computing time of 9657 seconds.

Two scenarios with different demands on control performance were proposed. For the case 1 the norm $\|M\|_1 < 1000$ and for the case 2 the norm $\|M\|_1 < 1500$. The weights *Wp* for both cases are*:* $Wp(s) = \frac{8s + 19.2}{s + 0.0001}$

Table 1. Numerical results for integrated synthesis and design with MPC for the case 1

Cost (MU)	0.13	Wu	0.0122
V_1 (m^3)	8640	Hp	9
A (m^2)	2728.9	Hc	3
S_1 (mg/l)	115.66	$\|N\|_\infty$	0.97
Qr_1 (l/hr)	371.47	$\|M\|_1$	987.47
Fk1	0.035	$\|Wp \cdot S\|_\infty$	0.92
Residence times	2.5		
Mass loads	0.08		
Hydraulic capacity	0.55		
Sludge age	2.08		

The results for the two scenarios are presented in tables 1 and 2. In both cases, the transfer functions and weights are referred to disturbances in si and qi. It is observed that the solution gives small economical plants that satisfy all the process and control constraints. It is important to notice the flexibility of the method for different limits imposed over the constraints leading to plants of different dimensions. In the case 1, where an stringent bound is imposed over l1 norm is obtained a plant with 8640m^3 reactor while, for the case 2, with a relaxed bound in l1 norm is possible to obtain an smaller plant with a reactor of 5858.1 m^3 which is reflected in cost.

The optimization case 1 produces a plant with better disturbance rejection because the weight Wp_1 is more restrictive for sensitivity function S. On the other hand, with a smaller bound for $\|M\|_1$, the magnitude of control is less relaxed than in case 2 giving a smaller range of action to the manipulated variable to reject disturbances. The values of Wesf for qr_1 and qr_2 control sensitivity functions are fixed to:

$$Wesf_{qr1}(s) = \frac{0.0117s + 0.14}{s + 0.0004} \qquad Wesf_{qr2}(s) = \frac{0.0183s + 0.22}{s + 0.0004}$$

Table 2. Numerical results for integrated synthesis and design with MPC for the case 2

Cost (MU)	0.064	Wu	0.0069
V_1 (m^3)	5858.1	Hp	8
A (m^2)	2178.4	Hc	3
S_1 (mg/l)	118.06	$\|N\|_\infty$	0.979
Qr_1 (l/hr)	273.9	$\|M\|_1$	1454.9
Fk1	0.021	$\|Wp \cdot S\|_\infty$	0.786
Residence times	4.11		
Mass loads	0.0856		
Hydraulic capacity	0.65		
Sludge age	5.03		

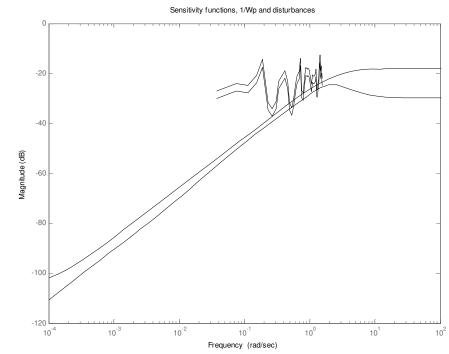

Fig.2. Sensitivity function *S*, Wp^{-1} and disturbances inverse spectrum for case 1

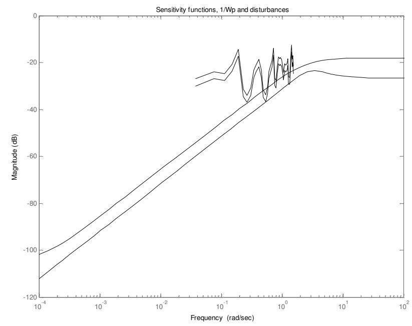

Fig.3. Sensitivity function *S*, Wp^{-1} and disturbances inverse spectrum for case 1

In figures 2 and 3 sensitivity functions S are presented for both cases. In the case 1 the inverse spectrum of disturbances is over Wp^{-1}, and in case 2 this weight is a bit more relaxed representing worse disturbance rejection. In figures 4 and 5 the dynamical responses of the optimal plants for both cases are presented, to illustrate the better disturbance rejection for case 1 as have been previously mentioned.

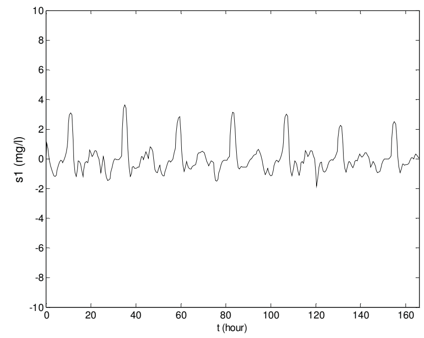

Fig. 4. Substrate response for case 1

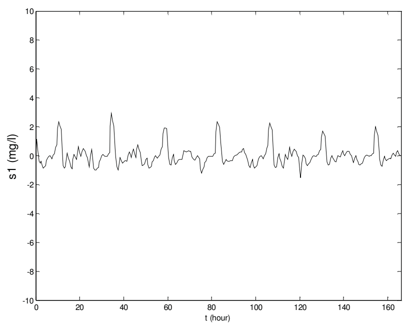

Fig. 5. Substrate response for case 2

5. CONCLUSIONS

In this work, the synthesis and integrated design of an activated sludge process with an advanced controller (MPC) was addressed. The problem was translated into a mixed-integer-non-linear optimization problem, with the evaluation of controllability norms to ensure the most economical design with a suitable control performance.

The MINLP was solved using a real-coded genetic algorithm which leads to good quality feasible solutions with desired disturbance rejection, which is the main control objective. The solutions obtained are sensible to the bounds imposed over controllability indices.

The controllability norms were set as constraints in the formulation of the optimization problem, but it could be formulated as a multiobjective optimization problem considering costs and controllability.

These results are encouraging for the development of simultaneous design and control approaches with advanced control schemes which usually results in complex optimization problems difficult to be solved. In this framework, the use of advanced control techniques represent a significant advance due to the advantages of these control strategies respect to conventional PID.

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