European Symposium on Computer Aided Process Engineering – 15 L. Puigjaner and A. Espuña (Editors) © 2005 Elsevier Science B.V. All rights reserved.

Algorithmic Synthesis and Integrated Design for Activated Sludge Processes Using Genetic Algorithms

Silvana Revollar^a, Rosalba Lamanna^a, Pastora Vega^b a Universidad Simón Bolívar. Dpto. de Procesos y Sistemas. Caracas 1081A, Venezuela b Departamento de Informática y Automática. Universidad de Salamanca. Spain.

Abstract

This work presents an approach for the Synthesis and Integrated Design of an activated sludge process. The mathematical formulation translates a superstructure that contains all the design alternatives into a mixed-integer dynamical optimization problem with non-linear constraints. A real-coded genetic algorithm is proposed for the solution of such complex problem as an alternative to classical optimisation techniques. Thus, the process synthesis considering open-loop-dynamical-performance indexes and also the closed loop integrated design for the plant are carried out. The results are encouraging for future application of these techniques to solve process synthesis problems

Keywords: Process synthesis, Integrated design, genetic algorithms, controllability

1. Introduction

The process design aims to select the economically optimal plant configuration, together with its dimensions and stationary working point. For chemical process design, several authors (Luyben, 1993; Luyben and Floudas, 1994) have suggested the integration of controllability issues at the early stage of process design in order to improve the dynamical behaviour of the resulting plants. Based on this idea, the integrated design is addressed to the systematic study of the influence of the process design and controllability of the system, even before the process flowsheet is defined. This methodology has been actually applied for chemical processes by Luyben and Floudas (1994) and Kookos and Perkins (2001).

This paper deals with the Integrated Synthesis and Design of an activated sludge process. We present the process synthesis following an optimization procedure where the constraints are posed to consider the dynamical performance of the process and the minimization of the investment and operation costs. Thus, the structure of the process is achieved, along with the set of the process variables that guarantees an acceptable dynamical behaviour for the plant.

The activated sludge process synthesis has been previously performed by Gutierrez and Vega (2002a) who used Generalised Benders Decomposition Algorithm to solve the optimisation problem. The closed loop design of an alternative plant structure was also

carried out by Gutierrez and Vega (2002b), however, they used controllability measures based in linearised models.

The mathematical formulation of the synthesis is presented, translating a superstructure that contains all the design alternatives into a mixed-integer non-linear optimisation problem (MINLP). The integration of controllability indexes to the process synthesis leads to a constrained mixed integer dynamical optimisation problem.

The classical optimization methods are being applied for solving mixed integer nonlinear problems, obtaining good solutions with reasonable computational effort. However, these techniques sometimes fail in presence of discontinuities, get trapped in local minimum and depend strongly on the starting points (Tsai and Chang, 2001). Therefore, alternative techniques are important issues to be considered, for instance, stochastic optimisation methods such as genetic algorithms which have been used with good results for MINLP problems (Costa and Oliveira, 2001).

Only few works have been published where GA are used for the synthesis or integrated design of chemical processes (Tsai and Chang, 2001; Revollar *et al.*, 2004). In this work, the application of a real-coded genetic algorithm is proposed to solve the problem issued from the synthesis and integrated design of the activated sludge process.

The paper is organised containing, first, the description of the process and the formulation of the optimization problem in section 2. The proposed genetic algorithm is described in section 3 and the analysis of the results is presented in section 4. Finally, conclusions and different projections of this work are included.

2. Formulation of the Optimization Problem

2.1. Process Description



Figure 1: Activated sludge process superstructure

The wastewater treatment process (Figure 1) has been selected for applying the proposed design methodology. The alternative structure consists in one or two aeration tanks and one secondary settler. The basis of the process lies on maintaining a microbial population (biomass) into each bioreactor, transforming the biodegradable pollution (substrate) with dissolved oxygen supplied through aeration turbines. Water coming out of each reactor goes to the settler, where the activated sludge is separated from the clean water and recycled to both bioreactors. The process superstructure and variables are presented in Figure 1. Biomass concentrations are denoted by "x" (mg/l), substrate concentrations are denoted by "s" (mg/l), "c" is used for the oxygen concentrations (mg/l), "q" for flow rates (m3/h) and "fk" for the aeration factors.

The control of this process aims to keep the substrate at the output, s_2 , bellow a certain value despite the large variations of the flow rate and the substrate concentration of the incoming water (qi and si).

2.2. Mathematical Modelling

The model of the process superstructure is a set of differential and algebraic equations which contains the process variables and integer variables (y_1, y_2) used to represent the existence of the second reactor and the recycle qr_2 , respectively. The problem is stated as a mixed integer NLP/DAE optimisation of the objective function which represents construction and operation costs, subject to process and controllability constraints. The cost function is:

$$f_1(x) = 0.5 \cdot v_1^2 + 0.5 \cdot v_2^2 + 0.3 \cdot A^2 + 0.6 \cdot fk_1^2 + 0.6 \cdot y_1 \cdot fk_2^2$$
(1)

where $v_{1,}v_{2}$ are the reactor volumes and A is the cross-sectional area of the settler. The process constraints on mass balances in aeration reactors (j=1,2) and mass balances in decanter to obtain a solution close to a steady state (ϵ close to zero), are:

$$\left| \mathbf{v}_{j} \frac{d\mathbf{x}_{j}}{d\mathbf{t}} \right| = \left| \boldsymbol{\mu}_{\max} \mathbf{y} \frac{\mathbf{s}_{j} \mathbf{x}_{j}}{\left(\mathbf{K}_{s} + \mathbf{s}_{j}\right)} \mathbf{v}_{j} - \mathbf{K}_{d} \frac{\mathbf{x}_{j}^{2}}{\mathbf{s}_{j}} \mathbf{v}_{j} - \mathbf{K}_{c} \mathbf{x}_{j} \mathbf{v}_{j} + \mathbf{q}_{j2} \left(\mathbf{x} i \mathbf{r}_{j} - \mathbf{x}_{j} \right) \right| \le \varepsilon$$

$$\tag{2}$$

$$\left| \mathbf{v}_{j} \frac{\mathrm{d}\mathbf{s}_{j}}{\mathrm{d}\mathbf{t}} \right| = \left| -\mu_{\max} \frac{\mathbf{s}_{j} \mathbf{x}_{j}}{\left(\mathbf{K}_{s} + \mathbf{s}_{j}\right)} \mathbf{v}_{j} + \mathbf{f}_{kd} \mathbf{K}_{d} \frac{\mathbf{x}_{j}^{2}}{\mathbf{s}_{j}} \mathbf{v}_{j} + \mathbf{f}_{kd} \mathbf{K}_{c} \mathbf{x}_{j} \mathbf{v}_{j} + \mathbf{q}_{j2} \left(\operatorname{sir}_{j} - \mathbf{s}_{j} \right) \right| \le \varepsilon$$
(3)

$$\left| \mathbf{v}_{j} \frac{\mathrm{d}\mathbf{c}_{j}}{\mathrm{d}\mathbf{t}} \right| = \left| \mathbf{K}_{\mathrm{la}} \mathbf{f} \mathbf{k} \left(\mathbf{c}_{\mathrm{s}} - \mathbf{c}_{j} \right) - \mathbf{K}_{01} \boldsymbol{\mu}_{\mathrm{max}} \frac{\mathbf{x}_{j}^{2}}{(\mathbf{K}_{\mathrm{s}} + \mathbf{s}_{j})} - \mathbf{q}_{j2} \mathbf{c}_{j} + \mathbf{W}_{\mathrm{l}j} \right| \le \varepsilon$$
(4)

$$\left| \mathbf{A} \cdot \mathbf{l}_{d} \cdot \frac{d\mathbf{x}_{d}}{dt} \right| = \left| \mathbf{q}_{sal} \mathbf{x}_{b} - \mathbf{q}_{sal} \mathbf{x}_{d} - \mathbf{A} \cdot vs(\mathbf{x}_{d}) \right| \le \varepsilon$$
(5)

$$\left| \mathbf{A} \cdot \mathbf{l}_{b} \cdot \frac{d\mathbf{x}_{b}}{dt} \right| = \left| \mathbf{q}_{22}\mathbf{x}_{2} - \mathbf{q}_{sal}\mathbf{x}_{b} - \mathbf{q}_{2}\mathbf{x}_{b} - \mathbf{A} \cdot \left(\mathbf{vs}(\mathbf{x}_{d}) - \mathbf{vs}(\mathbf{x}_{b}) \right) \right| \le \varepsilon$$
(6)

$$\left| \mathbf{A} \cdot \mathbf{l}_{b} \cdot \frac{d\mathbf{x}_{b}}{dt} \right| = \left| \mathbf{q}_{22}\mathbf{x}_{2} - \mathbf{q}_{sal}\mathbf{x}_{b} - \mathbf{q}_{2}\mathbf{x}_{b} - \mathbf{A} \cdot \left(\mathbf{vs}(\mathbf{x}_{d}) - \mathbf{vs}(\mathbf{x}_{b}) \right) \right| \le \varepsilon$$
(7)

The logical constraints for the activation and deactivation of continuous variables:

$$\mathbf{y}_2 - \mathbf{y}_1 \le \mathbf{0} \tag{8}$$

$$Z_2 - (1 - y_1)Z_1 \pm y_1U_j \le 0$$
(9)

$$qr_1 - (1 - y_2)q_2 \pm y_2 U_j \le 0 \tag{10}$$

$$W_{12} = y_1 q_{22} c_2 \tag{11}$$

where Z can be x, s or c and $W_{11}=0$. The logical constraints guaranteed the mathematical coherence of the model. If $y_1=0$, then $y_2=0$, $v_2=0$, $x_1=x_2$, $s_1=s_2$, $c_1=c_2$ and the balances in the second reactor become zero. If $y_2=0$ then $qr_1=q_2$. For $y_1=1$ and $y_2=1$ all the variables take values within their ranges.

Other process constraints as the residence times, the mass loads in the aeration tanks and the limits in hydraulic capacity can be found in Gutierrez and Vega (2002b).

The controllability constraints are stated to guarantee disturbance rejection capability, either in open or closed loop configurations. As controllability indices the ISE norm show in equation (12) and the H_{∞} norm of the disturbance transfer function were used.

$$ISE = \int_{t=0}^{T \max} (s_{2t} - s_2)^2 \cdot dt$$
(12)

 T_{max} is the simulation time and s_{2r} is the steady-state desired value for substrate.

$$\left\|\mathbf{G}_{d}\right\|_{\infty} = \max \,\overline{\mathbf{\sigma}}(\mathbf{w}) \tag{13}$$

 σ is the maximum singular value.

3. Solving the Problem Using Genetic Algorithms

Genetic algorithms are stochastic optimisation methods based on the principles of natural evolution. The optimisation process is carried out with a population of potential solutions for the problem, coded as chromosomes. A performance index based on the cost function is assigned to each chromosome. The population evolves toward better regions in the search space by means of genetic operators as selection, crossover and mutation. After several generations, the algorithm converges to the best individual, which represents an optimal solution to the problem.

For this particular case the chromosome coding is defined to handle simultaneously continuous and integer variables. Therefore, it contains continuous variables encoded as real numbers in the range [0 1] and two binary variables: $[x_1, s_1, c_1, x_2, s_2, c_2, x_d x_b x_r q_r q_{r1/} q_r q_p f_{k1} f_{k2} v_1 v_{1/}v_2 A y_1 y_2]$. The ratio $v_{1/}v_2$ and $q_{r1/}q_r$ are included into the chromosome instead of v2 and q_{r2} to manipulate easily these variables because they are change according to the integer y_1 and y_2 . An appropriated technique as the quadratic penalty term in the addition form is applied to deal with constraints (Gen and Chen, 2000).

The tournament operator is used as a selection procedure. The "arithmetic crossover" (Gen and Chen, 2000) is used to generate new candidate solutions. For this crossover operator, given the parents x, y, the genes of the offspring (zi) are calculated as shown in equation (14).

$$\mathbf{z}_{i} = \lambda_{1} \cdot \mathbf{x}_{i} + \lambda_{2} \cdot \mathbf{y}_{i}$$

(14)

where $0 \le \lambda_1 + \lambda_2 \le 2$. For the integer variables $0 \le \lambda_1 + \lambda_2 \le 1$ and $z_i = int eger(z_i)$.

For the closed loop design, the chromosome contains also the controller parameters, because the algorithm will explore the space of possible controllers together with the plant parameters. The controller search is improved including a few chromosomes which represent identical plants with different controllers into the initial population.

The optimization problems presented in this work are solved using a population size of 30 individuals and a maximum generation number of 300. For the evaluation of the dynamical performance indexes a simulation of the non-linear model considering the disturbances in "qi" and "si" is carry out for each possible chromosome. The deviation of the ISE norm respect to a desired value is added to the penalty term.

4. Integrated Synthesis and Design Results

Three scenarios are presented to study the synthesis and integrated design problem. First, the design was performed to optimise only investment and operation costs. The results are shown in table 1 and compared with results given by Gutierrez and Vega (2002a). The second case is focused in open loop design considering the mentioned controllability constraints; finally, the integrated design of the plant with a PI controller is performed. These results are presented in table 2.

Parameters	Economical synthesis	Economical synthesis	
		(Gutierrez and Vega, 2002a)	
V1 (m ³)	4014	3421	
$A(m^2)$	2140	2944	
S_1 (mg/l)	91.79	81.14	
Cost	0.2352	0.2474	

Table 1: Results of the economical synthesis

T 11 1	D 1.	C .1			,	• • • •	, ,	
Table 1.	Pagulta	ot th	10 CIMATI	00010	and	intomatod	1 1	agian
Tume 2.	пеминя	or u	ie sviii	lesis	unu	iniegraiea	u	esign
		- J						

Parameters	Synthesis with controllability constraints	Synthesis and closed loop design
V1 (m ³)	7784	9664
$A(m^2)$	2447	2405
S_1 (mg/l)	51.41	59.00
ISE	158080	75114
Cost	0.104	0.55
Norm H_{∞}	0.1609	0.1274

In all the cases, the flexibility of the genetic algorithm allows the achievement of the optimal design even thought dynamical constraints were imposed. The economical design results are comparable to the reported by Gutierrez and Vega (2002a). The best plant configuration for each case corresponds to the simple structure with one aeration tank and one secondary settler (y=1 and $y_2=0$).



Figure 2: Substrate and flow disturbances at the influent

The set of disturbances (Figure 2) proposed by Vanhooren and Nguyen (1996) were used for testing the dynamical response of the plant. The plant responses shown in figure 3 and controllability indexes presented in table 2 indicates that the plants obtained following the integrated design procedure exhibits better disturbance rejection than the economically optimal plant but with higher costs. For the closed loop design, the ISE norm and disturbance rejection are much better than the open loop design indicating an appropriated controller tuning.



Figure 3: Response of the plants resulting from open loop (left) and closed loop (right) design

5. Conclusions

In this paper, an approach for the synthesis of the activated sludge process which considers dynamical-performance indexes was presented. A real-coded genetic algorithm was proposed for the solution of the resulting mixed-integer non linear dynamical optimisation problem, showing good results in open loop and closed loop design. The non-linear model of the plant is satisfied, as well as the operation and process constraints. This methodology allows obtaining plants which are economically optimal and feature optimum disturbance rejection.

Results are very encouraging because of AG seems suitable for solving mixed integer dynamical optimisation problems derived from process synthesis or integrated design.

Acknowledgments

The authors acknowledge the support of the FONACIT project S1-99000111 and of Spanish Government through the CICYT project DPI2000-0665-C02-02

References

- Costa, L. and P. Oliveira, 2001, Evolutionary algorithms approach to the solution of mixed integer-non-linear programming problems, Comp. Chem. Eng. 25, 257.
- Gen, M. and R. Chen, 2000, Genetic algorithms and engineering optimisation. J. W. and Sons.
- Gutiérrez, G. and P. Vega, 2002, Integrated design of chemical processes and their control system including closed loop properties for disturbances rejection. 15th IFAC Triennal World Congress. Barcelona.
- Gutiérrez, G. and P. Vega, 2002, Process synthesis applied to activated sludge processes: A framework with MINLP optimisation models. 15th IFAC Triennial World Congress. Barcelona.
- Kookos I. and J. Perkins, 2001, An algorithm for simultaneous process design and control, Ind. Eng. Chem. Res. 40, 4079.
- Luyben, W., 1993, Trade-offs between design and control in chemical reactor systems. J. Proc. Cont. 3, 17.
- Luyben, M. and C. Floudas, 1994, Analyzing the interaction of design and control-1. A multiobjective framework and application to binary distillation synthesis, Comp. Chem. Eng. 18, 933.
- Revollar, S, Vega, P. and R. Lamanna, 2004, Algorithmic synthesis and integrated design of chemical reactor systems using genetic algorithms. World Automation Conference. Sevilla.
- Vanhooren H. and K. Nguyen, 1996, Development of a simulation protocol for evaluation of respirometry-based control strategies. Report University of Gent and University of Ottawa.
- Tsai, M. and Ch. Chang, 2001, Water usage and treatment network design using genetic algorithms Ind. Eng. Chem. Res. 40, 4874.