INTEGRATED DESIGN AND CONTROL OF CHEMICAL PROCESSES – PART II : ILLUSTRATIVE EXAMPLES

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Abstract— In this paper, the integrated design paradigm is illustrated with several examples taken from the wide range of methodologies developed in last decades and presented in the first article of this series [Part 1]. The techniques included here belong to the category of simultaneous design and control in an optimization framework, and they have been developed by the authors' research group and applied to the simultaneous process and control system design of the activated sludge process in a wastewater treatment plant (WWTP). In the present article, new aspects and results of those methodologies are presented for further understanding. The scope of the problem considers both a fixed plant layout and the plant structure selection by defining a simple superstructure. The control strategy chosen is a linear Model Predictive Controller (MPC) with terminal penalty in order to guarantee stability. As for the evaluation of the controllability, norm based indexes have been considered, and a multi-model approach to represent the uncertainty and assure robustness. The formulation of the optimization problem can be stated either as a multiobjective one considering costs and controllability, or as monoobjective adding some controllability constraints. Several strategies for solving the optimization problem are presented, mixing stochastic and deterministic methods, and genetic algorithms.

Keywords—Process synthesis, integrated design, controllability, activated sludge process, model predictive control

1. INTRODUCTION

The design of a chemical process is an extensive and challenging task that begins with the description and definition of a product and its specifications. The task is completed once the quantitative definition of all the structural and operating variables of the production plant satisfying the product requirements and process restrictions is achieved. The process design is, typically, based on steady state analysis and economical considerations. The control-systems design is carried out in a subsequent stage, separated from the process design in itself. Sometimes, in this stage, the engineers realize that the possibilities of the control systems may be significantly reduced due to adverse plant dynamics. This problem is usually solved by process re-design or by increasing the size of process units and equipment to achieve acceptable process operation in suboptimal conditions.

Therefore, now it is widely accepted that the process controllability analysis must be an integral part of the process design, in order to satisfy at the same time the economical objectives and those of plant dynamics. In the last thirty years, several researchers have been focused in the study of controllability and its metrics (Ziegler and Nichols, 1943; Skogestad and Wolff, 1992; Wolff et al., 1992; Luyben, 1993; Skogestad; 1994; Skogestad and Postlethwaite, 1996; Soloyev and Lewin, 2003, Ochoa, 2005; Araujo and Skogestad, 2006; Muñoz et al., 2008; Alvarez, 2012) as well as the development of different methodologies to include controllability criteria in the early stages of process design, establishing the idea of Integration of Design and Control (ID).

The *Integrated Design* has emerged as a systematic design procedure where process design and plan-dynamics analysis are carried out simultaneously even along with the control-systems design. Several methodologies developed in order to assess the trade-off between economical benefits and controllability in process design have been reported. In the literature related to integrated design and control it is possible to distinguish a wide variety of methodologies that focus on different aspects of the problem, such as the scope, the controllability issues, the way to quantify the dynamical performance, the formulation of the optimization problem and the resolution techniques. Some excellent reviews can be found (Lewin, 1999; Sakizlis et al. 2004; Seferlis y Georgiadis, 2004; Ricardez-Sandoval et al., 2009a, Yuan et al., 2012). However, due to the wide variety of works presented in the literature and

the continuous advances in the field, a detailed classification of the different approaches and developments on the Integrated Design Methodology supported on a comprehensive review is being published as PART I of this study. Such classification is helpful to systematize the research in this field, showing up the most interesting developments and indentifying the challenging aspects to be assessed and the possibility to integrate other approaches.

As a complement to the previous paper, the present one is dedicated to a brief presentation of several applications of simultaneous design and control of the activated sludge process in a real Wastewater Treatment Plant (WWTP of Manresa, Spain). The wastewater treatment plants must operate at the lowest possible cost with the most efficient control strategies. Therefore, the minimization of the investment and operational costs and the achievement of the effluent quality requirements may result into a conflict of interests that can be addressed by the integrated design methodology. The non-linear characteristics of the process model, makes the activated sludge process an interesting application to test the *integrated design* approach.

The paper is organized as follows. First, the activated sludge process is explained followed by the MPC formulation and its application to the process. Then, the general integrated design methodology is presented together with the particular optimization problems stated depending on the specific controllability indexes considered. The optimization strategies used to solve those problems are presented in the next point, to end with some detailed results and conclusions to the article.

2. DESCRIPTION OF THE PROCESS

A model representing the activated sludge process (ASP) in the wastewater treatment process of the Manresa plant, Spain (Moreno 1994; Gutierrez, 2000) is used herein as a working example, to show several applications of integrated synthesis and design. It has been selected to avoid the excessive complexity of models such as the ASM1. It is founded on the classical Monod and Maynard-Smith model and it is assumed that the reactions take place in one perfectly-mixed tank.

The simplified plant diagram considered in the model is presented in Fig. 1, and Table 1 shows the nomenclature, the values of biological and physical parameters in the model and typical operating conditions.

The differential equations that describe the rate of change of the biomass, organic substrate and dissolved oxygen concentrations in the aeration tank are described below. A detailed explanation of the equations can be found in Revollar et al. (2010a)

$$\frac{dx}{dt} = \mu_{\text{max}} y \frac{sx}{\left(K_c + s\right)} - K_d \frac{x^2}{s} - K_c x + \frac{q}{V_1} \left(xir - x\right) \tag{1}$$

$$\frac{ds}{dt} = -\mu_{\text{max}} \frac{sx}{\left(K_s + s\right)} + f_{kd} K_d \frac{x^2}{s} + F_{kd} K_c x + \frac{q}{V_1} \left(sir - s\right) \tag{2}$$

$$\frac{dc}{dt} = K_{la}Fk_1(c_s - c) - OUR - \frac{q}{V}c \tag{3}$$

The Fk_1 parameter in the equation (3) for oxygen transfer is an aeration factor which is proportional to the speed of working turbines.

The algebraic equations obtained from the mass balances for xir and sir are:

$$xir = \frac{x_i \cdot q_i + x_r \cdot q_r}{q} \tag{4}$$

$$sir = \frac{s_i \cdot q_i + s \cdot q_r}{q} \tag{5}$$

The oxygen uptake rate (OUR) is:

$$OUR = -K_{01}\mu_{\text{max}} \frac{x \cdot s}{(K_s + s)} \tag{6}$$

In the secondary clarifier (settler), the operation is described by the mass balances and the expression for the settling of activated sludge:

$$A \cdot l_d \frac{dx_d}{dt} = q_{sal} x_b - q_{sal} x_d - A \cdot vs(x_d) \tag{7}$$

$$A \cdot l_b \frac{dx_b}{dt} = qx_1 - q_{sal}x_b - q_2x_b + A \cdot vs(x_d) - A \cdot vs(x_b)$$
(8)

$$A \cdot l_r \frac{dx_r}{dt} = q_2 x_b - q_2 x_r + A \cdot vs(x_b) \tag{9}$$

The settling rate is calculated as:

$$vs(x_i) = nr \cdot x_i \cdot e^{(-ar \cdot x_i)}$$
(10)

2. MPC FORMULATION AND APPLICATION TO THE ASP

A linear MPC with terminal penalty has been considered to apply the ID methodology. The MPC formulation consists of the on line calculation of the future control moves by solving the following optimization problem subject to constraints on inputs, predicted outputs and inputs increments. The objective function is the following:

$$\min_{\Delta \mathbf{u}} V(k) = \min_{\Delta \mathbf{u}} \left(\left\| \mathbf{x} (k + H_c) \right\|_P^2 + \sum_{i=0}^{H_c - 1} \left(\left\| \mathbf{x} (k + i) \right\|_Q^2 + \left\| \Delta \mathbf{u} (k + i) \right\|_R^2 \right) \right)$$
(11)

where k denotes the current sampling point, $\mathbf{x}(k+i)$ is the predicted state vector at time k+i, depending of measurements up to time k, $\Delta \mathbf{u}$ is the vector of the changes in the manipulated variables, H_c is the control horizon, R and Q are positive definite matrices representing the weights of the change of control variables and the weights of the set-point tracking errors respectively, and P is a terminal penalty matrix. In this work the matrices R and Q are diagonal but not time dependent and the reference is fixed to zero.

The MPC prediction model is a linear discrete state space model of the plant obtained by linearizing the first-principles nonlinear model of the process (Maciejowski, 2002).

The terminal penalty arises from an infinite horizon formulation, guaranteeing closed loop stability. In this case an unconstrained LQR (Linear Quadratic Regulator) controller has been considered from sampling time H_c to infinity (Scokaert and Rawlings, 1998), and matrix P is obtained from Riccati equation:

$$P = A'PA - A'PB(B'PB + R)^{-1}B'PA + Q$$

$$\tag{12}$$

The control problem for the ASP considered for this ID example consists of maintaining the output substrate (s_1) below a certain value imposed by the environmental regulations. The process disturbances $\mathbf{d} = (s_i, q_i)$ are the variations of the flow rate (q_i) and the substrate concentration of the incoming water (s_i) . The recycling flow (q_r) is the manipulated variable and the substrate (s_1) is the controlled variable so that: $u(k) = q_r$; $y(k) = s_1$ (Fig. 1). The biomass (x_1) in the reactor is a bounded variable. Different sets of disturbances have been considered from COST 682 program and its benchmark [36], and particularly the set for dry and storm weather (Fig. 2). These sets are used here for normalizing purposes and for validating simulations.

The MPC dynamic constraints imposed are the following:

$$s_{1d} < s_1 < s_{1u}$$

$$x_{1d} < x_1 < x_{1u}$$

$$q_{rd} < q_r < q_{ru}$$

$$\Delta q_{rd} < \Delta q_r < \Delta q_{ru}$$

$$(13)$$

where s_{Id} , s_{Iu} ; x_{Id} , x_{Iu} ; q_{rd} , q_{ru} ; Δq_{rd} , Δq_{ru} are the bounds for substrate, biomass, recycling flow and the increments of recycling flow respectively.

2. INTEGRATED DESIGN METHODOLOGY AND APPLICATION TO THE ASP

The Integrated Design methodology described in this paper belongs to the group of simultaneous process and control system design by means of an optimization problem, in the framework of the classification presented in Part I of this work. More precisely, it is a nonlinear optimization problem with nonlinear constraints, including economic and control considerations (Sakizlis et. al. 2004), with the following general formulation:

$$\min_{\mathbf{p}, \mathbf{c}, \mathbf{x}, \mathbf{z}} \mathbf{J}(\mathbf{x}, \mathbf{z}, \mathbf{u}, \mathbf{p}, \mathbf{\delta})$$

$$\mathbf{f}(\dot{\mathbf{x}}, \mathbf{x}, \mathbf{z}, \mathbf{u}, \mathbf{p}, \boldsymbol{\delta}, \boldsymbol{\theta}) = 0$$

$$\mathbf{h}(\mathbf{x}, \mathbf{z}, \mathbf{u}, \mathbf{p}, \boldsymbol{\delta}, \boldsymbol{\theta}) = 0$$

$$\mathbf{g}(\mathbf{x}, \mathbf{z}, \mathbf{u}, \mathbf{p}, \boldsymbol{\delta}, \boldsymbol{\theta}) \leq 0$$

$$\varphi(\dot{\mathbf{x}}, \mathbf{x}, \boldsymbol{\xi}, \mathbf{y}, \mathbf{u}, \mathbf{c}, \boldsymbol{\delta}) = 0$$

$$\eta(\mathbf{x}, \boldsymbol{\xi}, \mathbf{y}, \mathbf{u}, \mathbf{c}, \boldsymbol{\delta}) = 0$$
(15)

where \mathbf{x} denotes the state variables, \mathbf{z} are the algebraic variables, \mathbf{u} are the control variables, \mathbf{p} are the time invariant process design variables, \mathbf{c} are the controller tuning parameters, $\mathbf{\delta}$ are the binary variables that define the process and control system structure, \mathbf{f} denotes the differential equations of the process (mathematical model), \mathbf{h} are the algebraic equations, \mathbf{g} are the inequality constraints (physical constraints, process constraints, controllability constraints, etc.), $\mathbf{\varphi}$ are the differential equations of the controller, $\mathbf{\eta}$ are the algebraic equations of the controller, $\mathbf{\chi}$ are the differential variables of the controller, and $\mathbf{\xi}$ are the algebraic variables of the controller. In this work, a steady state solution \mathbf{x}_0 is sought, so $\dot{\mathbf{x}} = 0$ in the first equation of (15). The function J is the objective function. It can be expressed as a vector when several objectives are present, or some of the constraints (15) are considered as objectives (multiobjective problem):

$$\mathbf{J} = (f_1, \dots, f_i) \quad i=1 \dots n \quad (n= \text{ number of objectives})$$
 (16)

The aim of the integrated-design-of-process-and-control-system problem is to obtain the optimal process design parameters (**p**) and controller parameters (**c**), together with a steady state working point (\mathbf{x}_0) and related algebraic variables (**z**).

The integrated design of the ASP is set in general to obtain the most economical plant that satisfies the desired control performance. Several applications, varying the scope of the problem, the controllability measures and the statement of the optimization problems, are presented in the following paragraphs. The optimization problems are selected depending on the specific controllability indexes included and the scope of the problem.

2.1 Integrated Design including a mixed sensitivity index

This example of application of the ID methodology considers a mixed sensitivity index as the main controllability measure. The cost function for the optimization problem can be expressed as $J = (f_1, f_2)$, where f_I represents the construction cost (proportional to plant dimensions) and operational costs (pumping energy) (Vega et. al., 1999) and f_2 represents the process controllability:

$$f_1(\mathbf{p}, \mathbf{c}, \mathbf{x}, \mathbf{z}) = w_1 \cdot V_{1n}^2 + w_2 \cdot A_n^2 + w_3 \cdot q_2^2$$
(17)

$$f_2(\mathbf{p}, \mathbf{c}, \mathbf{x}, \mathbf{z}) = \|\mathbf{N}\|_{\infty} \tag{18}$$

where V_{In} and A_n are the normalized values for the reactor volume and the cross-sectional area of the settler, q_2 is the total recycling flow, $\mathbf{p}=(V_I,A)$, $\mathbf{x}=(s_I,x_I,c_I,x_d,x_b,x_r)$, $\mathbf{z}=(q_r,q_p)$ and $\mathbf{c}=(R,H_c)$ are the optimization variables, and $w_i=1$ (i=1,2,3) are the weights in the cost function.

The controllability is here included via norm based indices considering that sensitivity functions can be obtained for the unconstrained MPC (see block diagram of Figure 3). Firstly, the f_2 objective function is defined as an H_{∞} mixed sensitivity function that takes into account disturbance rejection and control efforts (dependence on Laplace variable s has been omitted for brevity):

$$N_0 = \begin{pmatrix} W_p \cdot S_0 \cdot R_{d0} \\ W_{esf} \cdot s \cdot M_0 \end{pmatrix}$$

$$R_{d0} = G_{d0} + K_2 G_0$$

$$(19)$$

where S_0 is the output sensitivity function, M_0 is the control sensitivity function, G_{d0} and G_0 are the nominal plant transfer functions.

Parameters W_p and W_{esf} are suitable weights chosen empirically to achieve closed loop performance specifications for disturbance rejection and to reduce the control efforts respectively.

As in the ASP there are two main load disturbances, weights $\mathbf{W}_{p}(s)$ and $\mathbf{W}_{esf}(s)$ and sensitivity functions $\mathbf{S}(s)$, $\mathbf{M}(s)$, $\mathbf{R}_{d}(s)$, $\mathbf{N}(s)$ are vectors and matrices with two elements (dependence in the Laplace variable s for signals and transfer functions is omitted):

$$\mathbf{W_{p}} = \begin{pmatrix} W_{p_{si}} & W_{p_{qi}} \end{pmatrix}; \mathbf{W_{esf}} = \begin{pmatrix} W_{esf_{si}} & W_{esf_{qi}} \end{pmatrix}; \mathbf{S} = \begin{pmatrix} \frac{s_{1}}{\tilde{s}_{i}} & 0 \\ 0 & \frac{s_{1}}{\tilde{q}_{i}} \end{pmatrix}; \mathbf{M} = \begin{pmatrix} \frac{q_{r}}{s_{i}} & 0 \\ 0 & \frac{q_{r}}{q_{i}} \end{pmatrix}; \mathbf{R_{d}} = \begin{pmatrix} G_{ds_{i}} + K_{2}G & 0 \\ 0 & G_{dq_{i}} + K_{2}G \end{pmatrix};$$

$$\mathbf{N} = \begin{pmatrix} \mathbf{W}_{p} \cdot \mathbf{S} \cdot \mathbf{R}_{d} \\ \mathbf{W}_{osf} \cdot \mathbf{s} \cdot \mathbf{M} \end{pmatrix}; \ \mathbf{G}_{d} = \begin{pmatrix} G_{ds_{i}} & G_{dq_{i}} \end{pmatrix}$$
 (20)

For the correct operation of the ASP, the following process and controllability constraints are included, together with physical bounds for all variables:

• Residence time and mass load in the reactor limited between $[ml_d, ml_u]$ and $[ret_d, ret_u]$:

$$ret_d \le \frac{V_1}{q} \le ret_u \; \; ; \; \; ml_d \le \frac{q_i \cdot s_i + q_r \cdot s_1}{V_1 \cdot x_1} \le ml_u \tag{21}$$

• Limits in hydraulic capacity of the settler [ch] and sludge age $[sa_d, sa_u]$:

$$\frac{q}{A} \le ch \; ; \; sa_d \le \frac{V_1 \cdot x_1 + A_d \cdot l_r \cdot x_r}{q_n \cdot x_r \cdot 24} \le sa_u \tag{22}$$

• Limits in the ratios between the input and recycled flows $[rec_d, rec_u]$ and between the recycled and purge flows $[purg_d, purg_u]$:

$$rec_d \le \frac{q_2}{q_i} \le rec_u; \quad purg_d \le \frac{q_p}{q_2} \le purg_u$$
 (23)

• Constraints over the nonlinear differential equations of the process to obtain a steady state solution with a tolerance. Particularly, all normalized derivates are constrained to be less than 10⁻⁵.

 Controllability constraints for robust performance considering a set of multiple models defined around the nominal one.

$$\left\|\mathbf{M}_{\mathbf{0}}\right\|_{1} < u_{\text{max}} \tag{24}$$

$$\left\| \mathbf{W}_{\mathbf{p}} \cdot \mathbf{S} \cdot \mathbf{R}_{\mathbf{d}} \right\|_{2} < 1 \tag{25}$$

Note that by means of the l_1 norm constraint (24) the maximum deviation value of the control (u_{max}) for the worst case of disturbances is constrained to be less than certain limits, in order to avoid saturations and to keep the control system in the linear region. On the other hand, the constraint (25) imposes robust disturbance rejection when applied in the limits of a polyhedral uncertainty region delimited by multiple linearized plant and disturbance models. The plant and MPC obtained are optimal in the region that they define.

2.2 Integrated Design including only l_1 norm indexes

The ID methodology presented can be formulated alternatively considering some disturbance rejection measures stated in (Kariwala and Skogestad, 2007), such as the minimum output error achievable considering bounded manipulated variables for the worst possible combination of disturbances, and the maximum disturbance allowed with inputs and outputs bounded. This approach is interesting because the disturbance rejection is directly characterized in the time domain, and the measures can be represented using l_1 norm-based indexes as the induced norm of the ∞ norm of a signal.

The first optimization problem consists of designing a plant with the MPC such as the output error is minimum, for the worst case of disturbances, when the manipulated variable and costs are bounded. Mathematically, the objective function can be posed in terms of the l_I norm of the closed loop transfer functions as follows:

$$f_{1}(\mathbf{p}, \mathbf{c}, \mathbf{x}, \mathbf{z}) = \|\mathbf{S}_{0}\mathbf{R}_{d0}\|_{1} \tag{26}$$

The minimization of f_1 is subjected to the following constraints:

• Controllability constraint (24), where u_{max} is the upper bound for the manipulated variable and the model is scaled so the maximum magnitude for disturbances is 1.

$$\left\|\mathbf{M}_{\mathbf{0}}\right\|_{1} < u_{\text{max}} \tag{27}$$

• Constraint over construction (plant dimensions) and operation costs (pumping energy), where β is a fixed upper bound:

$$w_1 \cdot V_{1n}^2 + w_2 \cdot A_n^2 + w_3 \cdot q_2^2 < \beta \tag{28}$$

Recall that the l_1 norm of a stable transfer function is defined as the maximum peak of the output divided by the maximum peak of the input, for the worst combination of inputs. This problem comes from the approach described in (Skogestad and Wolf, 1992), based on the maximum values of the signals in the closed loop system, expressed in this way for a SISO system:

$$\max_{\|d\|_{\infty} \le 1} \min_{\|u\|_{\infty} \le u_{\text{max}}} \|y\|_{\infty} \tag{29}$$

where

$$y = G_0 \cdot u + G_{d0} \cdot d \tag{30}$$

considering zero reference and normalized disturbances.

Another approach in this line consists of designing a plant that maximizes the largest possible magnitude of disturbances (d_{max}) such that for the worst possible combination of disturbances up to that magnitude, an acceptable output error is achieved with bounded manipulated variables. The objective function is:

$$f_1(\mathbf{p}, \mathbf{c}, \mathbf{x}, \mathbf{z}) = \frac{1}{d_{\text{max}}}$$
(31)

The optimization of f_1 is subjected to the following constraints, using the l_1 norm definition, where u_{max} is the upper bound of the manipulated variable and y_{max} is the upper bound of the output variable.

• Controllability constraints:

$$\left\|\mathbf{S_0}\mathbf{R_{d0}}\right\|_{1} \le \frac{y_{max}}{d_{\max}} \tag{32}$$

$$\left\|\mathbf{M}_{\mathbf{0}}\right\|_{1} \le \frac{u_{\text{max}}}{d_{\text{max}}} \tag{33}$$

Constraint over costs, where β is a fixed upper bound:

$$w_1 \cdot V_{1n}^2 + w_2 \cdot A_n^2 + w_3 \cdot q_2^2 < \beta \tag{34}$$

This problem can be stated as a multiobjective one because the dependence of d_{max} with the optimization parameters is only through the constraints in (32)-(33). The solution will be a maximum d_{max} that satisfies the equality limits of (32)-(33) and the constraint on costs. Then, considering (32)-(33) as equalities, the solution of this problem can be stated as a multiobjetive optimization one that searches for the maximum value of d_{max} that satisfies both equalities:

$$\min_{\mathbf{p}, \mathbf{c}, \mathbf{x}, \mathbf{z}} \left(\frac{\|\mathbf{M}_{\mathbf{0}}\|_{\mathbf{I}}}{u_{\text{max}}} \quad \frac{\|\mathbf{S}_{\mathbf{0}} \mathbf{R}_{\mathbf{d0}}\|_{\mathbf{I}}}{y_{\text{max}}} \right) \tag{35}$$

For both problems in this point, the (21)-(23) process constraints and the constraints over the non linear differential equations of the process are also included, together with physical bounds for all variables.

2.3 Integrated Design including process synthesis

The simultaneous design of the activated sludge process and its MPC control system has also been solved including the process synthesis. Two possible structural alternatives are proposed, which are represented in the superstructure shown in Figure 4. The alternatives consist of one or two aeration tanks and one secondary settler. The set of decision variables includes the process structure given by binary variable y_1 , plant dimensions, stationary working point and MPC controller parameters. The objective function is:

$$f_{1}(\mathbf{p}, \mathbf{c}, \mathbf{x}, \mathbf{z}) = \alpha_{1} \cdot V_{1}^{2} + \alpha_{1} \cdot V_{2}^{2} + \alpha_{2} \cdot A + \alpha_{3} \cdot q_{2}^{2} + \alpha_{4} \cdot fk_{1}^{2} + \alpha_{4} \cdot fk_{2}^{2}$$
(36)

where $\mathbf{p} = (V_1, V_2, A)$ are the time invariant process design variables, with V_I and V_2 the volumes of the first and second reactor respectively, and A the cross-sectional area of the settler; $\mathbf{c} = (R, H_p, H_c)$ are the MPC tuning parameters (the basic formulation of MPC is considered), $\mathbf{x} = (s_1, s_2, x_1, x_2, c_1, c_2, x_d, x_b, x_r)$ is the state vector including the concentrations on both reactors and the biomass in the settler, $\mathbf{z} = (q_{r1}, q_{r2}, q_p, fk_1, fk_2)$, with q_{r1} and q_{r2} the recycling flows to each reactor, q_p the purge flow, fk_1 and fk_2 the aeration factors for each reactor, and q_2 is

the overall recycling flow. The weights α_i with $i \in \{1, 2, 3, 4\}$ determine the relative importance of each factor in the cost function. The first three terms are associated with construction costs, the terms proportional to fk_1 , fk_2 represent the aeration turbine costs, and the term proportional to q_2 represents pumping costs (purge and recycling).

As in the previous points, the following process and controllability constraints are included, together with physical bounds for all variables. New parameters are added to make the constraints valid for both plant structures.

• Residence time in the reactors limited between $[ret_{dl}, ret_{ul}]$ and $[ret_{d2}, ret_{u2}]$ respectively:

$$ret_{d1} \le \frac{V_1}{q_{12}} \le ret_{u1}; \quad ret_{d2} \le \frac{V_2 + (1 - y_1) \cdot W_2}{q_{22}} \le ret_{u2}$$
 (37)

The last equation is written as:

$$V_2 + (1 - y_1) \cdot W_2 - ret_{u2} \cdot q_{22} \le 0 \tag{38a}$$

$$ret_{d_2} \cdot q_{22} - V_2 + (1 - y_1) \cdot W_2 \le 0$$
 (38b)

where the parameter W_2 is used to adjust the constraint to the actual number of bioreactors, $W_2 = ret_{u2} \cdot q_{22}$ for (38a) and $W_2 = -ret_{d2} \cdot q_{22}$ for (38b).

• Mass load in the reactors limited between $[ml_{d1}, ml_{u1}]$ and $[ml_{d2}, ml_{u2}]$ respectively:

$$ml_{d1} \le \frac{q_i s_i + q r_1 s_2}{V_1 x_1} \le ml_{u1}; \ ml_{d2} \le \frac{q_{12} s_1 + q r_2 s_2 - (1 - y_1) W_3}{v_2 x_2} \le ml_{u2}$$
(39)

where the parameter W_3 term is also included to adjust the constraint to the actual number of bioreactors:

$$W_3 = q_{12} \cdot s_1 \tag{40}$$

• Limits in hydraulic capacity of the settler [ch] and sludge age $[sa_d, sa_u]$:

$$\frac{q_{22}}{A} \le ch \; ; \; sa_d \le \frac{V_1 x_1 + V_2 x_2 + AL_r x_r}{q_v x_r 24} \le sa_u \tag{41}$$

• Limits in the ratios between the input and recycled flows [rec_d, rec_u] and between the recycled and purge flows [purg_d, purg_u]:

$$rec_d \le \frac{q_2}{q_i} \le rec_u; \ purg_d \le \frac{q_p}{q_2} \le purg_u$$
 (42)

• Constraints on the nonlinear differential equations of the process to obtain a solution close to a steady state. The activated sludge model described previously in the point 2, is extended for this process superstructure resulting in a set of differential and algebraic equations which takes the appropriated values for each structural alternative according to the binary y₁ (see Revollar et al., 2010a):

$$\left| V_{1} \frac{dx_{1}}{dt} \right| = \left| \mu_{\max} y_{c} \frac{s_{1}x_{1}}{\left(K_{s} + s_{1}\right)} V_{1} - K_{d} \frac{x_{1}^{2}}{s_{1}} V_{1} - K_{c} x_{1} V_{1} + \left(x_{i} \cdot q_{i} + x_{r} \cdot q_{r_{1}} - q_{12} \cdot x_{1}\right) \right| \le \varepsilon$$

$$(43)$$

$$\left| V_{1} \frac{ds_{1}}{dt} \right| = \left| -\mu_{\max} \frac{s_{1}x_{1}}{\left(K_{s} + s_{1}\right)} V_{1} + f_{kd} K_{d} \frac{x_{1}^{2}}{s_{1}} V_{1} + f_{kd} K_{c} x_{1} V_{1} + \left(s_{i} \cdot q_{i} + s_{1} \cdot q_{r1} - q_{12} \cdot s_{1}\right) \right| \leq \varepsilon$$

$$(44)$$

$$\left| V_{1} \frac{dc_{1}}{dt} \right| = \left| K_{la} f k_{1} \left(c_{s} - c_{1} \right) V_{1} - K_{01} \mu_{\text{max}} \frac{s_{1} x_{1}}{\left(K_{s} + s_{1} \right)} V_{1} - q_{12} c_{1} \right| \le \varepsilon$$

$$(45)$$

$$\left| V_2 \frac{dx_2}{dt} \right| = \left| \mu_{\text{max}} y_c \frac{s_2 x_2}{\left(K_s + s_2 \right)} V_2 - K_d \frac{x_2^2}{s_2} V_2 - K_c x_2 V_2 + \left(x_1 \cdot q_{12} + x_r \cdot q_{r2} - q_{22} \cdot x_2 \right) \right| \le \varepsilon$$
(46)

$$\left| V_2 \frac{ds_2}{dt} \right| = \left| -\mu_{\text{max}} \frac{s_2 x_2}{\left(K_s + s_2 \right)} V_2 + f_{kd} K_d \frac{x_2^2}{s_2} V_2 + f_{kd} K_c x_2 V_2 + \left(s_1 \cdot q_{12} + s_2 \cdot q_{r2} - q_{22} \cdot s_2 \right) \right| \le \varepsilon$$

$$(47)$$

$$\left| V_2 \frac{dc_2}{dt} \right| = \left| K_{la} f k_2 \left(c_s - c_2 \right) V_2 - K_{01} \mu_{\text{max}} \frac{s_2 x_2}{\left(K_s + s_2 \right)} V_2 - q_{22} c_2 + W_1 \right| \le \varepsilon$$
(48)

$$\left| A l_d \frac{dx_d}{dt} \right| = \left| q_{sal} x_b - q_{sal} x_d - A \cdot v_s \left(x_d \right) \right| \le \varepsilon \tag{49}$$

$$\left| A l_b \frac{dx_b}{dt} \right| = \left| q_{22} x_2 - q_{sal} x_b + A \cdot v_s \left(x_d \right) - A \cdot v_s \left(x_b \right) \right| \le \varepsilon \tag{50}$$

$$\left| A l_r \frac{dx_r}{dt} \right| = \left| q_2 x_b - q_2 x_r + A \cdot v_s \left(x_b \right) \right| \le \varepsilon \tag{51}$$

The flow relations are given by:

$$q_{12} = q_i + q_{r1} (52)$$

$$q_{22} = q_{12} + q_{r2} (53)$$

$$q_2 = q_{r1} + q_{r2} + q_{p} \tag{54}$$

where q_{12} and q_{22} are the input flows to both reactors.

It is important to mention that logical conditions must be imposed to guarantee the mathematical coherence of the model for any possible structure. If the second reactor does not exist $(y_1=0)$, then $V_2=0$, $x_1=x_2$

$$W_1 = (1 - y_1) q_{22} \cdot c_2 \tag{55}$$

If the second reactor exists, then, $y_i = 1$ and all the variables take values within their ranges.

• Controllability constraints are expressed as the limits over the norms described by eq. (19), (24),(25), where the transfer functions are referred to s_2 as the output (or s_1 if there is only one reactor), and recycling flows qr_1 , qr_2 as manipulated variables. The parameter u_{max} is an upper bound for the magnitude of both control variables.

$$\|\mathbf{N}\|_{\infty} < 1 \tag{56}$$

$$\left\| \mathbf{W_p} \cdot \mathbf{S_0} \cdot \mathbf{R_{d0}} \right\| < 1 \tag{57}$$

$$\left\|\mathbf{M}_{\mathbf{0}}\right\|_{1} < u_{\text{max}} \tag{58}$$

The control of this process aims to keep the substrate at the output of the reactors $(s_1 \text{ and } s_2)$ below a legal value despite the large variations of the incoming substrate concentration (si) and flow (qi). The disturbances are one of the main problems when trying to control the plant properly and disturbance rejection is therefore the main control objective. The set of disturbances used to evaluate the control performance while tuning the MPC has been taken from BSM1 benchmark (Copp, 2002). The manipulated variables are the recycle flows qr_1 and qr_2 .

The prediction model for the MPC is the linearized discrete state space model representing the superstructure, with the outputs and manipulated variables selected depending on the existing number of reactors. In the proposed superstructure, the control structure depends directly on the plant configuration. For y_1 =0, then V_2 =0 and q_{r2} =0 and the control system is SISO, the substrate s_1 is controlled manipulating q_{r1} and there is a scalar weight R associated to the control efforts. For y_1 =1, then V_2 ≠0 and q_{r2} ≠0, and then the control system is multivariable with a diagonal matrix weight R.

3 OPTIMIZATION STRATEGIES

Several optimization strategies have been developed according to the specific characteristics of the problem. The complexity of considering controller tuning and plant design, including real and integer parameters, makes attractive the two-step iterative algorithm with some variants detailed below. Genetic algorithms are also suitable for this kind of problems and they have been used in some cases. The choice of the strategy depends on several factors, such us convergence difficulties, the computing time or the scope of the problem. For more details about the implementation, see (Francisco et al., 2011).

• *Option 1*:

One option to solve the multiobjective optimization defined by (17) - (18) is to tune the controller in a first step, applying for example the method proposed in (Francisco et al., 2010) and in a second step perform the plant design using the goal-attainment method, or vice versa. The procedure presented in (Francisco et al.,2010) is, in turn, another two-step iterative algorithm based on norm controllability indexes (horizon tuning + weights tuning). This iterative procedure will stop when a convergence criteria is satisfied over the objective function and optimization variables.

The goal-attainment method consists of minimizing a slack variable γ which combines all objectives in the non linear constraints. Mathematically, if f_1^* , f_2^* , f_3^* are the goals for each objective, it is stated as follows:

$$\min_{\mathbf{x}, \mathbf{z}, \mathbf{p}, \mathbf{c}, \gamma} \gamma \tag{59}$$

s.t.
$$f_i(x) - w_i \gamma \le f_i^*$$
 $i=1...n$ (60)

where n is the number of objectives considered.

• *Option 2*:

This is also a two-step iterative algorithm, but considering on one side the optimization of all real parameters (plant parameters, working point and controller weights) and on the other side the tuning of the MPC control horizon. In this case, for the horizon tuning, a random search based on the Solis method is used [31, 37], and for the rest of real parameters, the presented goal-attainment method or a Sequential Quadratic Programming method if the problem is mono-objective. If the MPC horizon is fixed in advance, this option is eventually a one-step approach to solve the integrated design,

• *Option 3*:

The last option to solve the optimization problems generated in the ID is using Genetic Algorithms (GA) (Revollar *et al.*, 2010), For this particular case, GA real coding is proposed, thus, each chromosome contains the continuous variables corresponding to the normalized process variables in the range [0 1], controller parameters and a binary variable to set the structure of the plant. The roulette operator (Goldberg, 1989) is chosen for the selection procedure, also considering elitism. The "arithmetic crossover" (Gen and Chen, 2000) is selected for chromosome recombination, where the offspring (z) is obtained from the parents x, y, as:

$$z_i = \lambda \cdot x_i + (1 - \lambda) \cdot y_i \tag{61}$$

where $0 \le \lambda \le 1$. The random mutation operator (Goldberg, 1989) which decreases proportionally as the generations progress is also applied. The new candidate solutions are again manipulated to fulfill the logical conditions. The population in a succeeding generation consists of 50% of the best individuals from the previous generation and 50% of the individuals generated by crossover. To deal with constraints, an evaluation function with penalty term in the addition form is applied (Gen and Chen, 2000).

4 RESULTS

4.1. Results for optimization problem 2.1

Some results of ID considering the mixed sensitivity index, for different conditions of the optimization problem, are shown at this point. The influence of the uncertainty regions and the weights are addressed. Recall that the needed norm-based controllability indexes are obtained from the linearized model of the plant (state space models). Once the optimization is solved, the plant is validated using the full nonlinear set of ASP differential equations.

The weights for the controllability indexes are the following:

$$W_{p_{si}} = \frac{7 \cdot 10^{-3} \cdot \left(\frac{s}{M_p} + w_{B1}\right)}{s + w_{B1} \cdot A_p} \qquad W_{p_{qi}} = \frac{0.02 \cdot \left(\frac{s}{M_p} + w_{B2}\right)}{s + w_{B2} \cdot A_p} \quad \text{where } w_{B1} = 2500, w_{B2} = 2000, A_p = 10^{-4}, M_p = 10^{-3}$$
 (62)

$$W_{esf_{si}} = \frac{0.0175 \cdot \left(\frac{S}{M_{esf}} + w_{B3}\right)}{S + w_{B3} \cdot A_{arf}} \qquad W_{esf_{qi}} = \frac{0.0525 \cdot \left(\frac{S}{M_{esf}} + w_{B4}\right)}{S + w_{B4} \cdot A_{arf}} \quad \text{where } w_{B3} = 3, w_{B4} = 3, A_{esf} = 10^{-4}, M_{esf} = 3$$
 (63)

The weight $W_p(s)$ has been chosen considering condition (25) with benchmark and real disturbance spectra, while $W_{esf}(s)$ has been chosen to impose a certain penalty on control moves. Both weights have been determined empirically using the following procedure. First, the form of the gain has been determined, taking into account that $M_p(M_{esf})$ and $A_p(A_{esf})$ are the inverse weights gain at high and low frequencies respectively. The frequencies w_{B1} , w_{B2} , w_{B3} , w_{B4} are related to the bandwidth requirement [34]. Once the form is defined, the gains are modified in order to give proper disturbance rejection.

The numerical bounds for the process constraints are: ret_d =2.5 hours; ret_u =8 hours; ml_d =0.001; ml_u =0.1; ch=0.7 m/h; sa_d =2 days; sa_u =10 days; rec_d =0.05; rec_u =0.9; $purg_d$ =0.03; $purg_u$ =0.3. The dynamic constraints for MPC are: s_{1d} =20 mg/l; s_{1u} =150 mg/l; s_{1u} =400 mg/l; s_{1u} =3000 mg/l; s_{1u} =3500 mg/l; s_{1u} =150 mg/l; s_{1u} =1000 mg

In order to determine the uncertainty regions for robust ID, several criteria have been considered. The first one consists of varying the concentration of substrate s_1 10 mg/l around the current nominal value (CASE 1). The second criterion consists of modifying the influent characteristics (input flow q_i and substrate concentration at the input s_i) ($s_i\pm 100$ mg/l, $q_i\pm 220$ m³/h) (CASE 2). This is very interesting because the plant influent has always a large variability. The last criteria modifies the plant dimensions around nominal values ($V_1\pm 300$ m³, $A\pm 180$ m²), in order to give some flexibility to the designed plant or to give some error building margin (CASE 3).

In Table 2, Fig. 5 and Fig. 6, some results comparing performance at the more demanding point of the uncertainty regions are presented. The weights $W_p(s)$ and $W_{esf}(s)$ for the mixed sensitivity indexes are kept constant. A comparison with the ID case without considering robustness in the worst working point of the region of CASE 2 is also shown. In the last column of the table, CASE 2 and CASE 3 are considered together. The controllability constraint considered is $\|\mathbf{M}\|_1 < 3500$ and the control horizon is fixed to $H_c=10$ in order to reduce the computational effort. The effect of local minima on the procedure has been overcome by using different starting points for each ID case. In all cases, the constraint over $\|\mathbf{W}_p \cdot \mathbf{S}\|_{\infty}$ for disturbance rejection is satisfied except for the ID without multiple models, showing the advantages of performing ID with uncertainty. The cost of the ID without robustness is larger mainly because of the pumping energy represented by the value of q_{rl} . The weight R increases when more conditions are imposed to the calculation of the multiple models, but consequently, cost increases (dimensions are larger in order to satisfy performance condition throughout the region).

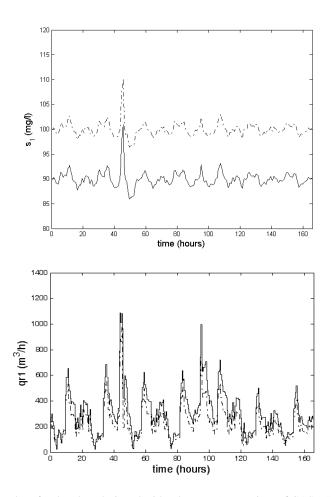


Fig. 5: A comparison of s_1 and q_r for the plant designed with robust ID (uncertainty of CASE 1), working in the nominal point (dash dotted line) and working in the limit of the region (solid line)

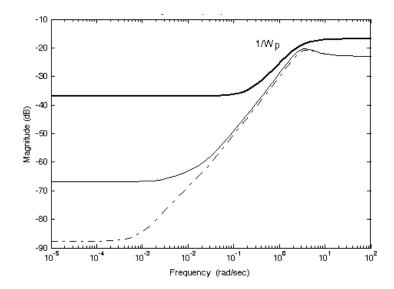


Fig. 6: Output sensitivity functions for the closed loop plant designed with robust ID with CASE 1 of multiple models, working in the limit of the region (solid line) and in the nominal point (dash dotted line), together with magnitude of weight $W_{p_{si}}^{-1}$ (solid thick line)

Influence of the weights in the controllability indexes

where $W_{B3} = 4$, $A_{esf} = 10^{-3}$, $M_{esf} = 3$

The influence of the weights in the controllability indexes is very important and in some cases determines the success of the methodology. In this section the influence of the weight $W_{\rm esf}$ in the mixed sensitivity index is presented, keeping $W_{\rm p}$ constant with values of (62). The following weights have been considered, where only the component $W_{\rm esf}$ is presented, because $W_{\rm esf}$ in also been modified proportionally in each case.

Weight 1:
$$W_{esf_{si}} = \frac{0.14 \cdot \left(\frac{s}{M_{esf}} + w_{B3}\right)}{s + w_{B3} \cdot A_{esf}}$$
; Weight 2: $W_{esf_{si}} = \frac{0.08 \cdot \left(\frac{s}{M_{esf}} + w_{B3}\right)}{s + w_{B3} \cdot A_{esf}}$; Weight 3: $W_{esf_{si}} = \frac{0.05 \cdot \left(\frac{s}{M_{esf}} + w_{B3}\right)}{s + w_{B3} \cdot A_{esf}}$;

In the Table 3 numerical results obtained are presented, together with some values of the controllability indexes. It is observed that for weights \mathbf{W}_{esf} with larger magnitude, which penalize more the control efforts, plant designs with larger weights R are obtained, which give worse disturbance rejection. In essence, weight \mathbf{W}_{esf} regulates control efforts of the MPC obtained in the ID. The uncertainty region of CASE1 has been considered and scaled dry-weather disturbances of BSM1. The optimization problem is solved using the *Option 1* with H_c =8 fixed.

Table 3. Results for ID with different W_{esf} Weight W_{esf} considered: Weight 1 Weight 2 Weight 3

| R | 0.0087 | 0.0056 | 0.0050 |
|--|--------|---------|--------|
| $\left(V_{1}\right)_{0} \ (\mathrm{m}^{3})$ | 4554.5 | 4507.9 | 4864.8 |
| $(A)_0$ (m ²) | 2202.5 | 2147.8 | 4618.7 |
| $(s_1)_0$ (mg/l) | 99.462 | 100.000 | 99.391 |
| $\operatorname{Cost}(f_1)$ | 0.1902 | 0.1839 | 0.4681 |
| $\left\ \boldsymbol{W}_{\!p} \cdot \boldsymbol{S}_{0} \cdot \boldsymbol{R}_{d0} \right\ _{\scriptscriptstyle \infty}$ | 0.9224 | 0.7040 | 0.6788 |
| $\left\ \mathbf{M}_{0} ight\ _{_{1}}$ | 1259.5 | 1516.5 | 1662.0 |
| $\left\ \mathbf{N} ight\ _{\infty}$ | 2.7514 | 1.7882 | 1.3097 |
| $\max \left s_1 - s_{1ref} \right \text{ (mg/l)}$ | 3.367 | 2.873 | 2.427 |

For other results about the influence of the optimization procedures and controllability constraints, and the influence of the controllability indexes considered see (Francisco et al., 2011).

4.2 Results for optimization problem 2.2

Here some ID results considering the disturbance rejection indices proposed in (Kariwala and Skogestad, 2007) are presented. Firstly, the ID has been solved to obtain a plant with the minimum output error achievable considering bounded manipulated variables and for the worst possible combination of disturbances. The numerical results for this case are summarized in table 4, showing that when cost is restricted the plant designed is smaller, satisfying constraint $\|\mathbf{M}_0\|_1 < 3000$ for the manipulated variable. The control horizon is fixed here to H_c =10.

Table 4
Results for ID with different bounds in cost

| | Without bound | Cost < 1.1 |
|---|---------------|------------|
| R | 0.0026 | 0.0025 |
| $V_1 (\mathrm{m}^3)$ | 10000 | 9919.6 |
| $A (m^2)$ | 1832.5 | 1800.4 |
| $s_1 (\text{mg/l})$ | 47.57 | 47.91 |
| $\left\ \mathbf{M}_{0}\right\ _{1}$ | 2984.6 | 3000 |
| Cost | 1.1122 | 1.100 |
| $\max \left s_1 - s_{1ref} \right \text{ (mg/l)}$ | 3.212 | 3.3150 |

Secondly, the ID has been solved considering the maximization of the largest possible magnitude of disturbances such that for the worst possible combination of disturbances up to that magnitude, an acceptable output error is achievable with the bounded manipulated variables. The problem has been stated as a multiobjective optimization problem and solved with the goal-attainment method. The results are shown in table 5, and in this case, when the bounds are relaxed either for the inputs or for the outputs, the value of the maximum allowed normalized disturbance d_{max} increases, for the corresponding plant obtained, as expected in a plant with larger control or output bounds. Costs are only constrained to be less than a fixed value Cost < 1, and in these cases it is given more importance to the magnitudes of inputs and outputs.

Table 5
Results for ID maximizing the largest possible magnitude of disturbances

| u_{ma} | $u_{\text{max}} = 4000$ u_{max} | $u_{\text{max}} = 3000$ $u_{\text{max}} = 300$ | 00 |
|----------|--|--|----|
| y_{ma} | $y_{\text{max}}=10$ y_{max} | $y_{\text{max}}=10$ $y_{\text{max}}=14$ | |

| 1/d _{max} | 0.747 | 0.87705 | 0.71469 |
|---|-----------|----------|----------|
| R | 0.0023371 | 0.003353 | 0.005432 |
| $V_I (\text{m}^3)$ | 8224.1 | 8898.8 | 9332.4 |
| $A (m^2)$ | 1809.9 | 1802.1 | 1467.6 |
| $s_1 (\text{mg/l})$ | 57.281 | 53.137 | 56.123 |
| $\ \mathbf{M_0}\ _{_1}$ | 2988 | 2631.2 | 2144.1 |
| $\max \left s_1 - s_{1ref} \right \text{ (mg/l)}$ | 3.3315 | 3.547 | 5.1761 |

4.3 Results for optimization problem 2.3

Some integrated design results with plant structure selection, considering different weights W_p for disturbance rejection and different bounds over $\|\mathbf{M}_0\|_1$, are presented in this paragraph. All weights are referred to disturbance s_i , which is the only one considered in this set of results, and the multivariable transfer functions have been obtained analogously to the equations (20).

Case 1:
$$W_{p1} = \frac{8s + 19.2}{s + 0.0001}$$
 and $\|\mathbf{M}_0\|_1 < 1000$. (65)

Case 2:
$$W_{p2} = \frac{4.4s + 10.56}{s + 0.0001}$$
 and $\|\mathbf{M}_0\|_1 < 450$. (66)

The values of W_{esf} for the mixed sensitivity function considering q_{rl} and q_{r2} are:

$$W_{esf_{qr1}} = \frac{0.0117s + 0.14}{s + 0.0004} \qquad W_{esf_{qr2}} = \frac{0.0183s + 0.22}{s + 0.0004}$$
(67)

The numerical bounds for the process constraints are: $ret_{dl} = 2.5$ hours; $ret_{ul} = 8$ hours; $ret_{d2} = 2$ hours; $ret_{u2} = 6$ hours; $ml_{dl} = 0.001$; $ml_{ul} = 0.12$; $ml_{d2} = 0.001$; $ml_{u2} = 0.12$; ch = 1.5 m/h; $sa_d = 2$ days; $sa_u = 10$ days; $rec_d = 0.05$; $rec_u = 0.9$; $purg_d = 0.07$; $purg_u = 0.3$.

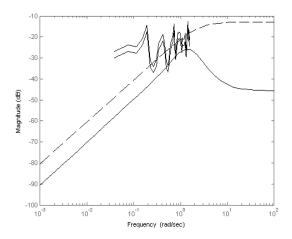
The cromosomes defined for the genetic algorithm include 19 real variables (normalized) and 3 integers (MPC horizons and plant structure):

$$\left[x_{ln}, x_{2n}, s_{ln}, s_{2n}, c_{ln}, c_{2n}, x_{dn}, x_{bn}, x_{rn}, q_{r1ss}, q_{r2n}, q_{pn}, fk_{ln}, fk_{2n}, V_{ln}, V_{2n}, A_n, R_{ln}, R_{2n}, H_p, H_c, y_1\right]$$

where R_{1n} and R_{2n} denote the control efforts MPC weights, conforming a diagonal matrix when y_1 =1 and a scalar when y_1 =0, implying in turn that R_{2n} =0.

In table 6 some numerical results are presented, showing that changes in the controllability conditions give plants with different structure and operating conditions. The plant of Case 1 has better disturbance rejection than the plant of Case 2. The weight W_{p1} is more restrictive and the more relaxed bound over $\|\mathbf{M}_{\mathbf{0}}\|_{\mathbf{1}}$ allows for a larger action of the manipulated variable to reject disturbances. No robustness conditions have been included in these results, and BSM1 profiles for disturbances are considered. In the figure 7, the sensitivity function for both cases together with the weights W_p and inverse spectrum of the influent disturbance s_i are shown (for dry and storm weather conditions). Here it is shown how in case 2 the separation between the weight W_{p2} and the sensitivity function is smaller, therefore with worse disturbance rejection.

In the AG, a population of 100 chromosomes, a maximum number of iterations of 1000, a decreasing mutation rate from 0.1 to 0.02 and a crossover probability of 80%.(Revollar *et al.*, 2006).



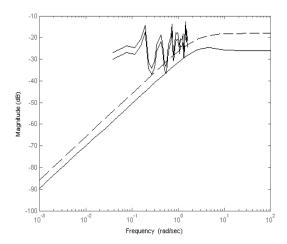


Fig. 7: Magnitude of the sensitivity function S_0R_{d0} for case 1 (left) and case 2 (right), together with line) and the inverse spectrum of influent disturbance s_i for dry and storm weather.

Table 6
Results for ID of the activated sludge process with MPC including plant structure selection

| plant structure selection | | |
|---|----------------|--|
| | Case 1 | Case 2 |
| R | 0.009 | $\begin{bmatrix} 0.347 & 0 \\ 0 & 0.052 \end{bmatrix}$ |
| H_p | 7 | 7 |
| $\overset{\cdot}{H_c}$ | 2 | 4 |
| $V_I \text{ (m}^3)$ | 5409.2 | 3442.7 |
| $V_2 \text{ (m}^3)$ | 0 | 2819.2 |
| $A (m^2)$ | 1253.1 | 1147.0 |
| $s_1 or s_2 (\text{mg/l})$ | $s_1 = 107.03$ | $s_2 = 93.86$ |
| $\left\ \mathbf{N_0} ight\ _{\infty}$ | 0.74 | 0.96 |
| $\ \mathbf{M}\ _{_{\mathrm{I}}}$ | 725.7 | 281.3 |
| $\left\ \mathbf{W_p \cdot S_0 \cdot R_{d0}} \right\ _{\scriptscriptstyle{\infty}}$ | 0.63 | 0.93 |
| $\operatorname{Max}(qr_1 \text{ or } qr_2)$ | 563.9 | 254.5 |
| $\max s_1 - s_{1ref} \pmod{l}$ | 17.7 | 36.5 |

5 CONCLUSIONS

In this paper, the review of the existing ID methodologies presented in the first part of this series has been illustrated with the Integrated Design of the activated sludge processes in a wastewater treatment plant with stable linear MPC. The problem is based on optimization including investment, operating costs, and dynamical indexes stated as the weighted sum of the H_{∞} and l_1 norms of different closed loop transfer functions matrices of the system, following a multiobjective methodology. Some robustness conditions are also included as constraints to guarantee that the resulting plant and control system designs are robust in the face of nonlinearities and disturbances acting on the process. The different aspects of the ID methodologies shown in this paper are the following:

- The integrated design of the activated sludge process with an advanced controller (linear MPC with terminal penalty) using mixed sensitivity norm-based controllability indices and a multiobjective formulation.
- The integrated design of the activated sludge process with an advanced controller (linear MPC with terminal penalty) using l₁ norm-based controllability indices.
- Finally, the mathematical formulation of the integrated synthesis, design and MPC control of the process, translated into a mixed-integer-non-linear optimization problem, with the evaluation of norm-based controllability indices to ensure the most economical design with a suitable control performance, and the application of Genetic Algorithms to solve the problem.

It was shown that the plants obtained applying the integrated synthesis and design procedure can be structurally different from the economical designs, which gives advice about the importance of including the process synthesis in the integrated design framework. Those plants are larger (with the corresponding increase in the investment and operation costs) but ensuring satisfactory values of dynamical performance indices.

Different optimization methods have been studied to solve the synthesis and integrated design problem of chemical processes, and particularly the activated sludge process. Special attention deserves the stochastic optimisation methods in the solution of the complex formulations that include integer and binary variables. It is important to mention that the stochastic algorithms select the process structure in a one step optimization procedure in contrast to the required decomposition algorithms found in the applications of classical optimization methods.

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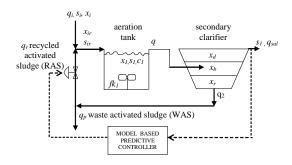


Figure. 1. Plant and controller layout for the simplified structure of Manresa's activated sludge process

Table 1. Operational, biological and physical parameters for the selected activated sludge process

| Symbol | Parameter | Value [units] |
|-------------------|---|------------------------|
| μ_{max} | Maximum growth rate of the | 0.1824 |
| 1 max | microorganisms | |
| y | Yield coefficient between cellular | 0.5948 |
| · | growth and substrate elimination | |
| fkd | Yield coefficient between biomass | 0.2 |
| J | endogenous and substrate | |
| | contribution to the medium | |
| K_d | Kinetic coefficient of biomass decay | 5.5e-5 |
| | by endogenous metabolism | [L/h] |
| K_s | Saturation constant | 300 |
| K_c | Kinetic coefficient of biomass decay | 1.333e-4 |
| | by biological waste | [L/h] |
| c_s | Saturation oxygen (DO) | 8 [mg/L] |
| - 3 | concentration in the aeration tanks | - [8] |
| Kla | Mass transfer coefficient in aeration | 0.7 [h ⁻¹] |
| | process | |
| OUR | Oxygen uptake rate | |
| K01 | Yield coefficient between the cellular | 0.0001 |
| | growth and the oxygen consumption | |
| | rate | |
| xi | Biomass concentration at the influent | 80 |
| | | [mg/L] |
| si | Substrate concentration at the | 366.67 |
| | influent | [mg/L] |
| qi | Influent flow | 1300 |
| | | $[m^3/h]$ |
| X | Biomass concentration at the output | [mg/L] |
| | of the aeration tanks | |
| S | Substrate (COD) concentration at the | [mg/L] |
| | output of the aeration tanks | F /F.1 |
| c | Dissolved oxygen (DO) | [mg/L] |
| | concentration at the output of the aeration tanks | |
| ~ | Bioreactor input flow | [m2/h] |
| q | Recycle flow | [m3/h] [m3/h] |
| qr xir | Bioreactor inlet biomass | |
| λιι | concentration | [mg/L] |
| sir | Bioreactor inlet substrate | [mg/L] |
| SII | concentration | [mg/L] |
| Fk_1 | Aeration factor | |
| V_I | Bioreactor volume | $[m^3]$ |
| $\stackrel{r}{A}$ | Settler area | $[m^2]$ |
| x_d | Biomass concentration at the surface | [mg/L] |

| of the settler | , |
|--|--|
| Biomass concentration in the settler | [mg/L] |
| second layer | |
| Biomass concentration at the bottom | |
| of the settler | |
| Settling rate of the activated sludge | |
| in the settler | |
| Empirical parameter for the settling | 3.1563 |
| rate relationship | |
| Empirical parameter for the settling | - |
| rate relationship | 0.000785 |
| Height of the first layer of the settler | 2m |
| Height of the second layer of the | 1m |
| settler | |
| Height of the third layer of the settler | 0.5m |
| | Biomass concentration in the settler second layer Biomass concentration at the bottom of the settler Settling rate of the activated sludge in the settler Empirical parameter for the settling rate relationship Empirical parameter for the settling rate relationship Height of the first layer of the settler Height of the second layer of the settler |

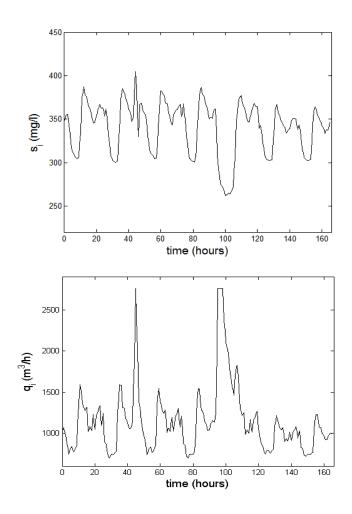


Figure 2: Storm weather disturbances at the influent (s_i, q_i)

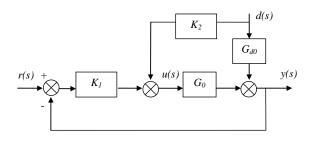


Figure 3: Nominal closed loop system

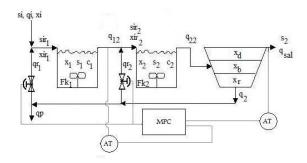


Figure 4. Activated sludge process superstructure

Table 2. Results for different robust Integrated Design cases when working in the worse point of the uncertainty region

| | ID with single models | CASE 1 | CASE 2 | CASE 2 CASE 3 |
|---|-----------------------|---------|---------|------------------|
| | | 0.00727 | 0.00647 | |
| R | 0.00699 | 0.00737 | 0.00647 | 0.00589 |
| $V_1(m^3)$ | 3605.5 | 3628 | 3923 | 4443 |
| $A(m^2)$ | 2452 | 2449.4 | 2445.5 | 2225.5 |
| $s_1 (mg/l)$ | 100.0 | 90.0 | 99.0 | 95.0 |
| $q_r (m^3/h)$ | 570.5 | 257.5 | 354.6 | 362.3 |
| $s_i(mg/l)$ | 400 | 340 | 400 | 400 |
| $q_i (m^3/h)$ | 1280 | 1150 | 1280 | 1280 |
| $\left\ \boldsymbol{W}_{\!p} \cdot \boldsymbol{S} \cdot \boldsymbol{R}_{\!d} \right\ _{\scriptscriptstyle \infty}$ | 33.829 | 1 | 1 | 1 |
| $\ \mathbf{M}\ _{_{1}}$ | 4889.5 | 3632.4 | 4889.5 | 5558.3 |
| Cost | 0.999 | 0.184 | 0.364 | 0.471 |
| max. deviation from s_1 (mg/l) | MPC non feasible | 17.9 | 26.3 | 23.7 |