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 MIDI 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 (Viswanathan 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
The activated sludge process was selected to study the simultaneous design and control of the activated sludge process. 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 $H_\infty$ 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.
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.

\[
\frac{dx}{dt} = \mu_{\text{max}}Y\frac{s}{(K_s + s)} - K_d x + \frac{q}{V_i} (x_{ir} - x) .
\]

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.

\[
\frac{ds}{dt} = -\mu_{\text{max}}\frac{s}{(K_s + s)} + f_{s0} K_s \frac{x^2}{s} + f_{s0} K_c x + \frac{q}{V_i} (s_{ir} - s) .
\]

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.

\[
\frac{dc}{dt} = K_d F k_i (c_{i} - c) - OUR - \frac{q}{V_i} c .
\]

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 \( F k_i \) is the aeration factor which is proportional to the speed of working turbines.

The algebraic equations obtained from the mass balances for \( x_{ir} \) and \( s_{ir} \) are:

\[
x_{ir} = \frac{x_i q_i + x_r q_r}{q} .
\]

\[
s_{ir} = \frac{s_i q_i + s_r q_r}{q} .
\]

The oxygen uptake rate (OUR) is:

\[
OUR = -K_{d0}\mu_{\text{max}}\frac{x}{(K_s + s)} .
\]

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.

\[
A_{11} \frac{dx_{1}}{dt} = q_{w1} x_{1} - q_{w2} x_{2} - A_{1} \cdot \text{vs} (x_{1}) .
\]

\[
A_{12} \frac{dx_{2}}{dt} = q_{r1} x_{2} - q_{r2} x_{3} + A_{1} \cdot \text{vs} (x_{2}) - A_{1} \cdot \text{vs} (x_{1}) .
\]

\[
A_{13} \frac{dx_{3}}{dt} = q_{r3} x_{3} - q_{r4} x_{4} + A \cdot \text{vs} (x_{3}) .
\]

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

\[
\text{vs} (x_j) = \text{nnr} \cdot x_j \cdot e^{-\text{nrr} x_j} .
\]

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

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Value [units]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu_{\text{max}} )</td>
<td>Maximum growth rate of the microorganisms</td>
<td>0.1824 [h(^{-1})]</td>
</tr>
<tr>
<td>( Y )</td>
<td>Yield coefficient between cellular growth and substrate elimination</td>
<td>0.5948</td>
</tr>
<tr>
<td>( f_{s0} )</td>
<td>Yield coefficient between biomass endogenous and substrate contribution to the medium</td>
<td>0.2</td>
</tr>
<tr>
<td>( K_d )</td>
<td>Kinetic coefficient of biomass decay by endogenous metabolism</td>
<td>5.5e-5 [1/h]</td>
</tr>
<tr>
<td>( K_{s0} )</td>
<td>Saturation constant</td>
<td>300</td>
</tr>
<tr>
<td>( K_{c0} )</td>
<td>Kinetic coefficient of biomass decay by biological waste</td>
<td>1.333e-4 [1/h]</td>
</tr>
<tr>
<td>( c_i )</td>
<td>Saturation oxygen (DO) concentration in the aeration tanks</td>
<td>8 [mg/L]</td>
</tr>
<tr>
<td>( K_{la} )</td>
<td>Mass transfer coefficient in aeration process</td>
<td>0.7 [h(^{-1})]</td>
</tr>
<tr>
<td>( \text{OUR} )</td>
<td>Oxygen uptake rate</td>
<td>0.0001</td>
</tr>
<tr>
<td>( xi )</td>
<td>Biomass concentration at the influent</td>
<td>80 [mg/L]</td>
</tr>
<tr>
<td>( si )</td>
<td>Substrate concentration at the influent</td>
<td>366.67 [mg/L]</td>
</tr>
<tr>
<td>( qi )</td>
<td>Influent flow</td>
<td>1300 [m(^3)/h]</td>
</tr>
<tr>
<td>( x )</td>
<td>Biomass concentration at the output of the aeration tanks</td>
<td>[mg/L]</td>
</tr>
<tr>
<td>( s )</td>
<td>Substrate (COD) concentration at the output of the aeration tanks</td>
<td>[mg/L]</td>
</tr>
<tr>
<td>( c )</td>
<td>Dissolved oxygen (DO) concentration at the output of the aeration tanks</td>
<td>[mg/L]</td>
</tr>
<tr>
<td>( q )</td>
<td>Bioreactor input flow</td>
<td>[m(^3)/h]</td>
</tr>
<tr>
<td>( q_{r} )</td>
<td>Recycle flow</td>
<td>[m(^3)/h]</td>
</tr>
<tr>
<td>( x_{ir} )</td>
<td>Bioreactor inlet biomass concentration</td>
<td>[mg/L]</td>
</tr>
<tr>
<td>( s_{ir} )</td>
<td>Bioreactor inlet substrate concentration</td>
<td>[mg/L]</td>
</tr>
<tr>
<td>( Fk_i )</td>
<td>Aeration factor</td>
<td></td>
</tr>
<tr>
<td>( V_i )</td>
<td>Bioreactor volume</td>
<td>[m(^3)]</td>
</tr>
<tr>
<td>( A )</td>
<td>Settler area</td>
<td>[m(^2)]</td>
</tr>
<tr>
<td>( x_s )</td>
<td>Biomass concentration at the surface of the settler</td>
<td>[mg/L]</td>
</tr>
<tr>
<td>( x_{sl} )</td>
<td>Biomass concentration in the settler second layer</td>
<td>[mg/L]</td>
</tr>
<tr>
<td>( x_r )</td>
<td>Biomass concentration at the bottom of the settler</td>
<td>[mg/L]</td>
</tr>
<tr>
<td>( vs )</td>
<td>Settling rate of the activated sludge in the settler</td>
<td>[h(^{-1})]</td>
</tr>
<tr>
<td>( nnn )</td>
<td>Empirical parameter for the settling rate relationship</td>
<td>3.1563</td>
</tr>
<tr>
<td>( aar )</td>
<td>Empirical parameter for the settling rate relationship</td>
<td>-0.000785</td>
</tr>
<tr>
<td>( l_{f1} )</td>
<td>Height of the first layer of the settler</td>
<td>2m</td>
</tr>
<tr>
<td>( l_{f2} )</td>
<td>Height of the second layer of the settler</td>
<td>1m</td>
</tr>
<tr>
<td>( l_{f3} )</td>
<td>Height of the third layer of the settler</td>
<td>0.5m</td>
</tr>
</tbody>
</table>
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.

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

The cost function is:

\[
f = p_1 \cdot v_1^2 + p_2 \cdot v_2^2 + p_3 \cdot A^2 + p_4 \cdot Fk_1^2 + p_5 \cdot Fk_2^2 + p_6 \cdot q_2^2 \]  
(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 \( v_2=0, \; s_1=s_2, \; c_1=c_2, \; Fk_2=0, \; qr_2=0 \). 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 \( \varepsilon \) is the tolerance allowed (a very small number).

\[
\begin{align*}
\frac{dx_1}{dt} &= \mu_{max} \frac{x_1}{(K_1 + s_1)} v_1 - K_1 \frac{x_1^2}{s_1} v_1 - K_2 x_1 v_1 + q_1 (x_{1r} - x_1) \\
\frac{dx_2}{dt} &= -\mu_{max} \frac{x_2}{(K_2 + s_2)} v_2 + f_{Kx1} K_1 \frac{x_1^2}{s_1} v_1 + q_2 (x_{2r} - x_2)
\end{align*}
\]  
(12)

\[
\begin{align*}
\frac{dx_3}{dt} &= \frac{\mu_{max} x_3}{(K_1 + s_1)} v_1 - f_{Kx1} K_1 x_1 v_1 + q_1 (x_{3r} - x_3)
\end{align*}
\]  
(13)

Figure 2. Activated sludge process superstructure

Figure 3. Schematic representation of the integrated synthesis, design and control approach
If the second reactor does not exist \( \left( y_1 = 0 \right) \), 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:

\[
W_1 = q_{22} \cdot c_2 \tag{21}
\]

The operation constraints for the activated sludge process are:

- Residence times:

\[
2.5 \leq \frac{V_2}{q_{i2}} \leq 8 \tag{22}
\]

\[
2 \leq \frac{V_2 + (1 - y_1) \cdot W_2}{q_{22}} \leq 6 \tag{23}
\]

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:

\[
0.001 \leq \frac{q_{i1} s_i + q r_{s1}}{v_i x_1} \leq ML_{\text{max}} \tag{24}
\]

\[
0.001 \leq \frac{q_{12} s_1 + q r_{s1} - (1 - y_1) \cdot W_s}{v_i x_2} \leq ML_{\text{max}} \tag{25}
\]

where \( W_s \) term is:

\[
W_s = (q r_s + q i) \cdot s_i \tag{26}
\]

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

- Sludge age in the settler:

\[
SA_{\text{min}} \leq \frac{v_i x_1 + v_2 x_2 + A l x_s}{q_p x_24} \leq 10 \tag{27}
\]

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

- Limits in hydraulic capacity:

\[
\frac{q_{22}}{A} \leq 1.5 \tag{28}
\]

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

\[
0.03 \leq \frac{q_p}{q_{i2}} \leq \frac{R_{p_{\text{max}}}}{q_{i2}} \leq 0.9 \tag{29} \]

the bounds \( R_{p_{\text{max}}} \) and \( R_{r_{\text{max}}} \) 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 \( (s_i) \) and flow \( (q_i) \). 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 \( (q r) \). The control law corresponds to a PI controller:

\[
q r = q r_{\text{ss}} + \frac{1}{T_{i2}} \int_{t=0}^{t} (s_{\text{ref}} - s_{t_{(1+y_1)})}) dt \tag{31}
\]

where \( q r_{\text{ss}} \) is the steady state \( q r \) 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.

\[
ISE = \left. \int_{t=0}^{T_{\text{max}}} (s_{\text{ref}} - s_{t_{(1+y_1)})})^2 \cdot dt \right. \tag{32}
\]

where \( T_{\text{max}} \) is the simulation time and \( s_{\text{ref}} \) is the desired value for substrate concentration.

The constraint over the ISE is set as follows:

\[
ISE \leq ISE_{\text{max}} \tag{33} \]

where \( ISE_{\text{max}} \) 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:

\[ [x_1, x_2, x_3, s_1, s_2, c_1, c_2, x_6, x_8, q_{r1s}, q_{r2}, q_p, F_{k1}, F_{k2}, v_1, v_2, A, Kp, T_i, y_1] \]

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 logic 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:

\[ z_i = \lambda \cdot x_i + (1-\lambda) \cdot y_i \]  \hspace{1cm} (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.

\[ F(x) = f(x) + R \left( \sum_{i=1}^{n} \max \{0, g_i(x)\} \right)^2 \]  \hspace{1cm} (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 \( g_i(x) \), 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 \( (\text{prob}) \) given by:

\[ \text{prob} = \exp \left( \frac{E_i - E_j}{K_b T} \right) \]  \hspace{1cm} (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

\[
P\text{(accept)} j = \begin{cases} 1 & \text{if } f(j) \leq f(i) \\ \exp\left(\frac{f(i) - f(j)}{c}\right) & \text{if } f(j) > f(i) \end{cases}
\]

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>
<thead>
<tr>
<th>Parameters</th>
<th>Scenario 1</th>
<th>Scenario 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>( ML_{max} )</td>
<td>0.06</td>
<td>0.12</td>
</tr>
<tr>
<td>( SA_{max} )</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>( Rp_{max} )</td>
<td>0.07</td>
<td>0.7</td>
</tr>
<tr>
<td>( Rg_{max} )</td>
<td>0.5</td>
<td>0.05</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Simulated Annealing</th>
<th>Average</th>
<th>Best solution</th>
<th>Repeatability</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c=0.78 )</td>
<td>0.19</td>
<td>0.17</td>
<td>0.04</td>
</tr>
<tr>
<td>( c=0.88 )</td>
<td>0.18</td>
<td>0.16</td>
<td>0.03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Genetic Algorithms</th>
<th>Average</th>
<th>Best solution</th>
<th>Repeatability</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R=0.001 )</td>
<td>0.1984</td>
<td>0.180</td>
<td>0.028</td>
</tr>
<tr>
<td>( R=0.01 )</td>
<td>0.1980</td>
<td>0.183</td>
<td>0.029</td>
</tr>
<tr>
<td>( R=0.1 )</td>
<td>0.2080</td>
<td>0.183</td>
<td>0.058</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Scenario 1</th>
<th>Scenario 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost</td>
<td>0.17</td>
<td>0.04</td>
</tr>
<tr>
<td>Number of reactors</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>$s_1 (mg/l)$</td>
<td>87.75</td>
<td>196.67</td>
</tr>
<tr>
<td>$s_2 (mg/l)$</td>
<td>-</td>
<td>92.43</td>
</tr>
<tr>
<td>$V_1 (m^3)$</td>
<td>5278.8</td>
<td>3709.6</td>
</tr>
<tr>
<td>$V_2 (m^3)$</td>
<td>-</td>
<td>3102.5</td>
</tr>
<tr>
<td>$A (m^2)$</td>
<td>1787.9</td>
<td>1456.4</td>
</tr>
<tr>
<td>$q_{r_1} (m^3/h)$</td>
<td>630.5</td>
<td>166.96</td>
</tr>
<tr>
<td>$q_{r_2} (m^3/h)$</td>
<td>-</td>
<td>11.6</td>
</tr>
<tr>
<td>$F_{k_1}$</td>
<td>0.076</td>
<td>0.005</td>
</tr>
<tr>
<td>$F_{k_2}$</td>
<td>-</td>
<td>0.215</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Genetic algorithm</th>
<th>Simulated Annealing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost</td>
<td>0.25</td>
<td>0.2911</td>
</tr>
<tr>
<td>$s_1 (mg/l)$</td>
<td>68.95</td>
<td>81.98</td>
</tr>
<tr>
<td>$s_2 (mg/l)$</td>
<td>27.02</td>
<td>25.68</td>
</tr>
<tr>
<td>$V_1 (m^3)$</td>
<td>6531.6</td>
<td>5281.5</td>
</tr>
<tr>
<td>$V_2 (m^3)$</td>
<td>3048.5</td>
<td>3964.9</td>
</tr>
<tr>
<td>$A (m^2)$</td>
<td>2517.1</td>
<td>2588.8</td>
</tr>
<tr>
<td>$q_{r_1} (m^3/h)$</td>
<td>643.49</td>
<td>643.4</td>
</tr>
<tr>
<td>$q_{r_2} (m^3/h)$</td>
<td>0.46</td>
<td>0.18</td>
</tr>
<tr>
<td>$F_{k_1}$</td>
<td>0.175</td>
<td>0.037</td>
</tr>
<tr>
<td>$F_{k_2}$</td>
<td>0.128</td>
<td>0.067</td>
</tr>
<tr>
<td>$K_p$</td>
<td>-2.58</td>
<td>-12.24</td>
</tr>
<tr>
<td>$T_i$</td>
<td>137.75</td>
<td>188.11</td>
</tr>
<tr>
<td>ISE</td>
<td>1875.9</td>
<td>1901.7</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Genetic algorithm</th>
<th>Simulated Annealing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost</td>
<td>0.1728</td>
<td>0.1611</td>
</tr>
<tr>
<td>$s_1 (mg/l)$</td>
<td>104.51</td>
<td>131.52</td>
</tr>
<tr>
<td>$s_2 (mg/l)$</td>
<td>32.65</td>
<td>27.72</td>
</tr>
<tr>
<td>$V_1 (m^3)$</td>
<td>4526.6</td>
<td>3737.8</td>
</tr>
<tr>
<td>$V_2 (m^3)$</td>
<td>3403.4</td>
<td>6100.1</td>
</tr>
<tr>
<td>$A (m^2)$</td>
<td>2208.8</td>
<td>2212.3</td>
</tr>
<tr>
<td>$q_{r_1} (m^3/h)$</td>
<td>265.34</td>
<td>234.82</td>
</tr>
<tr>
<td>$q_{r_2} (m^3/h)$</td>
<td>1.52</td>
<td>1.64</td>
</tr>
<tr>
<td>$F_{k_1}$</td>
<td>0.269</td>
<td>0.076</td>
</tr>
<tr>
<td>$F_{k_2}$</td>
<td>0.231</td>
<td>0.160</td>
</tr>
<tr>
<td>$K_p$</td>
<td>-39.32</td>
<td>-40.65</td>
</tr>
<tr>
<td>$T_i$</td>
<td>138.76</td>
<td>112.84</td>
</tr>
<tr>
<td>ISE</td>
<td>1046.7</td>
<td>823.98</td>
</tr>
</tbody>
</table>
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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