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Design and operation issues using NLP superstructure modeling

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Abstract

Till present, models that determined batch plants configurations in the chemical process industry resorted to models with binary variables to represent the different admissible options. This approach allowed representing the problem in a simple way while considering a significant number of alternatives. Nevertheless, the non-convexity that arises when dealing with detailed models for representing the involved units operation prevents its correct resolution or has a low performance. This work presents a representation of the problem through a superstructure that takes explicitly into account all the alternatives without resorting to binary variables. By using extremely simple modeling, it is possible to manage an appropriate number of options for this type of problems by means of a non-linear programming (NLP) model. Moreover, it is possible to consider duplication in series of production stages, which is an alternative that has not been used till now. This approach is posed for the case of a fermentors network. The solution is reached with very low requirements as regards employed computer time and without the aforementioned difficulties.

Keywords: NLP problems; Superstructure modeling; Optimization; Design and operation of batch plants

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Nomenclature

Subscripts

a	alternative, $a = 1, \ldots, A_p$
f	material used in the feeding
j	stage, $j = 1, \ldots, C_p$
last	last stage or last operation (j_{last} or p_{last}, respectively)
p	operation, $p = 1, \ldots, P$

Continuous variables

B^{e}_{paj}	entering batch volume [m^3]
B^{s}_{paj}	leaving batch volume [m^3]
E_{paj}	ethanol concentration [$kg\ m^{-3}$]
Feed_{paj}	set of feeding materials
G_j	number of in-phase duplicated stages in the MINLP model used for comparison
M_j	number of out-of-phase duplicated stages in the MINLP model used for comparison
PR	plant production rate [$kg\ h^{-1}$]
PR_{paj}	production rate of alternative a [$kg\ h^{-1}$]
S_{paj}	substrate concentration [$kg\ m^{-3}$]
S^{e}_{paj}	entering substrate concentration of unit j of alternative a [$kg\ m^{-3}$]
S^{s}_{paj}	output substrate concentration of unit j of alternative a [$kg\ m^{-3}$]
SF_{pajf}	feed substrate concentration of material f [$kg\ m^{-3}$]
T_{paj}	stage operating time [h]
TAC	total annual cost [$\$\ year^{-1}$]
TL	Plant cycle time [h]
V_{paj}	unit size [m^3]
VF_{pajf}	feed volume of material f [m^3]
X_{paj}	biomass concentration [$kg\ m^{-3}$]
X^{dead}_{paj}	non-active biomass concentration [$kg\ m^{-3}$]
Yx_{paj}	biomass yield coefficient
μ_{paj}	specific growth rate of biomass [h^{-1}]

Parameters

A_p	number of alternatives of each operation
C_p	upper bound on the number of stages
G_{paj}	number of in-phase duplicated stages in the NLP superstructure model
H	horizon time [$h\ year^{-1}$]
ks_{paj}	substrate saturation constant [$kg\ m^{-3}$]
M_{paj}	number of out-of-phase duplicated stages in the NLP superstructure model
OC	operating costs [$]
Q	demand [kg]

Ye_{paj}	product yield coefficient
α_p	cost coefficient
β_p	cost exponent
γ_f	cost of sugar substrate [\$ m^{-3}]
$\mu_{max,paj}$	maximum specific growth rate of biomass [h^{-1}]
υ_{paj}	biomass rate death [h^{-1}]

1. Introduction

The design problem of a batch process plant implies determining the plant structure, the number of units to be used at each stage and its size. Previously published works on this area resorted to mixed integer non-linear models (MINLP). Binary variables allowed for contemplating the different alternatives to organize units at each stage. The various models were characterized by a certain number of stages, which are the necessary steps to elaborate the product according to the previously settled recipe. This problem was initially modeled with this format by Grossmann and Sargent [1].

The aforementioned work and those that followed started from relating the sizes of the batches to be processed to the equipment size through linear factors called size factors. Different alternatives have been used for the case of operating time of process stages. The most frequently used models are those with fixed times and variable times depending on the batch size to be processed with a predetermined expression. These assumptions allowed for notably simplifying the model, since a posinomial structure was achieved, which assured the existence of a unique optimum of the problem [1]. Anyway, the different parameters that characterized the model were calculated on some determined operative conditions. In this way, the possibility of adjusting these values according to variations in the process operation was lost. However, this kind of models was widely used in subsequent works [2–6].

Taking into account the very strong limitation as regards the level of detail employed in representing the production process, some other approaches followed. Salomone and Irribarren [7] proposed performance models in which posinomial representation constants were calculated from models that considered other process decision variables. In this way, information on the process operation could be incorporated into design. In the first works [7,8], this approach was used for small plants and then it began to be considered for bigger processes [9,10]. In this way, it was possible to pose models with a greater level of detail as regards the process description. This led to both an increased complexity in resolution and a loss of the properties of the original posinomial model. The attained models presented a structure that strongly depended on the equations corresponding to performance models. For this reason, a non-convex model was generally obtained.

MINLP problems are usually solved through methodologies that successively solve mixed integer linear (MILP) approximations to the model, and NLP problems for fixed configurations, i.e. certain decisions as regards the value of binary variables [11]. For the case of a non-convex problem, this mechanism presents the drawback that successive linearizations usually cut part of the feasible region. In this way, some solutions to the problem are lost [12]. In addition, many

solutions of plant configurations, which are found through MILP, correspond to non-feasible structures, with which it is not possible to meet production requirements.

Another important aspect to be taken into account is that all works on this area start from a process in which the number of stages is settled by a decision made in a previous step. Thus, the only structural decision that remains is the one related to unit duplication at each previously determined stage. It is important to highlight that there are many operations that pose alternatives as regards the number of stages to be used. For example, in the case of fermentation depending on reaction velocity, equipment cost, or raw material availability, the number of units to be used and the way in which they should operate (in series or in parallel) may vary. It is interesting to consider these options in relation to the other previously described decisions. By means of this example, it is noted that there is a strong relationship among the number of stages, the way in which each stage is configured and the operative characteristics of stages, which has not been posed yet. This is due to the difficulties in solving a problem in which the number of stages in the plant is a model variable.

This work is intended to solve the aforementioned problems. Firstly, we start from a model with a high level of detail. Operations have been represented through discretized differential equations that describe mass balances (in this case mass balances of batch fermentors). Furthermore, constraints on feeds to each processing unit and equations of interconnections between stages are considered. It is a level of detail that has been posed by few authors. Some exceptions that can be mentioned are Bhatia and Biegler [13], even though with a simpler model since they work with a predetermined number of stages and they do not admit its duplication.

The option of determining the number of stages in series to be considered has not been included in general models of batch plants design. All of the elements that make up a plant structure have been solved in previous models resorting to binary variables. It should be stressed that, in many cases, when the level of detail of the operations included in the process was significant [13,14] this last option was not even considered. As previously pointed out, this led to difficulties or constrained the capacity for solving the model. For that reason, this work proposes the solution of the problem by explicitly including a superstructure that contemplates all possible options with units in series or in parallel. These options can be obtained by means of different mechanisms. A previous work [15] presented a heuristic procedure through a simplified optimization model that provides an upper bound over the number of stages of each operation. Another option is to pose an exhaustive detail of all the alternatives arisen from the upper bounds for the units in series or in parallel. The designer's criteria and his or her experience are also critical aspects taking into account that this approach is useful for expensive units with a significant impact on the complex process performance. The resulting model is a NLP, and thus it avoids difficulties of resolution methodologies of the outer approximation type that arise in non-convex programs. Therefore, the work presents a representation schema of the configuration options of the plant, which is extremely compact and allows for taking into consideration a significant number of alternatives.

The developed model is presented over the case of a fermentors network. It is a typical case for a number of reasons. First of all, it is often present in industrial plants. In addition, it is necessary to represent the process with a high level of detail, due to the high economic value of the various involved elements and its impact on the plant cost. Due to the operation characteristics, it is required to duplicate stages both in series and in parallel. On the other hand, the number of options to be contemplated in both cases is relatively bounded by operative considerations. It is important

to mention that this approach could be easily extended for another kind of operations. In the case a mono-product plant it is solved in the same way, but it could be easily extended to the multi-product case in which many products are made with the same equipment.

In the next section, the characteristics of the model are presented. Then, we describe its application to the case of a fermentors network. The resolution of this example allows contemplating the potentiality of the proposed approach. Finally, it is compared to a traditional formulation in which the structural decisions of the plant are represented by means of binary variables.

2. Model formulation

We consider a plant that produces only one product and must meet a certain demand Q for that product on the available time horizon H.

For the purpose of completing the product processing, P operations are required. Each operation is accomplished over several stages j, whose optimal number has to be determined. For each operation p, there is an upper bound C_p on the number of stages to be contemplated for this operation. In this way, there is an allowance for varying the number of stages to be considered for each operation. Therefore, for each operation p, there is a set of stages j ranging from 1 to C_p, whose utilization must be determined as a solution to the optimization problem.

It should be pointed out that this approach is more realistic when the operation of each stage can be represented by means of a detailed model and is not fixed by a size factor as in the first examples we referred to in the introduction section. In this way, it is possible to take into account the different tradeoffs that arise when considering different operative conditions. Therefore, the model to solve the batch operations design comes to be more appropriate when the description of the stages operation is explicitly contemplated.

For each operation p, alternatives $a = 1, \ldots, A_p$ are defined. These alternatives can be either automatically generated (through an optimization model, for example) or proposed by the designer, which is more effective, taking into account the feasible options for the kind of process they are working with. Each existing alternative a in operation p must be characterized. This implies defining the following elements:

- Number of stages to be included in the alternative.
- Determining the last stage being included in the alternative (basic information to allow for connection between successive operations).
- Number of in-phase (G_{paj}) and out-of-phase (M_{paj}) duplicated units for each stage included in the alternative.

The existing j stages in alternative a of operation p may vary between 1 and C_p. For each alternative, the number of stages is predetermined. Each one of these alternatives has structural options due to the duplication of the units included in it. These options are predetermined in each alternative a.

The transfer policy considered in this work is the zero wait (ZW) transfer. A stage-configuration option is in series duplication. In this case, the cycle time (problem variable) for a plant is determined as the longest time of all the stages over each operation involved in its production

process. This cycle time settles down the time between two successive batches. Therefore, all units that require less time for their operation have some idle time. With the aim of reducing this time, out-of-phase parallel units can be introduced into the stage in which the cycle time is reached. These units operate out-of-phase, thus allowing for reducing the time spent between two successive batches, and consequently the remaining unit size is diminished as a result of having less idle time.

The other configuration option for units duplicated at a stage corresponds to the in-phase case, in which duplicated units operate all together. In this case, when the batch enters that stage, it is split among all units making up the stage and, when finishing the process, the resulting batch is gathered together again. In this way, the processing capacity of a stage can be enhanced, which is important when the unit size reaches the upper bound.

Fig. 1 shows an example. An operation ($P = 1$) has $C_p = 3$ stages, which indicates that any alternative being used in this operation can have 3 stages at the most. The problem designer

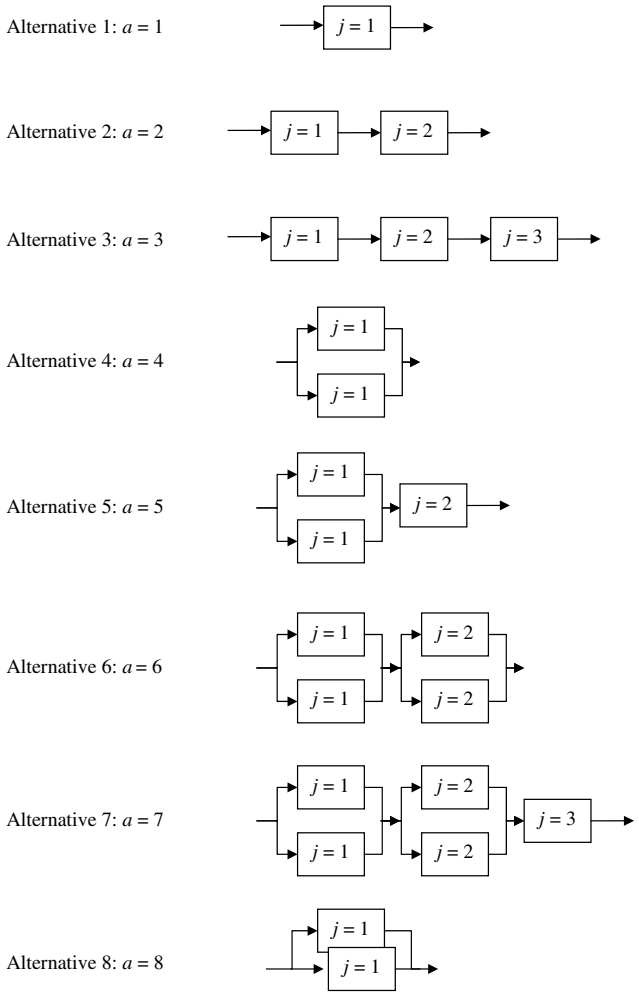

Fig. 1. Alternatives to be considered for a three-stage operation.

has settled that the $A = 8$ alternatives shown in Fig. 1 should be taken into account. The j stages used in the corresponding a alternative are also indicated. The first alternative includes only one stage, whereas the following two have added in series stages. The other alternatives have included out-of-phase duplicated units for various stages, except for the last one ($a = 8$), which is the only stage in which in-phase duplicated units are considered. This is shown through overlapped units in Fig. 1.

The model tries to determine a plant design that allows producing the required quantity Q in time horizon H at the lowest cost. This general presentation takes into account unit costs and operative costs. The objective function is total annual cost (TAC) minimization and is calculated from the following expression:

$$\text{Min TAC} = \sum_{p=1}^{P} \sum_{a=1}^{A_p} \sum_{j=1}^{C_p} \alpha_p M_{paj} G_{paj} V_{paj}^{\beta_p} + \text{OC}. \tag{1}$$

V_{paj} is unit j size in alternative a for operation p. Its cost is calculated from coefficients α_p and β_p that are usually used in this kind of problems [1–3]. M_{paj} and G_{paj} correspond to the number of out-of-phase and in-phase duplicated units, respectively, for stage j in alternative a for operation p (model data). OC represents operating costs that depend on how each operation is performed and thus it cannot be represented through a general expression.

In the previous expression, all stages j of all existing alternatives for operation p are considered. Taking into account that the objective function minimizes the units cost, only the best structural option will be chosen, driving to zero the size of all units that are not involved in the optimal structure. The simultaneous operation of two structures will always involve a greater cost taking into account that the exponent coefficient β_p is less than one. For that reason, the unit sizes of non-optimal alternatives will be equal to zero.

According to this information, a set of constraints are developed. First of all, the required demand should be satisfied. For that purpose, the plant production rate PR is employed, which is given by:

$$\text{PR} = \frac{Q}{H}. \tag{2}$$

At the last stage of the last operation, the final product is obtained. The sum of what is produced through all of the alternatives there defined must meet the settled requirements for the plant:

$$\sum_{a \in p_{\text{last}}} \text{PR}_{p_{\text{last}} a j_{\text{last}}} \geqslant \text{PR}, \tag{3}$$

where p_{last} corresponds to the last operation of the process and j_{last} to the last stage in each option a. For this operation, what is produced $\text{PR}_{p\text{last}}a$ is added in each available alternative for operation p_{last}, which are given by

$$\text{PR}_{p_{\text{last}} a j_{\text{last}}} = \frac{Q_{p_{\text{last}} a}}{\text{TL}} \quad \forall a = 1, \ldots, A_{p_{\text{last}}}, \tag{4}$$

$Q_{p_{\text{last}} a}$ corresponds to the quantity produced in alternative a in the last operation.

The total produced should be at least equal to the plant requirement. Logically, since the model tries to minimize costs, the quantity to be produced will be just PR, and will be reached by using only one alternative in operation p_{last}. This will be so because in case of using two alternatives it will be necessary to use equipment for both of them, which would notably increase the cost.

It is required to determine the plant cycle time TL. This is determined by the longest time required in the stages being used at the plant. Let T_{paj} be the unit operation time at stage j for alternative a in operation p. This value is calculated from the model that described that operation. Then, considering ZW policy, it should be

$$\text{TL} \geqslant \frac{T_{paj}}{M_{paj}} \quad \forall p = 1, \ldots, P;\ \forall a = 1, \ldots, A_p;\ \forall j = 1, \ldots, C_p, \tag{5}$$

M_{paj} corresponds to the number of out-of-phase duplicated units that exist at stage j of alternative a in operation p.

Connection balances should be performed between successive stages of each alternative of an operation. Let B^{e}_{paj} and B^{s}_{paj} be the batch volume that enters and leaves the unit of stage j in alternative a in operation p; then the balances are

$$B^{\text{e}}_{paj} = B^{\text{s}}_{pa,j-1} \quad \forall p = 1, \ldots, P;\ \forall a = 1, \ldots, A_p;\ \forall j \geqslant 2. \tag{6}$$

In case of handling several materials, this kind of connection constraint should be settled for each of them. As it will be seen in the example, this balance can also consider adding extra feeds at each stage.

Connection between successive operations must be also assured. For that reason, the last stage of an operation should get in contact with the first stage of the following operation:

$$\sum_{a_p \in p} B^{\text{s}}_{p,a,j_{\text{last}}} = \sum_{a_{p+1} \in p+1} B^{\text{e}}_{p+1,a,1} \quad \forall p = 1, \ldots, P-1. \tag{7}$$

In this case, the total obtained at the last stage j_{last} of all alternatives of operation p, must be equal to all material entering the first stage of all alternatives of the following operation.

The B_{paj} and T_{paj} values being used must be characterized through appropriate equations. Even the material to be considered could be decomposed into several components (substrate, biomass, product, etc.) as it will be shown in the example of this work. The existing relationship among the material to be processed, the equipment sizes and the time that will be required for processing arises from the model to be used for describing this operation.

Therefore, there is a set of constraints that closely depend on the characteristics of the process being used, so it is not possible to formalize them with a general format.

3. Fermentation process for ethanol production

In this example corresponding to fermentation for ethanol production, the previously described model is applied to a specific case. The detailed models that allow describing each unit operation are introduced.

Fermentation for ethanol production consists of two operations, namely: biomass fermentation and ethanol fermentation. At the first operation, only biomass is produced, while at the second

both ethanol and biomass are produced, even though the latter is produced at a growth velocity that is lower than that of the previous operation. All stages of both operations can be fed with a mixture of sugar substrates that provide different substrate concentrations. Water can be also added to dilute these substrates. Mass balances of these stages are described by the following differential equations:

$$\text{Biomass}: \frac{\mathrm{d}X_{paj}}{\mathrm{d}t} = \mu_{paj}X_{paj} - \upsilon_{paj}X_{paj}, \tag{8}$$

$$\text{Substrate}: \frac{\mathrm{d}S_{paj}}{\mathrm{d}t} = -\frac{\mu_{paj}X_{paj}}{Yx_{paj}}, \tag{9}$$

$$\text{Non-active biomass}: \frac{\mathrm{d}X^{\text{dead}}_{paj}}{\mathrm{d}t} = \upsilon_{paj}X_{paj}, \tag{10}$$

$$\text{Product}: \frac{\mathrm{d}E_{paj}}{\mathrm{d}t} = \frac{\mu_{paj}X_{paj}}{Ye_{paj}}, \tag{11}$$

where

$$\mu = \mu_{\max,paj}\frac{S_{paj}}{ks_{paj} + S_{paj}}, \tag{12}$$

where (8)–(12) are described for $\forall p = 1,\ldots,P$; $\forall a = 1,\ldots,A_p$; $\forall j = 1,\ldots,C_p$, X is biomass concentration, S is substrate concentration, X^{dead} is non-active biomass concentration, E is ethanol concentration. For this reason, Eq. (12) is not obtained in the first operation and μ is growth specific velocity. All these are problem variables. υ represents bacteria death velocity, Ye is ethanol yield coefficient and ks is a substrate saturation constant. These are known parameters for the model. Yx is biomass yield and is a function of the biomass fermentor feed at biomass fermentors and a constant in the ethanol fermentation operation [15].

These equations have been discretized using the trapezoidal method and included in the global model. This model also contains all constraints presented in the previous section: connections between stages of each alternative of each operation, connections between the last stage of an operation and the first stage of the following operation, constraints that define the time cycle, constraints to meet production requirements, and a set of balances that are similar to those given in Eqs. (6) and (7) that is performed for each component: biomass, substrate, non-active biomass and ethanol. For example, substrate balances between successive stages are expressed by

$$V_{paj}S^{\text{e}}_{paj} = \sum_{f\in\text{Feed}_{paj}} SF_{paj\text{f}}VF_{paj\text{f}} + V_{pa,j-1}S^{\text{s}}_{pa,j-1}, \quad \forall p = 1,2;\ \forall a = 1,\ldots,A_p;\ \forall j \geqslant 2, \tag{13}$$

where S^{e}_{paj} represents substrate concentration entering stage j of alternative a of operation p, f the various materials that constitute the feed for stage j and those that belong to the set Feed_{paj}. In this example we took. $\text{Feed}_{paj} = \{\text{molass}_{paj}, \text{filter\_juice}_{paj}, \text{vinasses}_{paj}, \text{water}_{paj}\}$, each one of them having a substrate concentration that is equal to $SF_{paj\text{f}}$ and volume equal to $VF_{paj\text{f}}$. $S^{\text{s}}_{pa,j-1}$ is the output substrate concentration of unit $j-1$ of alternative a. It should be noted that in this case, besides the material coming from the previous stage, other material from other sources

represented by the set Feed_{paj} is also allowed to enter. In a similar way, the balances for the remaining elements and interconnection balances between operations are posed.

Since variable feeds are considered, volume balances have been added:

$$V_{paj} = \sum_{f \in \text{Feed}_{paj}} VF_{paj\text{f}} + V_{pa,j-1} \quad \forall p = 1,2;\ \forall a = 1,\ldots,A_p;\ \forall j \geqslant 2. \tag{14}$$

The posed objective is minimizing total annual costs, which are computed as investment cost (given by equipment cost) in addition to operating costs. In this specific case, variable OC of expression (1) can be posed as shown by expression (15). This operating cost is the sum of the cost per m^3 of sugar substrates being used in feed f to stage j of alternative a of operation p. Let γ_f be cost per m^3 of the sugar substrate f being used in feed Feed_{paj}, then the total annual cost can be computed as:

$$\text{Min TAC} = \sum_{p=1}^{P}\sum_{a=1}^{A_p}\sum_{j=1}^{C_p} \alpha_p M_{paj} G_{paj} V_{paj}^{\beta_p} + \frac{H}{TL}\sum_{p=1}^{P}\sum_{a=1}^{A_p}\sum_{j=1}^{C_p}\sum_{f \in \text{Feed}_{paj}} \gamma_f VF_{paj\text{f}}. \tag{15}$$

4. Example resolution

The fermentation model for ethanol production that was established in the previous section has been solved. We will present three examples with different sets of data with the aim of evaluating the optimal design of the plant according to various problem conditions.

It is a problem with $P = 2$ operations. For both first examples, the chosen superstructure schema is shown in Fig. 2. This figure includes the diverse alternatives that were selected by the designer for each one of the two operations the plant comprises. It should be noted that this superstructure allows considering the combination of the different alternatives that are chosen for each operation.

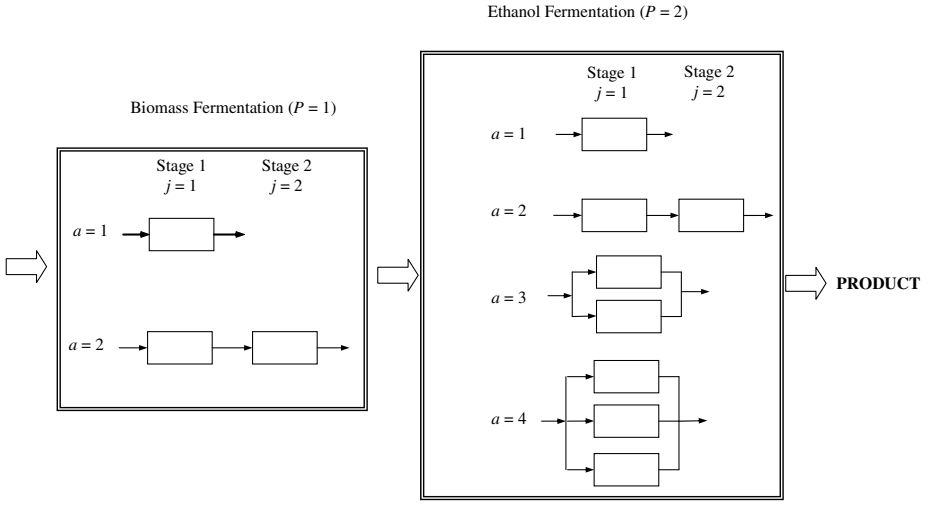

Fig. 2. Superstructure for ethanol fermentation model in Examples 1 and 2.

In the first operation, there are $C_1 = 2$ stages, so any alternative can have up to two stages. Fig. 2 also includes $A_1 = 2$ alternatives that are taken into account in this operation. In the first one, there is only one stage, while in the second one there are two stages in series. For the second operation, four alternatives of up to $C_2 = 2$ stages are considered. In this case, the first alternative consists of only one stage, the second one consists of two stages in series, the third one is the out-of-phase in parallel duplication of the first stage and the last one is the out-of-phase triplication of the first stage in parallel. The selection of alternatives for these operations is assumed to be based on the knowledge held by the designer on the problem as regards its feasibility from the engineering point of view. In this case, as the reaction velocity of the biomass fermentation operation is faster than that of the ethanol fermentation operation, processing time of the first operation tends to be lower than that of the following operation and therefore the option of in parallel stages duplication in not included in the first operation.

It is necessary to characterize each of the alternatives. Table 1 describes the elements of each alternative for biomass and ethanol fermentation. It indicates the number of in-phase and out-of-phase duplicated units at each stage making up each alternative. Moreover, it indicates the last stage of each alternative. This information is used for balances between stages and, in the case of the last one, for determining the process production.

The models have been implemented and solved in GAMS (General Algebraic Modeling System, [16]) in a CPU Pentium IV, 1.60 GHz. CONOPT 2 code was used to solve the NLP problem.

The model parameters values for the following examples are shown in Table 2.

As a first example, the model of the previously presented superstructure is solved by setting the equipment costs exponent β at 0.43 for both operations. The optimal configuration for producing 100 kg/h of ethanol corresponds to the first alternative of operation 1 and the first alternative of operation 2, i.e., alternatives $a = 1$ for $p = 1$ and $a = 1$ for $p = 2$. Fig. 3 shows the optimal solution. The values of some process and design variables are found in Table 3. Sub-index "*final*" of some variables denotes the value of the variable at final time (value corresponding to the last point of discretization). The time cycle of the plant is 16 hr 24 min and the total annual cost is \$287,865.

In the second example, we increase the production rate to 500 kg/h. The best alternative consists of using a biomass fermentor and two ethanol fermentors in series. Fig. 4 shows this solution

Table 1
Description of the alternatives of ethanol superstructure for Examples 1 and 2

	Operation: biomass fermentation			Operation: ethanol fermentation		
	Stage 1	Stage 2	Last stage	Stage 1	Stage 2	Last stage
Alternative 1	$M_{111} = 1$ $G_{111} = 1$	$M_{112} = 0$ $G_{112} = 0$	1	$M_{211} = 1$ $G_{211} = 1$	$M_{212} = 0$ $G_{212} = 0$	1
Alternative 2	$M_{121} = 1$ $G_{121} = 1$	$M_{122} = 1$ $G_{122} = 1$	2	$M_{221} = 1$ $G_{221} = 1$	$M_{222} = 1$ $G_{222} = 1$	2
Alternative 3	No	No		$M_{231} = 2$ $G_{231} = 1$	$M_{232} = 0$ $G_{232} = 0$	1
Alternative 4	No	No		$M_{241} = 3$ $G_{241} = 1$	$M_{242} = 0$ $G_{242} = 0$	1

Table 2
Parameters used in the ethanol production model

Parameter	Value
$\mu_{\max,1aj}$	0.5 h^{-1}
$\mu_{\max,2aj}$	0.1 h^{-1}
α_p	115,550
υ_{paj}	0.02 h^{-1}
Yx_{2aj}	0.124
Ye_{2aj}	0.23
H	7500 h $year^{-1}$
ks_{paj}	20 kg m^{-3}

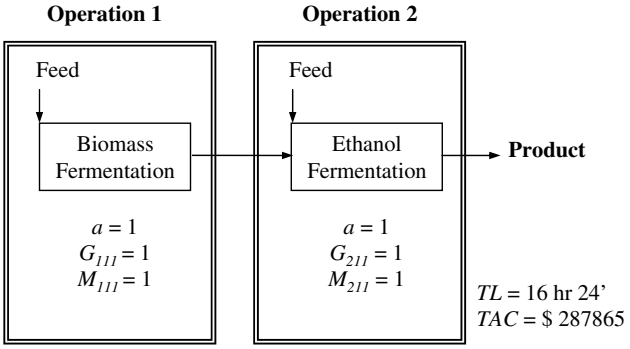

Fig. 3. Optimal solution for $\beta_p = 0.43$ and PR = 100 kg h^{-1}.

and Table 3 presents the values of some optimal design and process variables. The time cycle is 16 h 1 min and the Total annual cost is $883,732.

In the third example we decrease the equipment cost exponent of the first operation (β_1) to 0.3 and increase the second ones (β_2) to 1. For this case, we change the superstructure schema presented on Table 1. Table 4 presents the information about the superstructure for both biomass and ethanol fermentation operation, and Fig. 5 shows this superstructure schema. The optimal solution consists of the out-of-phase in parallel duplication of the first biomass fermentor followed by one biomass fermentor and two ethanol fermentors in series. This solution corresponds to Alternative 5 of the first operation and Alternative 2 of the second one. Fig. 6 shows this solution and Table 3 presents some of its optimal variables. In-parallel working equipment has the same operative and design characteristics (operation time, size, feeds, flows, etc.). The time cycle is in this case equal to 5 h 9 min 47 s and the total annual cost is $526,822.

5. A comparison with the traditional approach

A comparison will be made between the proposed approach, in which the different alternatives of the plant configuration are modeled without resorting to binary variables, and the traditional approach, in which the problem is represented through a MINLP program.

Table 3
Design and operating optimal solutions

	First example		Second example			Third example			
	Biomass fermentor	Ethanol fermentor	Biomass fermentor	Ethanol fermentor 1	Ethanol fermentor 2	Biomass fermentor 1	Biomass fermentor 2	Ethanol fermentor 1	Ethanol fermentor 2
Time (h)	16.44	16.44	16.017	16.017	16.017	10.326	5.163	5.163	5.163
Size (m^3)	6.719	31.89	11.29	57.84	98.09	4.075	4.169	4.675	5.33
$X_{initial}$ ($kg\,m^{-3}$)	0.1	7.45	0.1	6.74	8.6	0.1	5.75	31.86	34.94
X_{final} ($kg\,m^{-3}$)	35.38	15.39	34.53	14.58	16.43	5.88	35.73	39.8	42.83
X_{final}^{dead} ($kg\,m^{-3}$)	2.7	0.568	2.405	3.94	6.6	0.296	2.1	5.65	9.08
S_{final} ($kg\,m^{-3}$)	2.275	4.4	5.22	8.74	2.37	84.36	17.56	5.52	3.1
E_{final} ($kg\,m^{-3}$)	–	51.54	–	49.2	81.64	–	–	50.94	96.96

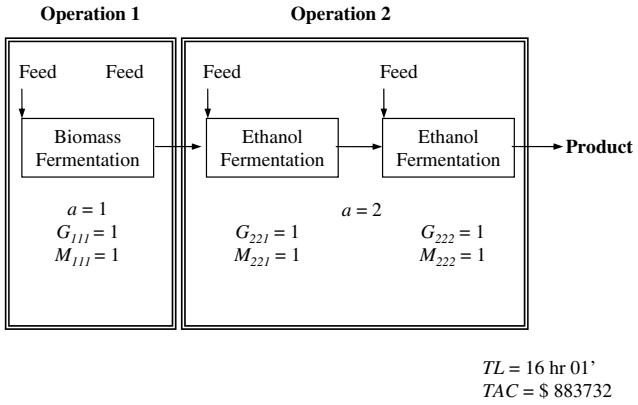

Fig. 4. Optimal solution for $\beta_p = 0.43$ and PR $= 500\ \mathrm{kg\ h^{-1}}$.

Table 4
Description of the alternatives of ethanol superstructure for Example 3

	Operation: biomass fermentation			Operation: ethanol fermentation		
	Stage 1	Stage 2	Last stage	Stage 1	Stage 2	Last stage
Alternative 1	$M_{111} = 1$ $G_{111} = 1$	$M_{112} = 0$ $G_{112} = 0$	1	$M_{211} = 1$ $G_{211} = 1$	$M_{212} = 0$ $G_{212} = 0$	1
Alternative 2	$M_{121} = 1$ $G_{121} = 1$	$M_{122} = 1$ $G_{122} = 1$	2	$M_{221} = 1$ $G_{221} = 1$	$M_{222} = 1$ $G_{222} = 1$	2
Alternative 3	$M_{131} = 2$ $G_{131} = 1$	$M_{132} = 0$ $G_{132} = 0$	1	$M_{231} = 2$ $G_{231} = 1$	$M_{232} = 0$ $G_{232} = 0$	1
Alternative 4	$M_{141} = 3$ $G_{141} = 1$	$M_{142} = 0$ $G_{142} = 0$	1	$M_{241} = 3$ $G_{241} = 1$	$M_{242} = 0$ $G_{242} = 0$	1
Alternative 5	$M_{151} = 2$ $G_{151} = 1$	$M_{152} = 1$ $G_{152} = 1$	2			
Alternative 6	$M_{161} = 1$ $G_{161} = 1$	$M_{162} = 2$ $G_{162} = 1$	2			

Firstly, it should be highlighted that traditional models do not solve this problem by considering in series stages duplication. Consequently, in order to perform a comparison, we assume that the number of plant stages is fixed, and thus we are facing a problem that is sensitively simpler than the one presented in this article. Therefore, the only way of comparing both approaches is solving a sequence of MINLP problems that contemplate all the alternatives. This work has been accomplished in this example because this includes a small number of operations and stages. In more realistic problems, this task can be extremely burdensome.

It is assumed that each MINLP model contemplates all the previously posed constraints. The difference lies in the fact that the number of stages on each operation is fixed, and the number of out-of-phase and in-phase parallel units for each stage is variable (M_j and G_j). In this case,

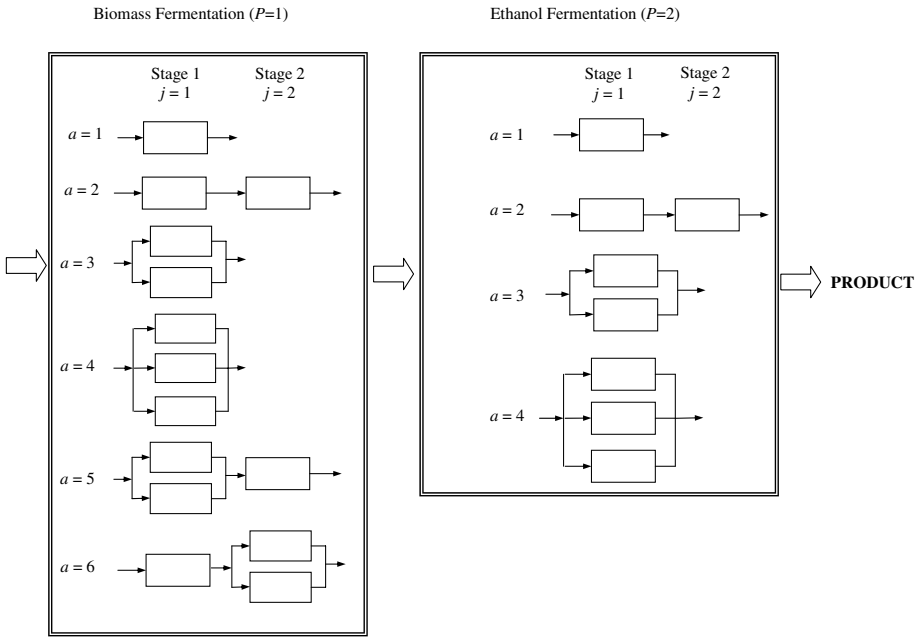

Fig. 5. Superstructure for ethanol fermentation model in Example 3.

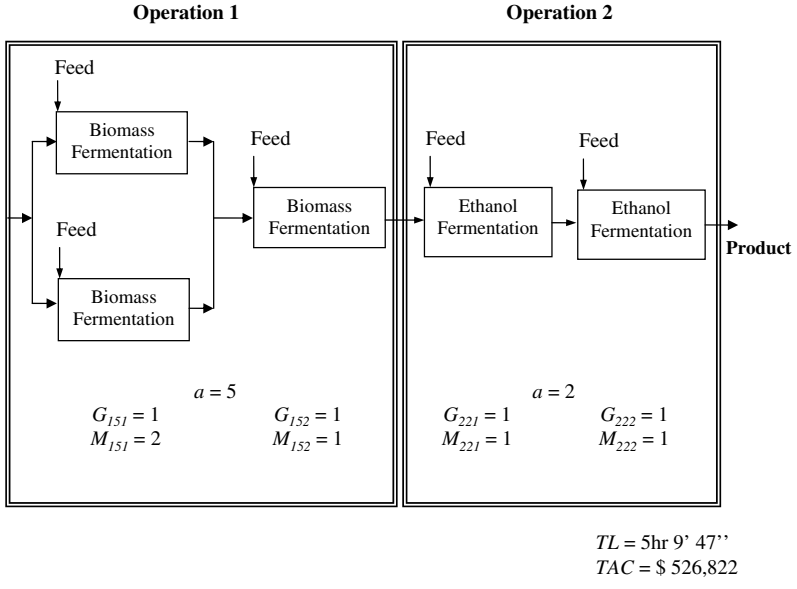

Fig. 6. Optimal solution for PR = 100 kg h^{-1}, $\beta_1 = 0.3$ and $\beta_2 = 1$.

sub-indexes p and a disappear and we only work with stages j that are included in the plant. M_{paj} and G_{paj}, which used to be parameters of each alternative, now become variables M_j and G_j, since

it is intended to determine the number of units composing each stage. All the previously posed equations remain.

Among the previously solved examples, the third example was chosen. The optimal solution there obtained had two biomass fermentation stages where the first one uses out-of-phase parallel duplicated units and two ethanol fermentation stages in series. In order to perform the comparison, four models are solved which contemplate the possible configurations using a predetermined number of units in series for each operation. For this example, up to two stages are used for each operation because this was obtained in the optimal solution of the NLP superstructure model. Then, the number of parallel units and size of each stage are to be determined.

This is obviously a much simpler problem but it is included with the object of evaluating the behavior of this kind of highly non-convex models when handling binary variables explicitly.

The cases modeled with binary variables are:

(i) one biomass fermentation stage and one ethanol fermentation stage,
(ii) one biomass fermentation stage and two ethanol fermentation stages,
(iii) two biomass fermentation stages and one ethanol fermentation stage,
(iv) two biomass fermentation stages and two ethanol fermentation stages.

The upper bounds for the M_j variables are shown in Table 5 for each previously mentioned case. In Table 6 the results for each studied case are shown, including the operations configuration, operating time, unit sizes, objective function value, number of constraints, number of continuous and discrete variables and CPU time to perform the solution.

The NLP superstructure model of Example 3 has 1707 continuous variables and 1617 constraints and the solution was performed in 10.5 CPU seconds. As it can be observed, the solutions of the MINLP cases were performed in a shorter CPU time, but in all cases the number of constraints and variables is smaller and the models are much simpler as it was previously mentioned. The solution of the model (iv) coincides with that obtained in the NLP superstructure model.

A commentary on the CPU resolution time is that the differences are not so significant (on the same order). Anyway this depends strongly on diverse factors, for example the initialization of variables, which can lead to changes in CPU resolution time. Nevertheless, it is necessary to emphasize that, ahead of the comparison of the resolution times, the MINLP model requires a greater effort for the generation of the different options. In this example only four options have been necessary, but in cases with more operations this number can be considerably increased,

Table 5
Out-of-phase parallel units upper bounds for MINLP models

Cases	Upper bound for M in biomass fermentation		Upper bound for M in ethanol fermentation	
	Stage 1	Stage 2	Stage 1	Stage 2
(i)	2	–	4	–
(ii)	2	–	3	3
(iii)	2	2	4	–
(iv)	2	2	3	3

Table 6
Optimal solutions of MINLP cases

	Case (i)		Case (ii)			Case (iii)			Case (iv)			
	Biomass fermentation	Ethanol fermentation	Biomass fermentation	Ethanol fermentation 1	Ethanol fermentation 2	Biomass fermentation 1	Biomass fermentation 2	Ethanol fermentation	Biomass fermentation 1	Biomass fermentation 2	Ethanol fermentation 1	Ethanol fermentation 2
Configuration	$M = 2$	$M = 1$	$M = 2$	$M = 1$	$M = 1$	$M = 2$	$M = 1$	$M = 1$	$M = 2$	$M = 1$	$M = 1$	$M = 1$
Time (h)	14.469	7.234	14.207	7.103	7.103	10.628	5.314	5.314	10.326	5.163	5.163	5.163
Size (m^3)	12.6	13.88	5.84	6.39	7.28	7.76	9.15	10.29	4.075	4.169	4.675	5.33
TAC ($)	643,687			583,410			605,692				526,822	
Constraints Num	252			387			359				494	
Continuous Variable Num	270			412			384				526	
Discrete Variable Num	8			12			12				16	
CPU time (s)	1.281			2.16			3.711				8.105	

because all possible combinations of alternatives must be done. Another subject to consider is the exigency of handling several models with different configurations, which leads to confusions.

6. Conclusions

This work presents a novel NLP model that serves to find the optimal configuration of plants with several operations, without resorting to binary variables to pose the different options. This approach gains more importance in cases for which operations can have several in series or in parallel duplicated stages (in-phase and out-of-phase). As regards the decision on how many stages in series have to be duplicated, there are no previous published works. For this reason, this methodology is an important tool. Furthermore, all possible options or those determined by the designer are simultaneously considered. This formulation is more appropriate and useful when detailed representations are posed. The resulting NLP model avoids difficulties that arise with resolution methodologies of MINLP problems applied to non-convex programs.

The model was described in a generic way and has a set of general constraints, but it also admits constraints that are specific to the operation to be designed and optimized.

This work presented the case of a fermentors network for ethanol production, whose operations were described in detail by means of a set of constraints that include dynamical equations. All constraints were included in the global model (superstructure) and simultaneously solved. Thus, optimal configuration, design and operation were found through a NLP problem.

Due to the characteristics of the operations on which this modeling technique is applied to real cases, the number of alternatives is restricted. Indeed, most of the time it is not necessary to apply all combinations among the various alternatives of the different operations because the designer can apply some criteria to describe only those that come out to be feasible for the process that is being optimized.

This model is simple to be written and includes a procedure to find initial solutions, which is generally known since it deals with real cases. Convergence and good solution are guaranteed in reasonable CPU time.

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