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Simultaneous Synthesis and Integrated Design of Chemical Processes Using IMC PID Tuning Methods

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This work presents the simultaneous synthesis, design and control of an activated sludge process. The mathematical formulation translates a process superstructure into a mixed-integer non-linear optimization problem. The optimization has been solved by the classical method of Branch and Bound using the SQP method for the evaluation of the nodes. The PID's are tuned using the SIMC (Simple Internal Model Control) method in order to avoid decomposition algorithms. The results of the integrated approach are compared to the obtained when classical methodology is applied, giving better controllable plants.

1. Introduction

The *simultaneous design and control* methodology is addressed to the systematic study of the influence of the process structure and design on the controllability of the plant. An important issue in the simultaneous design and control of processes is the selection of the appropriated controllability indicators. Some authors use the typical open-loop and closed-loop metrics, as RGAs, condition number and matrix norms of the system, however, these practical indices might fail due to the approximation to the linearized process model (Sakizlis et al, 2004). On the other hand, some authors propose the evaluation of economic objectives and a dynamic measure of performance, as the ISE for a more systematic analysis of the interactions of design and control.

In the literature dealing with *the integrated synthesis, design and control* of chemical processes (Schweiger and Floudas, 1994; Kookos and Perkins, 2001; Flores-Tlacuahuac and Biegler, 2008) a superstructure that contains all the design alternatives is translated into a mixed-integer non-linear dynamical optimization problem (MIDO). For solving the MIDO problem two major approaches are distinguished: a sequence of primal and master problems, where the primal problem corresponds to a dynamic optimization while the master problem is formulated as an MILP, and the full discretization of the dynamic model which is solved simultaneously with the optimization problem as an MINLP (Flores-Tlacuahuac and Biegler, 2008).

The complexity of the algorithms necessary to solve the MIDO problems arising from the integration of design and control has motivated the search of alternative methodologies for its solution.

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In this work, the classical method of Branch and Bound is applied for solving the *simultaneous synthesis, design and control* problem of a simplified activated sludge process. The SQP algorithm is used for the evaluation of each node. The PID controllers are tuned using the SIMC method (Skogestad, 2003). The control objectives are measured using open loop controllability metrics and dynamical performance indices for closed loop operation. A similar problem has been solved successfully using genetic algorithms (Revollar *et al*., 2005), however, it is interesting to explore non decomposition deterministic optimization methods for the solution of the problem.
The paper is organized containing, first, the process and control system description in section 2, the formulation of the optimization problem and optimization algorithm description in section 3, followed by the analysis of the results in section 4. Finally, conclusions and future work are included.

2. Process and control system description

The activated sludge process was selected as working example to apply the simultaneous synthesis and control system design methodology. This biological treatment, usually takes place in a series of bioreactors where microorganisms are used to reduce the substrate concentration in the water influent flow. They are followed by settlers used to separate the sludge from the clean water.

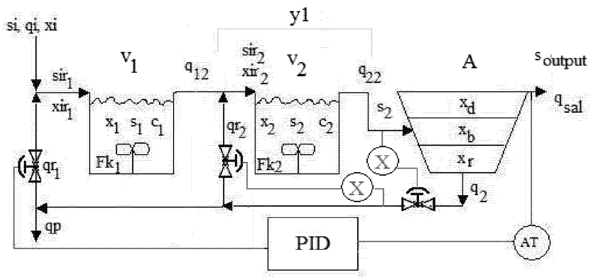

Fig. 1. Activated sludge process superstructure

The control objective is to keep the substrate concentration at the output below a legal value, despite the disturbances in the incoming substrate concentration (*si*) and flow (*qi*). A representative set of disturbances is taken from COST 624 program (Copp, 2002). The control strategy consists on manipulate the recycle flow (qr_1) to maintain the output substrate concentration (S_{output}) around its optimal working point. A ratio control scheme is used to keep the relation between the flows q_{22}, $q_{2,}$ qr_1 and qr_2 around the optimal value obtained for steady state operation.
As in previous work (Gutierrez and Vega, 2000a, Revollar et al., 2005), the two possible structural alternatives are *one reactor-one settler* and *two reactors-one settler*. A superstructure of the process with the control system is presented in figure 1. A binary variable y_1 represent the selection between both alternatives.
A detailed description of the model and process parameters for the specific case study can be found in Moreno, *et al*. (1992) and Francisco and Vega (2006). The most important equations for reactor (1-3) and the second settler layer (4) are given bellow:

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

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

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

$$A \cdot l_b \frac{dx_b}{dt} = qx_1 - q_{sal} x_b - q_2 x_b + A \cdot vs(x_d) - A \cdot vs(x_b) \tag{4}$$

3. Optimization Formulation and Solution

3.1 Mathematical Formulation of the Simultaneous Synthesis, Design and Control

In the simultaneous synthesis, design and control framework for the activated sludge process is considered:

- A set of binary and continuous decision variables that includes: plant structure (y_1), dimensions (reactor volumes, v_1, v_2 and the cross-sectional area of the settler A), working point (the aeration factors Fk_1 and Fk_2, the flows q_{r1}, q_{r2}, q_p and the biomass x_j, substrate s_j and oxygen concentration c_j, where j is the index for reactor or settler layer) and PID controller parameters.
- Some economic and control objectives and constraints over the expected controllability indices that the plant must satisfied.

The optimization objective is to determine the best structure, dimensions, working point and controller parameters which minimize de investment and operation costs as well as dynamical performance indices and controllability metrics based on the linearized process model. The formulation translates into a mixed-integer non-linear problem that includes the evaluation of dynamical indices.

The cost function is:

$$f = p_1 \cdot v_1^2 + p_1 \cdot v_2^2 + p_2 \cdot A^2 + p_3 \cdot Fk_1^2 + p_3 \cdot Fk_2^2 + p_4 \cdot q_2^2 \tag{5}$$

The first three terms are associated to the construction cost and the terms proportional to Fk and q_2 (overall recycle flow) represent the aeration and pumping costs, respectively. The process constraints are:

- Constraints as $\left| v_1 \frac{dx_1}{dt} \right| \le \varepsilon$ imposed over mass balances for each reactor and settler layer (eq 1 to 4) to ensure a stationary working point in the absence of disturbances.
- Logical constraints to guarantee the model mathematical coherence for any possible structure. As example: for y_1=0 $\Rightarrow$ v_2=0, x_1=x_2, s_1=s_2, c_1=c_2, Fk_2=0, qr_2=0.
- Constraints to satisfy the operational requirements over residence time, mass loads, sludge age, hydraulic capacity given by eq. (8) to (11) for one reactor structure and the range for the flow ratio $\frac{q_p}{q_2}, \frac{q_2}{q_i}$ demanded by environmental regulations.

$$2.5 \le \frac{v_1}{q_{12}} \le 8 \tag{6}$$

$$0.001 \le \frac{q_i s_i + qr_1 s_1}{v_1 x_1} \le 0.06 \tag{7}$$

$$3 \le \frac{v_1 x_1 + AL_r x_r}{q_p x_r 24} \le 10 \tag{8}$$

$$\frac{q_{12}}{A} \le 1.5 \tag{9}$$

A complete description of the process constraints can be found in Francisco and Vega (2006) and Francisco and Vega (2008).

Controllability constraints:

An analysis of the possible controllability measures to be included in the optimization problem was carried out previously in plant designs with different structures and dimensions. It was performed to avoid the conflict between controllability indices and to define the bounds to be imposed. The proposed indices were the Integral Square Error (ISE), Effluent Quality (EQ), Aeration Energy (AE), Pumping Energy (PE), sensitivity function maximum peak (Ms), condition number and the $H\infty$ norm. These indices are described in Skogestad and Postlethwaite (1996) and Copp (2002).

Based on this analysis, the condition number of the plant and disturbance were selected as open loop controllability metric used to determine how well the plant can be controlled before the controller tuning.

The selected closed loop controllability indices were the ISE, as a measure of the controller performance, the PE as a measure of the control efforts and the Ms.

Thus, the following controllability constraints are set:

- Condition number.

$$\gamma \le 20 \tag{10}$$

- Disturbance condition number

$$\gamma_p \le \gamma \tag{11}$$

- Sensitivity function maximum peak

$$1 \le Ms \le 1.7 \tag{13}$$

- Integral Square Error:

$$ISE \le 80000 \tag{14}$$

- Pumping energy:

$$PE \le 2800 \tag{15}$$

3.2 Optimization algorithm

The optimization is solved using the classical method of Branch and Bound. The non linear subproblems (NLP) at each node are solved applying the Sequential Quadratic Programming (SQP) using the MATLAB ® Optimization Toolbox.

In order to reduce the complexity of the optimization problem avoiding the controller optimization, the PID parameters for each possible plant design are determined using the SIMC (Simple Internal Model Control) method for the ideal PID in parallel form (Skogestad, 2003). The dynamical performance of the plant with the controller is considered in the global optimization by the evaluation of constraints (13) to (15).

4. Results and discussion

The simultaneous synthesis, design and control of the activated sludge process was performed successfully using the optimization algorithm described in 3.2. The non-linear model of the plant is satisfied, as well as the process and controllability constraints.
The design considering only economical objectives and process constraints (Classical design) was carried out also, to compare the features of the plants obtained using both methodologies. These results are presented in table 1.
In table 1 is possible to observe that both designs are structurally different, evidencing the influence of process design in controllability. The dynamical response shown in figure 2 and controllability indexes (table 1) reveal that the plant obtained using the integrated approach exhibits superior disturbance rejection and dynamical behaviour over the economically optimal plant, but the investment and operation cost increases.

Table 1. Results of the simultaneous synthesis, design and control of the activated sludge compared to the economical design

	Economical Design	Integrated Approach		Economical Design	Integrated Approach
Cost (MU)	*0.17*	*0.30*	Parameters		
v_1 (m^3)	5279.00	6142.20	Kp	-24.00	-8.67
v_2(m^3)	-	2891.30	Ti	28.70	1.66
A (m^2)	1788	2691.20	Td	1.63	0.41
Fk_1	0.08	0.1	Indices		
Fk_2	-	0.1	Ms	0.99	1.45
qr_1 (m^3/h)	630.5	326.70	ISE	80722	20564
qr_2 (m^3/h)	-	300.90	PE (Kwh/d)	1747	993
qp (m^3/h)	19.5	22.50	γ	21.73	6.43
S_{output}(mg/l)	87.5	30.00	γ_p	21.73	6.39

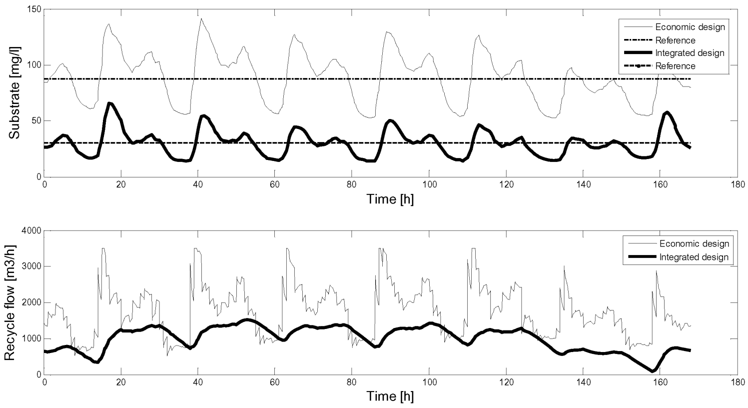

Figure 2. Response of the integrated and economical plants under disturbances.

5. Conclusions

In this work, the simultaneous synthesis, design and control of an activated sludge process was addressed. This problem translates into a mixed-integer non-linear problem including the evaluation of dynamical performance indices and controllability metrics based on the linearized process model.
An optimization technique based on Branch and Bound method, combined with SQP and the SIMC method for the tuning of PID controllers was used for solving the problem, obtaining simultaneously the plant structure, dimensions, working point and control system It is important to note that the introduction of a PID tuning method reduces the complexity of the optimization problem that results when deterministic methods are applied.

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