STOCHASTIC OPTIMIZATION FOR THE SIMULTANEOUS SYNTHESIS AND CONTROL SYSTEM DESIGN OF AN ACTIVATED SLUDGE PROCESS

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***Abstract*—This work presents two stochastic optimization methods to perform the integrated synthesis and design of an activated sludge process. The process synthesis and design are carried out simultaneously with the control system design to obtain the most economical plant which satisfies the desired control system performance. The mathematical formulation of this objective translates the process superstructure into a mixed-integer optimization problem with non-linear constraints and dynamical-performance-indices evaluations. The proposed stochastic optimization algorithms, namely simulated annealing and a real-coded genetic algorithm, are valid alternatives to classical optimization techniques for the solution of such complex problems. The results are encouraging for future applications, because the easy implementation and the quality of the solutions obtained make not only possible but practical the solution of the integrated synthesis and design problem.**

***Keywords*—Process synthesis, integrated design, genetic algorithms, simulated annealing, controllability.**

I. INTRODUCTION

The advantage of considering controllability issues in the early stage of process design has been broadly recognized in the literature (Ziegler and Nichols, 1942; Luyben, 1993; Luyben and Floudas, 1994). Based on this idea, several authors have proposed different methodologies for the simultaneous design and control of chemical processes (Sakizlis *et al*., 2004), addressing the systematic study of the influence of the process design on the controllability and dynamic behavior of the plant. Several authors perform the integrated design considering an economic objective and a dynamic measure of performance, for instance the integral-square-error, for a more systematic analysis of the interactions of design and control (Schweiger and Floudas, 1997; Gutiérrez and Vega, 2002; Kookos and Perkins, 2001; Revollar *et al*., 2005; Francisco and Vega, 2006; Revollar *et al*, 2006).

Thus, *the integrated design and control methodology*, leads to a non-linear optimization problem where economic objectives, operability specifications and control performance are considered. The most comprehensive applications also contemplate the process synthesis or the control structure selection, Tlacuahuac-Flores and Biegler (2008), resulting into a mixed-integer-non-linear optimization problem (MINLP). The controllability analysis may require the evaluation of dynamic performance indices, which translates the problem into a mixed-integer-dynamical optimization (MIDO). Therefore, this approach involves the use of advanced algorithms that handle both continuous and discrete decisions, to lead the design to economically optimal processes operating in an efficient dynamic mode around the nominal working point.

Several deterministic mathematical programming optimization techniques have been applied successfully to solve mixed integer non-linear optimization problems in different process engineering problems. However, in complex problems these algorithms, at times, fail to give any solution and their effectiveness decreases when discontinuities and non convexities are present (Tsai and Chang, 2001; Costa and Oliveira, 2001).

Some works addressing the MINLP or MIDO that arise from *integrated design and control* of chemical processes are found in the literature. Narraway and Perkins (1994) studied the problem of selecting an economically optimal multi-loop proportional-integral control structure using non-linear models. The solution was found using dynamic optimization and the OA/ER/ AP (Viswanatan and Grossman, 1990) technique for the MINLP, however, they reported a poor performance of the method due to the non-convexity of the problem.

On the other hand, Schweiger and Floudas (1997) presented a methodology for analyzing the interaction of design and control that resulted in a multi-objective Mixed Integer Optimal Control Problem. A control parameterization technique was used to transform the MIOCP into a MINLP with Differential and Algebraic Constraints problem, which was then decomposed in a NLP/DAE primal and MILP master problem to provide upper and lower bounds of the solution. Three chemical engineering examples were effectively solved using this procedure.

More recently, Kookos and Perkins (2001) proposed a decomposition algorithm for the simultaneous design of structure and parameters of the process and the control system, based on the generation of lower and upper bounds on the optimal economical performance of the

plant. The authors found good results with convergence in two to five iterations, for three cases considered corresponding to different chemical processes.

The complexity of the decomposition algorithms and special formulations that are necessary to solve the aforementioned problems is a tangible weakness of the methods, even in the presence of good results. Therefore, alternative techniques such as stochastic optimization methods are important to consider. Genetic algorithms and simulated annealing have been used with good results for mixed integer non-linear problems related to the process engineering area (Costa and Oliveira, 2001; Tsai and Chang, 2001; Revollar *et al*., 2005; Francisco and Vega, 2006). In this work, we are concerned with the *Integrated Design* of an activated sludge process incorporating the plant structure selection to the simultaneous design and control formulation. The simultaneous design and control, for a given plant structure, was carried out in Gutierrez and Vega (2002) who used SQP based methods and considered controllability measures using the linearized model of the plant. Francisco and Vega (2006) also performed the *integrated design* for a particular configuration of the activated sludge plant, using linear measures as the H_∞ norm and dynamical performance indices. The stochastic optimization algorithms were used as an alternative to the SQP conventional method. The effectiveness of both methods for solving this complex problem was comparable.

The more complicated problem of integrated synthesis, design and control of the activated sludge process, was performed by Revollar *et al*. (2005) using a real coded genetic algorithm. They translated a superstructure containing two possible plant structures into a mixed-integer-non-linear optimization problem. They took into account economics along with the Integral Square Error (ISE) as a dynamical performance index. The genetic algorithm exhibited a good performance giving reasonable feasible solutions.

In this paper, we compare two stochastic optimization algorithms for the integrated synthesis, design and control of the activated sludge process, namely Simulated Annealing and a real-coded Genetic Algorithm. Basically, the optimization focuses on the minimization of the investment and operation costs and the desired dynamical performance is achieved by imposing a bound over the ISE. The problem results in a mixed-integer non-linear optimization which incorporates the evaluation of dynamical performance indices.

This paper is organized as follows: in Section 2, the process and the formulation of the optimization problem are described; then, in Section 3, the proposed algorithms are presented, followed by the analysis of the results in Section 4. Finally, conclusions and different projections of this work are included.

II. FORMULATION OF THE OPTIMIZATION PROBLEM

The activated sludge process was selected to study the simultaneous synthesis and control system design methodology. The worldwide trend to protect the environment has increased the demands for cost- reasonable technologies for wastewater treatment. The main problem is designing plants that appropriately accomplish the stringent environmental regulations with the lowest possible cost, which leads to the search of more efficient control strategies for their adequate operation (Samuelsson, *et al.,* 2005). The minimization of the investment and operational costs and the achievement of the effluent quality requirements can result into a conflict of interest that is compatible with the integrated design philosophy. On the other hand, the complexity and variability of the biological processes involved introduce non-linear characteristics to the process model, which makes the activated sludge process an interesting application to test the *integrated design* approach. In this work, a model developed by Moreno *et al*. (1992) based on the wastewater treatment process of the Manresa plant (Spain) is used as a working example.

A. Activated sludge process

The water treatment plants usually comprise three stages: the mechanical treatment, the chemical treatment and the biological treatment. In biological treatment, the microorganisms are used to remove the organic matter present in the incoming wastewater.

The activated sludge process is a typical biological treatment corresponding to the secondary 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. This biomass degrades the organic substrate converting it into inorganic products, more biomass and water. The dissolved oxygen required is provided by a set of aeration turbines. Water coming out of each reactor is passed to the settler, where the activated sludge is separated from the clean water and recycled to both bioreactors. After this process, the water contains approximately 10% of the waste material and is discharged to the river. Part of the settled activated sludge is recycled to re-inoculate the reactors.

Several models are available for the activated sludge process, but the most commonly used is the ASM1 developed for the International Association on Water Pollution Research and Control (IAWPRC). Since the primary goal of this work is to focus on the application of the integrated design methodology, the model presented in Moreno *et al*. (1992) has been selected, to avoid the excessive complexity of models such as the ASM1.

The model by Moreno *et al.* (1992) is founded in the classical Monod and Maynard-Smith model. It is assumed that the reactions take place in only one perfectly-mixed tank. Some of the parameters of this model are known (such as the volume of the aeration tanks or the area of the settler), but the rest are calculated to minimize a function expressed as the difference between the model output and real data from the plant when the same inputs are applied to both systems. The simplified plant diagram considered in the model is presented in Fig. 1.

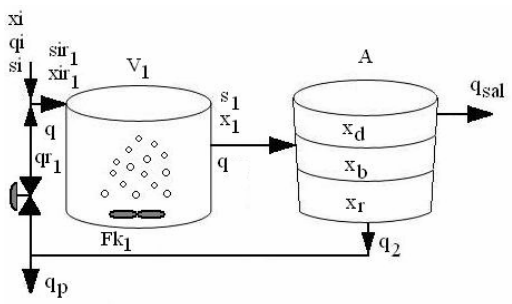

Figure. 1. Simplified structure of Manresa's activated sludge process

The rate of change of the biomass, organic substrate and dissolved oxygen concentrations in the aeration tank are described below. Table 1 shows the nomenclature and values for the operational, biological and physical parameters in the model.

$$\frac{dx}{dt} = \mu_{\max} Y \frac{sx}{(K_s + s)} - K_d \frac{x^2}{s} - K_c x + \frac{q}{V_1}(xir - x) \ . \quad (1)$$

The first term describes the biomass growth following the Monod model, the second describes cell death (as in the Volterra-Leslie modified model), the third describes the biological waste, and the final term quantifies the dilution effects.

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

In this equation, the first term expresses the decrease of the substrate through the activity of the biomass (Monod model), the second and third terms describe the transformation of the dead biomass and biological waste into organic substrate, and the last term is the difference between the input and output substrate mass flows.

$$\frac{dc}{dt} = K_{la} Fk_1 (c_s - c) - OUR - \frac{q}{V_1} c \ . \quad (3)$$

The oxygen balance follows the classic literature: the first term is the rate of oxygen transferred to the water, the second describes the rate of oxygen used by the microorganisms, and the final term quantifies the dilution effects. The Fk_1 is the aeration factor which is proportional to the speed of working turbines.

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

$$xir = \frac{xi \cdot qi + x_r \cdot q_2}{q} \quad (4)$$

$$sir = \frac{si \cdot qi + s \cdot q_2}{q} \quad (5)$$

The oxygen uptake rate (*OUR*) is:

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

In the secondary clarifier (settler), the operation is described by the mass balances and the expression for the settling of activated sludge. The model takes into account the difference in settling rates between layers of increasing biomass concentration. This model was presented in Moreno *et al.* (1992) as an attempt to capture the dynamic behaviour of the clarifiers, but is a simple representation.

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

$$A \cdot l_b \frac{dx_b}{dt} = q x_1 - q_{sal} x_b - q_2 x_b + A \cdot vs(x_d) - A \cdot vs(x_b) \quad (8)$$

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

The settling rate is calculated experimentally, the parameters are evaluated to fit a curve defined by experimental points:

$$vs(x_j) = nnr \cdot x_j \cdot e^{(-aar \cdot x_j)} \quad j : d, b, r \quad (10)$$

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

Symbol	Parameter	Value [units]
μ_{max}	Maximum growth rate of the microorganisms	0.1824 [h^{-1}]
Y	Yield coefficient between cellular growth and substrate elimination	0.5948
fkd	Yield coefficient between biomass endogenous and substrate contribution to the medium	0.2
K_d	Kinetic coefficient of biomass decay by endogenous metabolism	5.5e-5 [1/h]
K_s	Saturation constant	300
K_c	Kinetic coefficient of biomass decay by biological waste	1.333e-4 [1/h]
c_s	Saturation oxygen (DO) concentration in the aeration tanks	8 [mg/L]
Kla	Mass transfer coefficient in aeration process	0.7 [h^{-1}]
OUR	Oxygen uptake rate	
K_{01}	Yield coefficient between the cellular growth and the oxygen consumption rate	0.0001
xi	Biomass concentration at the influent	80 [mg/L]
si	Substrate concentration at the influent	366.67 [mg/L]
qi	Influent flow	1300 [m^3/h]
x	Biomass concentration at the output of the aeration tanks	[mg/L]
s	Substrate (COD) concentration at the output of the aeration tanks	[mg/L]
c	Dissolved oxygen (DO) concentration at the output of the aeration tanks	[mg/L]
q	Bioreactor input flow	[m^3/h]
q_2	Recycle flow	[m^3/h]
xir	Bioreactor inlet biomass concentration	[mg/L]
sir	Bioreactor inlet substrate concentration	[mg/L]
Fk_1	Aeration factor	
V_1	Bioreactor volume	[m^3]
A	Settler area	[m^2]
x_d	Biomass concentration at the surface of the settler	[mg/L]
x_b	Biomass concentration in the settler second layer	[mg/L]
x_r	Biomass concentration at the bottom of the settler	[mg/L]
vs	Settling rate of the activated sludge in the settler	[h^{-1}]
nnr	Empirical parameter for the settling rate relationship	3.1563
aar	Empirical parameter for the settling rate relationship	-0.000785
l_d	Height of the first layer of the settler	2m
l_b	Height of the second layer of the settler	1m
l_r	Height of the third layer of the settler	0.5m

B. Mathematical Optimization Problem

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 PI controller is tuned to achieve the desired closed loop dynamics. The dynamical performance is quantified using the Integral Square Error (ISE).

The two possible structural alternatives proposed for the plant are represented in a superstructure shown in Fig. 2. These alternatives consist on one or two aeration tanks and one secondary settler. The set of decision variables includes the process structure given by binary (y_1), dimensions, stationary working point and the PI controller parameters.

The activated sludge model described above 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 y_1.

The mathematical formulation of the process synthesis and design results in a mixed-integer non-linear optimization problem where the objective is to minimize a cost function considering as decision variables: the structure, dimensions of the plant and the controller parameters. Several constraints based on the process model are set to find dimensions and an initial working point. Specific constraints are imposed over the dynamical performance index to measure the controllability of the plant with the particular controller.

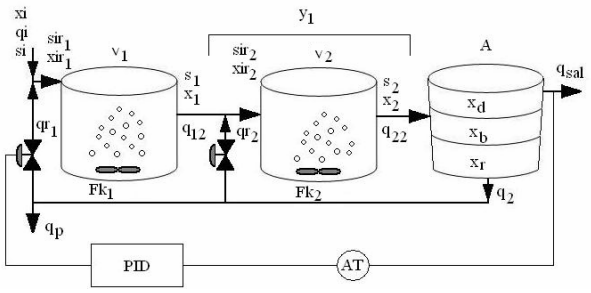

Figure 2. Activated sludge process superstructure

The formulation of the integrated approach is represented schematically in Fig. 3.

The cost function is:

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

where v_1, v_2 are the reactor volumes, 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 with the construction cost, considering that this cost is proportional to the volume of the reactors and the area of the settler (the height is fixed). 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).

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 $v_2=0$, $x_1=x_2$, $s_1=s_2$, $c_1=c_2$, $Fk_2=0$, $qr_2=0$. If the second reactor exists, then, $y_1=1$ and all the variables take values within their ranges.

The constraints imposed over mass balances in aeration tanks and settler, are used to define the plant dimensions and the initial stationary working point. Terms in the following equations are defined as in Table 1 and Fig. 2 and ε is the tolerance allowed (a very small number).

$$\left| v_1 \frac{dx_1}{dt} \right| = \left| \begin{array}{l} \mu_{\max} Y \dfrac{s_1 x_1}{(K_s + s_1)} v_1 - K_d \dfrac{x_1^2}{s_1} v_1 - K_c x_1 v_1 \\ + q_{12}(xir_1 - x_1) \end{array} \right| \le \varepsilon \quad (12)$$

$$\left| v_1 \frac{ds_1}{dt} \right| = \left| \begin{array}{l} -\mu_{\max} \dfrac{s_1 x_1}{(K_s + s_1)} v_1 + f_{kd} K_d \dfrac{x_1^2}{s_1} v_1 \\ + f_{kd} K_c x_1 v_1 + q_{12}(sir_1 - s_1) \end{array} \right| \le \varepsilon \quad (13)$$

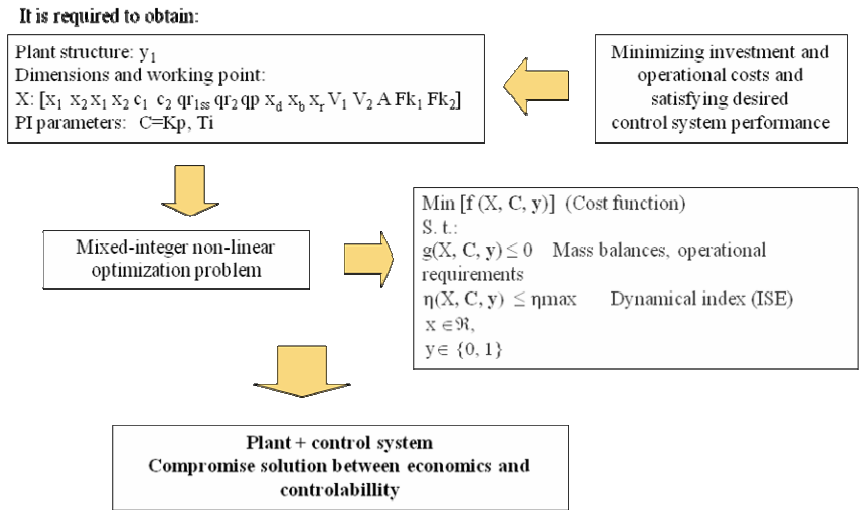

Figure 3. Schematic representation of the integrated synthesis, design and control approach

$$\left| v_1 \frac{dc_1}{dt} \right| = \left| \begin{array}{l} K_{la} Fk_1 \left(c_s - c_1 \right) v_1 - K_{01} \mu_{\max} \dfrac{s_1 x_1}{\left(K_s + s_1 \right)} v_1 \\ -q_{12} c_1 \end{array} \right| \le \varepsilon \quad (14)$$

$$\left| v_2 \frac{dx_2}{dt} \right| = \left| \begin{array}{l} \mu_{\max} Y \dfrac{s_2 x_2}{\left(K_s + s_2 \right)} v_2 - K_d \dfrac{x_2^2}{s_2} v_2 - K_c x_2 v_2 \\ +q_{22} \left(xir_2 - x_2 \right) \end{array} \right| \le \varepsilon \quad (15)$$

$$\left| v_2 \frac{ds_2}{dt} \right| = \left| \begin{array}{l} -\mu_{\max} \dfrac{s_2 x_2}{\left(K_s + s_2 \right)} v_2 + f_{kd} K_d \dfrac{x_2^2}{s_2} v_2 \\ +f_{kd} K_c x_2 v_2 + q_{22} \left(sir_2 - s_2 \right) \end{array} \right| \le \varepsilon \quad (16)$$

$$\left| v_2 \frac{dc_2}{dt} \right| = \left| \begin{array}{l} K_{la} Fk_2 \left(c_s - c_2 \right) v_2 - K_{01} \mu_{\max} \dfrac{s_2 x_2}{\left(K_s + s_2 \right)} v_2 \\ -q_{22} c_2 + W_1 \end{array} \right| \le \varepsilon \quad (17)$$

$$\left| Al_d \frac{dx_d}{dt} \right| = \left| q_{sal} x_b - q_{sal} x_d - A \cdot nnr \cdot x_d \exp\left(aar \cdot x_d \right) \right| \le \varepsilon \quad (18)$$

$$\left| Al_b \frac{dx_b}{dt} \right| = \left| \begin{array}{l} q_{22} x_2 - q_{sal} x_b + A \cdot nnr \cdot x_d \exp\left(aar \cdot x_d \right) \\ -A \cdot nnr \cdot x_b \exp\left(aar \cdot x_b \right) \end{array} \right| \le \varepsilon \quad (19)$$

$$\left| Al_r \frac{dx_r}{dt} \right| = \left| q_2 x_b - q_2 x_r + A \cdot nnr \cdot x_b \exp\left(aar \cdot x_b \right) \right| \le \varepsilon \quad (20)$$

If the second reactor does not exist (y_1=0), the values of the variables given by the logical conditions mentioned above, will set Eqs. (15) and (16) to zero. Another logical condition arises to cancel Eq. (17) fixing parameter W_1 as:

$$W_1 = q_{22} \cdot c_2 \quad (21)$$

The operation constraints for the activated sludge process are:

–Residence times:

$$2.5 \le \frac{v_1}{q_{12}} \le 8 \quad (22)$$

$$2 \le \frac{v_2 + (1 - y_1) \cdot W_2}{q_{22}} \le 6 \quad (23)$$

The last equation is written as:

$$v_2 + (1 - y_1) \cdot W_2 - 6 \cdot q_{22} \le 0 \quad (23a)$$

$$2 \cdot q_{22} - v_2 + (1 - y_1) \cdot W_2 \le 0 \quad (23b)$$

where the W_2 term is used to adjust the relation to the actual number of bioreactors $W_2 = 6 \cdot q_{22}$ for (23a) and $W_2 = -2 \cdot q_{22}$ for (23b).

–Mass loads in the aeration tanks:

$$0.001 \le \frac{qisi + qr_1 s_2}{v_1 x_1} \le ML_{\max} \quad (24)$$

$$0.001 \le \frac{q_{12} s_1 + qr_2 s_2 - \left(1 - y_1 \right) W_3}{v_2 x_2} \le ML_{\max} \quad (25)$$

where W_3 term is:

$$W_3 = \left(qr_1 + qi \right) \cdot s_1 \quad (26)$$

and $ML_{\max}$ is the maximum value admitted for the mass load, that can be changed according to the case studied.

– Sludge age in the settler:

$$SA_{\min} \le \frac{v_1 x_1 + v_2 x_2 + Al_r x_r}{q_p x_r 24} \le 10 \quad (27)$$

where $SA_{\min}$ is the minimum value for the sludge age in the settler.

– Limits in hydraulic capacity:

$$\frac{q_{22}}{A} \le 1.5 \quad (28)$$

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

$$0.03 \le \frac{q_p}{q_2} \le Rp_{\max} \quad (29)$$

$$Rr_{\min} \le \frac{q_2}{q_i} \le 0.9 \quad (30)$$

the bounds $Rp_{\max}$ and $Rr_{\min}$ are selected according to the actual operational requirements.

C. Process Control

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 of the incoming substrate concentration (si) and flow (qi). These disturbances are one of the main problems when trying to control the plant properly. The set of disturbances used to evaluate the control performance while tuning the PI has been taken from COST 624 program (Copp, 2002).

The controllability constraints are set to guarantee an appropriated dynamical response of the plant in terms of control objectives. The controlled variable is the output substrate concentration and the control signal is the recycle flow (qr_1). The control law corresponds to a PI controller:

$$qr_1 = qr_{1ss} + K_p . \left(s_{ref} - s_{(1+y_1)} \right) + \frac{1}{\tau_i} \int_{to}^{t} \left(s_{ref} - s_{(1+y_1)} \right) d\tau \quad (31)$$

where qr_{1ss} is the steady state qr_1 value.

The Integral Square Error (ISE) is applied as a dynamical index to provide a measure of the effect of the control strategy over the quality of the operation.

$$ISE = \int_{t=0}^{T\,max} \left(s_{ref} - s_{(1+y_1)} \right)^2 \cdot dt \quad (32)$$

where $Tmax$ is the simulation time and s_{ref} is the desired value for substrate concentration.

The constraint over the ISE is set as follows:

$$ISE \le ISE_{\max} \quad (33)$$

where $ISE_{\max}$ is the ISE upper bound that is selected according to the problem conditions and represent the minimum dynamic response requirements.

III. SOLVING THE PROBLEM USING STOCHASTIC OPTIMIZATION

A. Genetic algorithms (GA)

Genetic algorithms are stochastic optimization methods based on the principles of natural evolution (Goldberg, 1989). The optimization process is carried out with a population of potential solutions for the problem, coded as chromosomes. A fitness function is assigned to each chromosome as a measure of performance, associated with the objective function. The population evolves toward better regions in the search space by means of the genetic operators: selection, crossover and mutation (Goldberg, 1989). After several generations, the algorithm converges to the best solution of the problem.

Conventional genetic algorithms are binary coded. However, the use of real parameters makes possible the representation of large domains, which is difficult to achieve in binary implementations, and, additionally, improves the effectiveness for problems with a large number of constraints (Summanwar *et al*, 2002; Elliot *et al*., 2006). Another advantage of the real coding is that slight changes in the variables correspond to slight changes in the objective function (Elliot *et al*., 2006), which increases the capacity for the local tuning of the solutions. Here, a fixed length real coded chromosome is defined, which contains the continuous variables corresponding to the normalized process variables, controller parameters (*Kp, Ti*) and a binary variable to set the structure of the plant:

$$[x_1, x_2, s_1, s_2, c_1, c_2, x_d, x_b, x_r, qr_{1ss}, qr_2, q_p, Fk_1, Fk_2, v_1, v_2, A, Kp, Ti, y_1]$$

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

The genetic algorithm starts by randomly generating a population of a specific number of possible solutions that contains the same quantity of individuals for the two structural alternatives (y_1=0 and y_1=1). Each solution in this population is manipulated to fulfill the logical conditions mentioned in section 2.2, according to the actual value of y_1.

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:

$$z_i = \lambda \cdot x_i + (1-\lambda) \cdot y_i \tag{34}$$

where $0 \leq \lambda \leq 1$. 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.

The simplest way of solving constrained optimization problems is to search the optimal only in the feasible region, but it requires an intensive computational effort (Summanwar *et al.,* 2002). Therefore, an appropriate technique to deal with constraints is needed. A general approach borrowed from conventional optimization is to incorporate the constraints into the objective function as a penalty term.

$$F(x) = f(x) + R\left(\sum_{k=1}^{p}\left[\max\{0, g_k(x)\}\right]^2\right) \tag{35}$$

where x is the chromosome, F is the fitness function, f is the cost function, R is the penalty coefficient associated with the inequality constraints $g_k(x)$, and p is the number of inequality constraints. This penalization strategy focuses on the constraints over mass balances, the operational specifications and the controllability indices. The logical constraints and the ranges for the variables are handled in the chromosome coding.

As a technique to improve the agreement in the ISE controllability constraint, some of the individuals with the best ISE index (10% of population size) are selected to survive in the successive generation.

The problem is solved using a population size of 200 individuals and 1500 maximum iterations. The mutation rate decreases with generations from 0.1 to 0.02 and the crossover probability used is 85%.

B. Simulated annealing (SA)

The simulated annealing is a computational stochastic technique for solving different optimization problems. The method is inspired from the thermodynamic process of annealing of molten solids to attain the minimum energy state by decreasing the temperature slowly. In the initial state, the particles are arranged in a highly structured lattice and the energy of the system is minimal.

This physical process can be modeled by considering a simple algorithm that generates a sequence of states of the solid. Given a current state i with energy E_i, a new state with energy E_j is created applying some perturbation mechanism. If the energy decreases, the new state is accepted as the current state, but if it increases, the new state is accepted with a certain probability (*prob*) given by:

$$prob = \exp\left(\frac{E_i - E_j}{K_B T}\right) \tag{36}$$

where T is the temperature of the solid and K_B is the Boltzmann constant. If the lowering of T is sufficiently slow, the solid can reach thermal equilibrium at each temperature. This is achieved in the method by generating a large number of transitions at every temperature.

In the simulated annealing, an analogy is assumed between the physical system and the optimization problem, based on the following equivalences: solid states represent candidate solutions, and their energy is the cost associated with each of them. There is also a control parameter, which is equivalent to the temperature of the system.

The simulated annealing algorithm works as follows: starting with a random initial point, a sequence of

states (candidate solutions) is generated iteratively using the following acceptance criteria: if i is the current solution with cost $f(i)$, and j is a new generated candidate with cost $f(j)$, the acceptance probability of taking j as new candidate solution is

$$P(accept\ j)=\begin{cases}1 & if\ f(j)\le f(i)\\ \exp\left(\dfrac{f(i)-f(j)}{c}\right) & if\ f(j)>f(i)\end{cases} \tag{37}$$

where c is the control parameter that decreases with iterations.

The search strategy is such that at the start almost any solution is accepted, because c is large, but when this parameter decreases, the algorithm becomes more selective in accepting new solutions. By the end, only the improving moves are accepted in practice. This acceptance probability (37), which allows the algorithm to select solutions that increase cost, avoids local minima. The decreasing schedule for control parameter c is usually problem-dependent and is called cooling schedule. For a review of different approaches see (Salamon, 2002, Suman, 2004).

In this work a simple linear cooling is used to get proper results, with rate of 0.88. This rate is selected in order to get a particularly slow decreasing of c, providing a wide search in the first stage of the algorithm.

Candidate solutions are encoded as normalized vectors as presented in the genetic algorithm. They contain real numbers for the plant and controller parameters. The last element of the solution is the binary variable for the plant selection. The generation of a new candidate occurs by randomly changing four variables of the solution at the same time, together with the binary variable providing a more complete search of the space. The number of iterations for each temperature (chain length) starts as 120 and increases by a factor of $\beta=1.02$. The initial temperature is 50, which has been selected to provide an initial acceptance rate of 0.9. The total number of iterations is 120, which is long enough to achieve convergence.

As for constraints handling, a similar approach to the genetic algorithm is implemented. The constraints are added to the cost function as penalty terms, modulated by weights.

C. Stochastic Optimization Procedure and Algorithm Evaluation

The problems that arise from the *integrated approach* of the activated sludge process design are solved applying the algorithms described above.

For each candidate solution the evaluation of the optimization model proceeds as follows:

- The chromosome or state (for GA or SA, respectively) is decoded to take the real values of variables between their lower and upper bound.
- The mass balances and operation requirements Eqs. (12) to (30) are evaluated. The candidates that satisfy these constraints contain appropriated values for dimensions and stationary initial working point. On the other hand, if the constraints are not satisfied, a penalization term is added to the objective function.
- A simulation of the process model under disturbances is performed to calculate the ISE and verify Eq. (33). If this equation is not satisfied a term proportional to the deviation is included in the penalization of the objective function. For the candidate solutions that give unstable plants the simulation is avoided and a larger penalization value is assigned to the objective function.

In previous results (Revollar *et al,* 2005; Francisco and Vega, 2006) it has been observed that the stringent process conditions of the Manresa plant impose significant limitations on the control performance. Therefore, in this work, the optimization has been carried out contemplating two scenarios:

Scenario 1: considering the original operational conditions shown in Table 2 for Eqs. (22) to (30) (Moreno *et al.*, 1992)

Scenario 2: considering the relaxation of the operational conditions, as shown in the second column in Table 2, in order to improve the controllability of the plant.

Scenario 1 is selected to test the sensitivity of the stochastic algorithms to changes in their tuning parameters. In Table 3 the average cost value, the best solution cost, and the repeatability (measured as the difference between maximum and minimum costs) are presented (only for AG and SA) for the Scenario 1.

The SA has been evaluated changing the parameter c (0.78; 0.88; 0.95), which is a factor that determines the decreasing speed of the temperature in the algorithm. The optimal value for c is 0.88, giving the best repeatability, cost value, and percentage of feasible solutions. For the largest c parameter evaluated (c=0.95), there is not enough repeatability to report the results. The performance of the AG for different parameter combinations is also shown in table 3, where it can be observed that the variation of these parameters affects only the repeatability.

Table 2: Bounds for constraints for the two scenarios studied

Parameters	Scenario 1	Scenario 2
ML_{max}	0.06	0.12
SA_{min}	3	2
Rp_{max}	0.07	0.7
Rr_{min}	0.5	0.05

Table 3: Algorithms sensitivity to tuning parameters for the activated sludge process economical plant for scenario 1

Simulated Annealing	Average	Best solution	Repeatability
c=0.78	0.19	0.17	0.04
c=0.88	0.18	0.16	0.03
Genetic Algorithms	**Average**	**Best solution**	**Repeatability**
R=0.001	0.1984	0.180	0.028
R=0.01	0.1980	0.183	0.029
R=0.1	0.2080	0.183	0.058

IV. RESULTS

In order to compare the effectiveness of stochastic and deterministic methods, the design considering only the economical objectives (economical design) is carried out for both scenarios using the stochastic methods studied and a deterministic Branch and Bound algorithm.

The solution obtained with the B&B algorithm for *Scenario 1*, is a plant containing only one reactor, with a cost of 0.17. The stochastic algorithms give solutions close to the optimum solutions with small relative errors of 7 % for SA, and 5 % for AG. The three algorithms give the same solutions for the Scenario 2. Detailed results are presented below in Table 4. These results are to be compared to those obtained using the integrated approach to show the advantages of the integrated design considering cost and the global performance of the plant.

Scenario 1.

The results of the integrated design considering scenario 1 are shown in Table 5. As can be seen, the best plant corresponds to the two reactors structure ($y_1=1$), with larger dimensions than the economically optimal plant (Table 4). Larger plants provide better controllability which allows to satisfy the imposed ISE constraint ($ISE<2500$).

The simulations of the s_2 for both cases are shown in Fig. 4 and compared to the economical plant response. The effect of the control system is evidenced by comparing these responses and observing the significant reduction in the variations produced by the disturbances in the substrate concentration.

Table 4: Results for the plant designed considering only economical objectives

Parameters	Scenario 1	Scenario 2
Cost	0.17	0.04
Number of reactors	1	2
s_1 (mg/l)	87.75	196.67
s_2 (mg/l)	-	92.43
V_1 (m^3)	5278.8	3709.6
V_2 (m^3)	-	3102.5
A (m^2)	1787.9	1456.4
qr_1 (m^3/h)	630.5	166.96
qr_2 (m^3/h)	-	11.6
Fk_1	0.076	0.005
Fk_2	-	0.215

Table 5: Algorithms performance for the integrated synthesis and design of the activated sludge process with PI control for scenario 1

Parameters	Genetic algorithm	Simulated Annealing
Cost	0.25	0.2911
s_1 (mg/l)	68.95	81.98
s_2 (mg/l)	27.02	25.68
V_1 (m^3)	6531.6	5281.5
V_2 (m^3)	3048.5	3964.9
A (m^2)	2517.1	2588.8
qr_1 (m^3/h)	643.49	643.4
qr_2 (m^3/h)	0.46	0.18
Fk_1	0.175	0.037
Fk_2	0.128	0.067
Kp	-2.58	-12.24
Ti	137.75	188.11
ISE	1875.9	1901.7

Scenario 2.

In order to improve the controllability of the plant, a second scenario was selected for the synthesis and control system design, relaxing process constrains as mentioned previously. The ISE constraint was reduced to ISE<2000, because the plant is more controllable. The results, considering the ISE as controllability index, are presented in Table 6.

The solutions are plants with two reactors, but with smaller costs. The output substrate concentrations are similar to those obtained in scenario 1, but the recycling flow is much smaller, providing larger range for acceptable control actions and smaller costs.

The simulations of the s_2 response are shown in Fig. 5, exhibiting similar characteristics to scenario 1 when compared to the economical plant response.

Generally speaking about the simultaneous synthesis and control system design results, it is important to remark that the stochastic algorithms select the process structure in a one step optimization procedure in contrast to the required decomposition algorithms found in the literature.

V. CONCLUSIONS AND FUTURE WORK

In this work, the integrated synthesis and design of an activated sludge process was addressed. This problem translates into a mixed-integer-non-linear optimization problem which requires the evaluation of dynamical-performance-indices for the simultaneous process and control system design. Two stochastic methods: a genetic algorithm and simulated annealing are applied and compared to solve this challenging optimization problem.

The structure of the plants obtained applying the integrated synthesis and design procedure consists on two-reactors-one-settler, which is structurally different to the one-reactor-one-settler economical designs. Those plants are larger (with the corresponding increase in the investment and operation costs) but they show a significant improvement in the dynamical performance indices.

Table 6: Algorithms performance for the integrated synthesis and design of the activated sludge process with PI control for scenario 2

Parameters	Genetic algorithm	Simulated Annealing
Cost	0.1728	0.1611
s_1 (mg/l)	104.51	131.52
s_2 (mg/l)	32.65	27.72
V_1 (m^3)	4526.6	3737.8
V_2 (m^3)	3403.4	6100.1
A (m^2)	2208.8	2212.3
qr_1 (m^3/h)	265.34	234.82
qr_2 (m^3/h)	1.52	1.64
Fk_1	0.269	0.076
Fk_2	0.231	0.160
Kp	-39.32	-40.65
Ti	138.76	112.84
ISE	1046.7	823.98

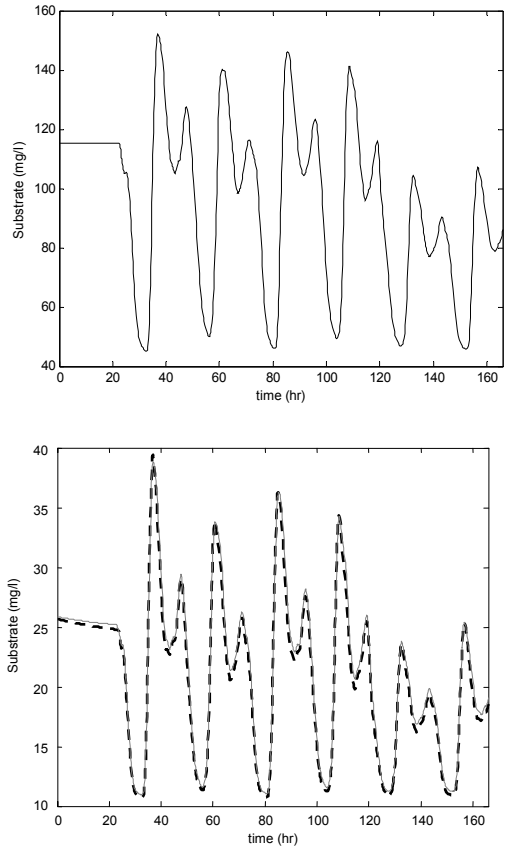

Figure 4: Output substrate response for the economical plant (upper figure) and the plant obtained by synthesis and control system design for scenario 1(lower figure). SA (dotted) and AG (solid).

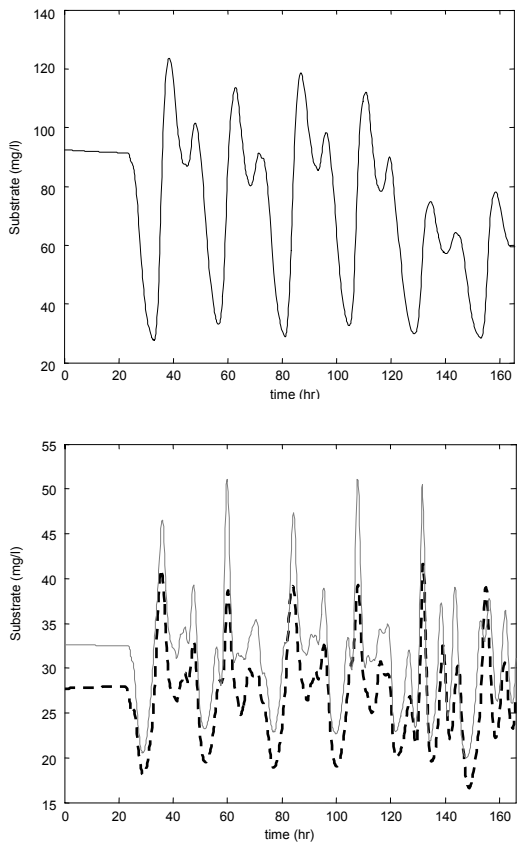

Figure 5: Output substrate response for the economical plant (upper figure) and the plant obtained by synthesis and control system design for scenario 2 (lower figure). SA (doted) and AG (solid).

As was expected, the performance of both algorithms in the basic case of economical synthesis and design was similar. The relevance of the stochastic methods as an alternative was evidenced in the complex problem of simultaneous synthesis, process and control-system design (Synthesis and integrated design), because they are able to automatically select the plant configuration, producing solutions with enhanced controllability indices.

The controllability indices were handled by the stochastic algorithms as constraints in the formulation of the optimization problem. This strategy was useful and easy to apply. However, in future work it would be more appropriated to consider each quality (cost and controllability) as separate objectives in a multi-objective optimization problem.

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REFERENCES

Copp, J.B., "The COST Simulation Benchmark: Description and Simulator Manual". *Office for Official Publications of the European Community.* (2002).

Costa, L. and P. Oliveira. "Evolutionary algorithms approach to the solution of mixed integer-non-linear programming problems," *Comp. Chem. Eng.,* **25**, 257-266 (2001).

Elliott, L., D. Ingham, A. Kyne, N. Mera, M. Porkashanian and S. Whittaker, "Reaction mechanism reduction and optimization for modeling aviation fuel oxidation using standard and hybrid genetic algorithms," *Comp. Chem. Eng.,* **30**, 889–900 (2006).

Francisco, M. and P. Vega, "Diseño Integrado de procesos de depuración de aguas utilizando Control Predictivo Basado en Modelos". *Rev. Ibero-americana de Automática e Informática Industrial*, **3**, 88-98 (2006).

Gen, M. and R. Chen, *Genetic algorithms and engineering optimisation*. J.W. and Sons (2000),

Goldberg, D.F, *Genetic Algorithm in Search, Optimization and Machine Learning*. Addison-Wesley, Reading, MA. (1989).

Gutiérrez, G. and P. Vega, "Integrated design of chemical processes and their control system including closed loop properties for disturbances rejection," *15th IFAC Triennal World Congress*. Barcelona (2002).

Kookos, I. and J. Perkins, "An algorithm for simultaneous process design and control," *Ind. Eng. Chem. Res*. **40**, 4079-4088 (2001).

Luyben, W., "Trade-offs between design and control in chemical reactor systems," *J. Proc. Cont.,* **3**, 17-41 (1993).

Luyben, M. and C. Floudas, "Analyzing the interaction of design and control–1. A multiobjective framework and application to binary distillation synthesis," *Comp. Chem. Eng*., **18**, 933-969 (1994).

Moreno, R., C. De Prada, J. Lafuente, M. Poch and G. Montague, "Non-linear predictive control of dissolved oxygen in the activated sludge process," *IFAC BIO,* **2** 289-298 (1992).

Narraway, L.T. and J.D. Perkins, "Selection of process control structure based en economics," *Comp. Chem.. Eng.,* **18**, S511-S515 (1994).

Revollar, S, R. Lamanna and P Vega, "Algorithmic synthesis and integrated design for activated sludge processes using genetic algorithms," *ESCAPE 15,* Barcelona, 725-730 (2005).

Revollar, S., R. Lamanna and P Vega, "Genetic Algorithms for simultaneous design and control of Continuous Stirred Tank Reactor System". *Proceedings Chemical Process Control, 7*, Lake Louise (2006).

Sakizlis, S., J. Perkins and E. Pistikopoulos, "Recent advances in optimization-based simultaneous process and control design," *Computers and Chemical Engineering*, **28**, 2069-2086 (2004).

Salomon, P., P. Sibani and R. Frost, "Facts, Conjectures, and Improvements for Simulated Annealing," *SIAM Monographs on Mathematical Modelling and Computation* (2002).

Samuelsson, P., B. Halvarsson and B. Carlsson, *Cost-Efficient Operation of a Denetrifying Activated Sludge Process – An initial Study,* Technical reports from the Department of Information Technology. Upsala Universitet. (2005)

Schweiger, C and C. Floudas, "Interaction of design and control: Optimization with dynamic models," In W. Hager and P. Pardalos (Eds.) *Optimal control: Theory, algorithms and Applications,* Kluwer Academic Publishers, 388-435 (1997).

Suman, B., "Study of simulated annealing based algorithms for multiobjective optimization of a constrained problem," *Computers and Chemical Engineering*, **28**, 1849-1871 (2004).

Summanwar, V., V. Jayaraman, H. Kulkarni, H., Kusumakar, K. Gupta and J. Rajesh, "Solution of constrained optimization problems by multiobjective genetic algorithm," *Computers and Chemical Engineering*, **26**, 1481-1492 (2002).

Viswanathan, J. and I. Grossman, "A compiled penalty function and outer approximations method for MINLP optimization," *Computers and Chemical Engineering*, **14**, 769-780 (1990).

Tlacuahuac-Flores, A and L. Biegler, "Integrated Control and Process Design During Optimal Polymer Grade Transitions Operations," *Computers and Chemical Engineering*, **31**, 2823-2837 (2008).

Tsai, M. and C. Chang, "Water usage and treatment network design using genetic algorithms," *Ind. Eng. Chem. Res.* **40**, 4874-4888 (2001).

Ziegler, J.G. and N.B. Nichols, "Optimum settings for automatic controllers," *Transactions of ASME*, **64**, 759-768 (1942).

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