15th Triennial World Congress, Barcelona, Spain

PROCESS SYNTHESIS APPLIED TO ACTIVATED SLUDGE PROCESSES: A FRAMEWORK WITH MINLP OPTIMISATION MODELS

G. Gutierrez* and P. Vega**

(*) Dpt. Ingenieria de Sistemas y Automatica. Facultad de Ciencias. Universidad de Valladolid. C/ Prado de la Magdalena, S/N. 47011, Valladolid,. Spain.
e-mail: gloria@autom.uva.es

(**) Dpt. Informatica y Automatica. Escuela Superior de Ingenieria Industrial. Universidad de Salamanca. C/ Pedro Ballesteros s/n , Bejar (Salamanca), Spain.
e-mail: pvega@gugu.usal.es

Abstract: Process Synthesis seeks to develop systematically process flowsheets that convert raw materials into desired products. In recent years, the optimization approach to process synthesis has shown promise in tackling this challenge. It requires the development of a network of interconnected units, the process superstructure, that represents the alternative process flowsheets. The mathematical modeling of the superstructure has a mixed set of binary and continuous variables and results in a mixed-integer optimization model. Due to the nonlinearity of chemical models, these problems are generally classified as Mixed Integer Nonlinear Programming (MINLP) problems. In this work presents the illustrative example of Process Synthesis applied to the activated sludge process.

Keywords: Optimization problems, Processes, Process models , Controllability, Design.

1. INTRODUCTION

The Synthesis Process Problem aim is to obtain the optimal process flowsheet, the sizes of the process units and the operating point that will allow for the transformation of some specified inputs to the desired final products while addressing the minimisation of a performance criteria. The cost function to be minimised usually takes into account different objectives like the minimisation of the capital and the operating costs, the product quality, environmental and safety issues, etc. To determine the optimal process flowsheets according to the performance criteria, some answers must be given to the following questions: Which process unit should be used in the process flowsheets?, How should the process units be interconnected?, What are the optimal operating conditions?, Which are the optimal values for the sizes of the selected process units?, etc. The optimisation approach to process synthesis considered in this paper, has been developed to address the mentioned issues and it has led to some the major theoretical and algorithmic advances in mixed-integer non-linear optimisation, (Adjiman, *et all*., 1998). In this paper, we present a mathematical approach for the algorithmic synthesis of the mentioned above biotechnological processes. The whole procedure is illustrated by taking as reference model a real wastewater treatment plant located in Manresa (Spain).

The paper is organised as follows. First of all, the MINLP problem is explained for a general case. After this, a superstructure is defined for the case of Activated Sludge Processes and some integer variables are associated to the process units belonging to this superstructure. In the following section, the mathematical first principle model of the process superstructure together with the set of operation and physical constraints are written in terms of these binary variables and in terms of the process real variables. This model is then completed through the definition of a multiobjective cost function and a set of logical constraints. The optimisation model is, in this way, presented as a mixed-integer non-linear programming problem (MINLP) with constraints. The solution of this problem for the case of activated sludge processes is obtained and is widely explained in one of the last sections, where some comments, about the numerical optimization algorithm GBD, are also made. Some results, obtained by using the MINOPT package, are shown and some conclusion are given at the end of the paper.

2. OPTIMIZATION IN THE SYNTHESIS PROCESS

The Optimization in the Process Synthesis problem involves the following elements:

a) A representation of the alternatives structures of the process through the definition of the, so-called, superstructure of the process.

b) A mathematical model of the superstructure, usually a non linear first principle model, and a set of constraints (process and physical constraints).

c) Statement of the MINLP optimisation model based on a) and b)

d) Algorithmic development for the solution of the optimisation model.

The superstructure must contain lots of alternative process flowsheets, i.e., the whole set of process configurations that are of interest.

The MINLP model is composed by a cost function, the model of the superstructure and the set of constraints. They should be written in terms of binary variables that indicate the existence of the units in the process, and in terms of continuous variables representing flow rates, compositions, temperatures and sizing of process units, etc.

The resulting formulation is a Mixed Integer Nonlinear Programming Problem of the form:

$$
\begin{aligned}
&\min_{x,y} \quad f(x,y) \\
&\text{s.a.} \quad h(x,y)=0 \\
&\qquad\;\; g(x,y)\le 0 \\
&\qquad\;\; x\in X\subseteq \Re^n \; y\in Y \text{ entero}
\end{aligned}
\qquad (1)
$$

being x: is a vector of n continuous variables, y: is a vector of integer variables; $f(x,y)$is the objective function that represents the design criteria, $h(x,y)=0$: are the *m* equality constraints (mass and energy balances, and equilibrium expressions) and $g(x,y)\le 0$ are the *p* inequality constraints (design specifications, logical constraints)

3. SUPERSTRUCTURE OF ACTIVATED SLUDGE PROCESS AND INTEGER VARIABLES DEFINITION

The basis of the activated sludge process lies in maintaining a microbial population (biomass) inside the reactors to transform the biodegradable pollution (substrate) in the presence of dissolved oxygen supplied through aeration turbines. Water coming out the reactors goes to the corresponding settler, where the activated sludge is separated from the clean water and recycled to the reactors.

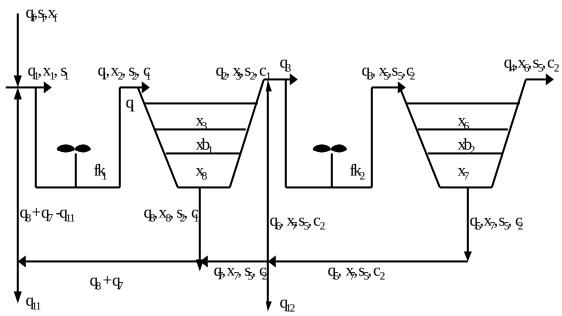

Fig. 1. The superestructure of the activated sludge process.

The selected superstructure of the process is shown in Figure 1. In the figure, we can observe that see that the decanters (D_1 y D_2), the second reactor (R_1), the recycling flow q_7 and the purge flow q_{12}, are the process elements that may exist or may not. They are actually represented by dotted lines. The existence or non-existence of these units defines the three alternative structures. In order to be able to obtain a mathematical model of the superstructure including the models for the three alternative structures as particular cases the following integer variables are defined:

The variable y_{r2} is associated to the second reactor with the following meaning: If y_{r2} =1 then the second reactor exists and the volumen V_2 has be calculated, but, If y_{r2} =0 then the second reactor does not exist and the volume V_2 has to be equal to zero.

The integer variables, y_{D1} and y_{D2}, are associated to the first and the second decanters and y_{q7} and y_{q12} to the flow rates q_7 and to q_{12}, respectively. These variables have the same meaning as y_{r2}. For example, If y_{D1} =1 then the first decanter exists and its crossing area A_1 has to be calculated, but if y_{D1} =0 then the first decanter does not exist and the crossing area must be zero. Note that A_2 will denote the crossing area for the second decanter.

Once the integer variables are defined and taking into account that the global objective is to find the optimal alternative process (the optimal structure, the optimal operations and investment costs), satisfying some operations constraints imposed to the process, the MINLP optimisation model can be easily define as it can be seen in next section.

4. THE MINLP OPTIMIZATION MODEL

The optimisation model consists of the objective function, a set of constraints associated to a stationary model of the superstructure of the process and a set of physical and process operation constraints.

Taking into account that we want to minimise the investment costs, as the reactors volumes and the decanter cross sections, and the operation costs, which are given by the aeration factor of the turbine.

The MINLP model can be written as:

$$\min_{x,y} \quad 0.5V_1^2+0.5V_2^2+0.3A_1^2+0.3A_2^2+0.6fk_1^2+0.6fk_2^2$$

subject to: (2)

Mass balances equations of the first reactor:

$$\mu y\frac{s_2x_2}{k_s+s_2}-k_d\frac{x_2^2}{s_2}-k_cx_2v_1+\frac{q_fx_f}{v_1}+\frac{q_8x_8}{v_1}+$$
$$+\frac{(q_5-q_6)(1-y_{q12})x_7}{v_1}-$$
$$-\frac{q_{11}}{v_1}\left(\frac{q_8x_8+(q_5-q_6)(1-y_{q12})x_7}{q_8+(q_5-q_6)(1-y_{q12})}\right) \tag{3}$$
$$-\frac{q_1x_2}{v_1}=0$$

$$-\mu\frac{s_2x_2}{k_s+s_2}+f_{kd}k_d\frac{x_2^2}{s_2}+f_{kd}k_cx_2+\frac{q_fs_f}{v_1}+$$
$$+\frac{q_8s_8}{v_1}+\frac{(q_5-q_6)(1-y_{q12})s_5}{v_1}+\frac{q_5s_2(1-y_{R2})}{v_1}-$$
$$-\frac{q_{11}}{v_1}\left(\frac{q_8s_2+(q_5-q_6)(1-y_{q12})s_5+q_5s_2(1-y_{R2})}{q_8+q_5s_2(1-y_{R2})}\right)-$$
$$-\frac{q_1s_2}{v_1}=0 \tag{4}$$

$$k_{la}fk_1(c_s-c_1)-k_{01}\mu\frac{x_2s_2}{k_s+s_2}-\frac{q_1c_1}{v_1}=0 \tag{5}$$

The equilibrium equations:

$$q_1=q_f+q_8+(q_5-q_6)(1-y_{q12})-q_{11} \tag{6}$$
$$q_3=q_6+q_2+q_1(1-y_{D1}) \tag{7}$$
$$q_2=(q_1-q_8)y_{D1} \tag{8}$$
$$q_6=(q_5-q_7-q_{12})y_{R2} \tag{9}$$

The mass balances equations of the first decanter:

$$(xb_1-x_8)q_8+A_1vsxb_1=0 \tag{10}$$
$$(q_1-q_8)xb_1-q_2x_3-A_1vsx_3=0 \tag{11}$$
$$q_1x_2-xb_1(q_2+q_8)+A_1[vsx_3-vsxb_1]-$$
$$-q_1x_2(1-y_{D1})=0 \tag{12}$$

The mass balances equations of the second reactor:

$$v_2\mu y\frac{s_5^2x_5}{k_s+s_5}-k_dx_5^2v_2-k_cx_5s_5v_2$$
$$+_2\ x_3s_5++q_1x_2s_5(1-y_{D1})+ \tag{13}$$
$$q_6x_7s_5-q_3x_5s_5=0$$

$$-v_2\mu\frac{s_5^2x_5}{k_s+s_5}+f_{kd}k_dx_5^2v_2$$
$$+f_{kd}k_cx_5s_5v_2+ \tag{14}$$
$$+q_2s_2s_5+q_1s_2s_5(1-y_{D1})$$
$$+q_6s_5^2-q_3s_5^2=0$$

$$v_2k_{la}fk_2(c_s-c_2)-k_{01}\mu\frac{x_5s_5}{k_s+s_5}v_2+$$
$$+(q_f+q_7-q_{11})c_1- \tag{15}$$
$$(q_f+q_5-q_{11}-q_{12})c_2-$$
$$-(c_1(q_f+q_7-q_{11}))(1-y_{R2})=0$$

The mass balance equations of the second decanter:

$$(q_3-q_5)xb_2-q_4x_6-A_2vsx_6=0 \tag{16}$$

$$q_3 x_5 + q_3 x_3 (1 - y_{R2}) + q_3 x_2 (1 - y_{D1}) -$$
$$- q_3 x_2 (1 - y_{D1}) y_{R2} - q_4 xb_2 - q_5 xb_2 + \quad (17)$$
$$+ A_2 (vsx_6 - vsxb_2) - x_3 q_3 (1 - y_{D2}) = 0$$

$$q_5 (xb_2 - x_7) + A_2 vsxb_2 = 0 \quad (18)$$

The logical constraints:

$1 - y_{D1} - y_{D2} \le 0$ (One decanter must exist, i.e., either yd1 or yd2 must be equal to 1)

$y_{q7} - y_{D2} \le 0$ (If decanter 2, D2, does not exist then y_{q7} must be zero)

$$y_{q12} - y_{R2} \le 0 \qquad y_{q12} - y_{D1} \le 0$$
$$y_{q12} - y_{D2} \le 0 \qquad y_{q7} + y_{q12} \le 1 \quad (19)$$

$$y_{q7} + y_{q12} - y_{R2} \ge 0 \quad (20)$$

The process constraints that can be found in (Gutiérrez, 2000).

5 OPTIMIZATION ALGORITHM (GBD) AND SOLUTION OF THE PROBLEM

The solution of the problem has been obtained by using the MINOPT package (Schweiger and Floudas, 1998), developed by C. Floudas and coo-workers in the University of Princeton. MINOPT is able to handle a wide variety of models described in the MINLP form since it actually handles variables of the following type: continuous time invariant, continuous dynamic, and integer variables. It also deals with constraints of the following type: linear, non-linear, dynamic, dynamic path and point constraints involving integer and real variables.
After the definition of the MINLP optimisation problem was carried out the Generalized Benders Decomposition (GBD) algorithm was executed to derive the solution numerically.

The basic idea behind GBD is the generation of upper and lower bounds on the solution of the MINLP model through the iterative solution of several sub-problems (master and primal problems) formulated from the original problem (1). The upper bound is the result of the solution of the primal problem. The primal problem corresponds to the solution of the original problem with the values of the **y** variables fixed. This problem is then solved in the x space and its solution provides information about Lagrange multipliers for the constraints. The master problem is formulated by making use of the Lagrange multipliers and the non-linear duality theory. Its solution provides a lower bound as well as a new set of **y** variables. The algorithm iterates between the primal and master problem generating a sequence of upper and lower bounds, which converge in a finite number of iteration (Floudas, 1995).

The obtained solution was the following:

Binary variables => Optimal Flowsheet

Y_{R2}=0 => Reactor 2 does not exist
Y_{A1}=1.=> Decanter 1 exists
Y_{A2}=0 => Decanter 2 does not exist
The rest were equal to zero.

This means that the optimal structure is the one represented in Figure 2.

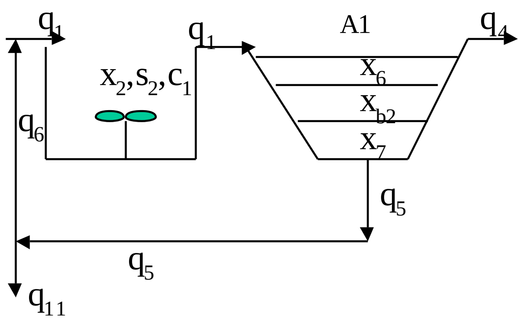

Fig.2. Optimal structure

Continuous variables =>Operation point and dimensions

x2: 2095.646, x6: 145.28 x7: 10000.00, xb2: 825.23,
s2: 91.79272, c1: 1.000000, q1: 1605.809, q4: 1288.0
q5: 317.8087,q11: 12.0000, V1: 4014.522,
A2: 2140.84, fk1: 0.08, vsx6: 409.1, vsxb2: 1361.99

6 CONCLUSIONS

The optimal activated sludge structure, the process units dimensions and a working point were evaluated simultaneously, by solving a mixed-integer non-linear optimisation problem. The problem resolution involved the definition of a superstructure of the process and a set of integer variables. A MINLP optimisation model for this example was obtained, next, and the optimisation was carried out numerically by using the MINOPT software. Although the design of the plant was obtained taking into account the operation and investment costs in stationary state, without any dynamics or any controllability characteristics, their consideration is straight forward, since, the method is general and any set of constraints can be included and any cost function can be defined.

The MINOPT software allows to solve nonlinear mixed integer optimization problems with algebraical constraints. Dynamic equations can be only considered via discretization methods (collocation methods, for instance)

REFERENCES

Adjiman, C. A., Schweiger, C. A., Floudas, C. A., (1998). Mixed-Integer Nonlinear Optimization in Process Synthesis. Handbook of Combinatorial Optimization. Kluwer Academic Publishers.

Floudas, C. A., (1995). *Nonlinear and Mixed-Integer Optimization*. Kluwer Academic Publishers. Princeton University.

Schweiger, C. A. and Floudas, C. A., (1998). MINOPT: A Modeling Language and Algorithmic Framework for Linear, Mixed-Integer, Nonlinear, Dynamic, and Mixed-Integer Nonlinear Optimization. Princeton University.

Gutiérrez, G. (2000). Integrated Design and Synthesis Process Applied to the Activated Sludge Process. Ph.D. Thesis. Universidad de Valladolid.