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

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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 al., 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:

\[
\begin{align*}
\min_{x,y} & \quad f(x,y) \\
\text{s.a.} & \quad h(x,y) = 0 \\
& \quad g(x,y) \leq 0 \\
& \quad x \in X \subseteq \mathbb{R}^n \quad y \in \mathbb{Y} \end{align*}
\]

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 \(g(x,y) \leq 0\) 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.

![Superstructure of the activated sludge process](image)

Fig. 1. The superstructure 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 (D₁ y D₂), the second reactor (R₂), the recycling flow q₁ and the purge flow q₁₂, 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 \(y_{12}\) is associated to the second reactor with the following meaning: If \(y_{12} = 1\) then the second reactor exists and the volumen \(V₂\) 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:

\[
\min_{\mathbf{y}, \mathbf{v}} 0.5V_1^2 + 0.5V_2^2 + 0.3A_1^2 + 0.3A_2^2 + 0.6k_1^2 + 0.6k_2^2
\]

subject to:

\[
\text{Mass balances equations of the first reactor:}
\]

\[
\begin{align*}
\mu y \frac{s_2 x_2}{k_s + s_2} - k_x \frac{x_2^2}{s_2} - k_c x_1 y_1 + q_{11} x_1 + q_{12} x_2 + q_{13} s_2 \frac{x_2}{v_1} + q_{14} x_1 + & \\
+ q_{15} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - q_{16} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{17} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{18} x_2 \frac{v_1}{v_i} = 0
\end{align*}
\]

\[
\text{Mass balances equations of the second reactor:}
\]

\[
\begin{align*}
\mu y \frac{s_2 x_2}{k_s + s_2} + f_{id} k_4 \frac{x_2^2}{s_2} + f_{id} k_c x_2 + q_{13} s_2 \frac{x_2}{v_1} + & \\
+ q_{14} s_2 + q_{15} (1 - y_{r2}) x_2 \frac{v_1}{v_i} + q_{16} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{17} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{18} s_2 \frac{v_1}{v_i} = 0
\end{align*}
\]

The equilibrium equations:

\[
q_1 = q_{f1} + q_{a} + (q_{s} - q_{a})(1 - y_{r2}) - q_{11}
\]

\[
q_3 = q_{f6} + q_{a} + q_{1}(1 - y_{r1})
\]

\[
q_2 = (q_{1} - q_{v}) y_{r1}
\]

\[
q_6 = (q_{1} - q_{7} - q_{12}) y_{r2}
\]

The mass balances equations of the first decanter:

\[
\begin{align*}
\mu y \frac{s_2 x_2}{k_s + s_2} - k_x \frac{x_2^2}{s_2} - k_c x_1 y_1 + q_{11} x_1 + q_{12} x_2 + q_{13} s_2 \frac{x_2}{v_1} + & \\
+ q_{14} x_1 + q_{15} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - q_{16} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{17} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{18} x_2 \frac{v_1}{v_i} = 0
\end{align*}
\]

The mass balances equations of the second decanter:

\[
(q_{1} - q_{v}) y_{r2} = 0
\]

\[
\mu y \frac{s_2 x_2}{k_s + s_2} - k_x \frac{x_2^2}{s_2} - k_c x_1 y_1 + q_{11} x_1 + q_{12} x_2 + q_{13} s_2 \frac{x_2}{v_1} + & \\
+ q_{14} x_1 + q_{15} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - q_{16} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{17} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{18} x_2 \frac{v_1}{v_i} = 0
\]

The mass balances equations of the second reactor:

\[
\begin{align*}
\mu y \frac{s_2 x_2}{k_s + s_2} - k_x \frac{x_2^2}{s_2} - k_c x_1 y_1 + q_{11} x_1 + q_{12} x_2 + q_{13} s_2 \frac{x_2}{v_1} + & \\
+ q_{14} x_1 + q_{15} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - q_{16} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{17} (1 - y_{r2}) x_2 \frac{v_1}{v_i} - & \\
- q_{18} x_2 \frac{v_1}{v_i} = 0
\end{align*}
\]
The logical constraints:

\[ 1 - y_{D1} - y_{D2} \leq 0 \]  
(One decanter must exist, i.e., either \( y_{D1} \) or \( y_{D2} \) must be equal to 1)

\[ y_{q7} - y_{D2} \leq 0 \]  
(If decanter 2, \( D_2 \), does not exist then \( y_{q7} \) must be zero)

\[ y_{q12} - y_{R2} \leq 0 \]  \[ y_{q12} - y_{D1} \leq 0 \]  \[ y_{q7} + y_{q12} \leq 1 \]  \[ y_{q7} + y_{q12} - y_{R2} \geq 0 \]  
(19) 
(20)

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.

**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 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).

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\( Y_{A2} = 0 \) => 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

\( x_2: 2095.646, x_6: 145.28, x_7: 10000.00, \)  
\( x_{b2}: 825.23, \)  
\( s_2: 91.79272, c_1: 1.000000, q_1: 1605.809, q_4: 1288.0, \)  
\( q_5: 317.8087, q_{11}: -41.00000, V_1: 4014.522, A_2: 2140.84, f_{k1}: 0.08, v_{sx6}: 409.1, v_{sx2}: 1361.99 \)
characteristics, their consideration is straightforward, 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