MATHEMATICAL MODELING APPROACHES FOR OPTIMIZATION OF CHEMICAL PROCESSES

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NOVA

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PREFACE

Mathematical modeling is a powerful tool for solving optimization problems in chemical engineering. In this work several models are proposed aimed at helping to make decisions about different aspects of the processes lifecycle, from the synthesis and design steps up to the operation and scheduling. Using an example of the Sugar Cane industry, several models are formulated and solved in order to assess the trade-offs involved in optimization decisions. Thus, the power and versatility of mathematical modeling in the area of chemical processes optimization is analyzed and evaluated.

Chapter 1

INTRODUCTION

Mathematical modeling is a powerful tool to solve different problems which arise in chemical engineering optimization. Problems as designing a plant, determining the number of units for a specific task, assigning raw materials to different production processes and deciding the production planning or production targets are some of the issues that can be solved through mathematical modeling. In other words, the mathematical formulations are used to make decisions at different levels, from the synthesis and design of the process up to its operation and scheduling.

In this work, different possible mathematical modeling in chemical engineering are developed. Generic formulations are presented and applied to a particular study case of the Sugar Cane industry: the simultaneous production of sugar and derivative products. Through the examples, several models will be posed corresponding to different considered conditions or decisions. Moreover, different scenarios will be considered and trade-offs between decisions will be represented and analyzed.

In general, the aforementioned problems in chemical engineering can be faced either sequentially or simultaneously. The sequential approach deals with each decision separately, one after the other. For example, the plant configuration is first determined, then the unit sizes, after that the processing variables e.g. processing times and flowrates, and lastly the production planning. Sometimes depending on the scenario, when the plant configuration or unit sizes are known, only the operating, scheduling or planning problem are solved separately. On the other hand, modeling all or some decisions simultaneously implies to consider in an overall model all the necessary variables and constraints in order to solve the plant synthesis, design, operation and planning, all together.

Some definitions, concepts and known methodologies of process system engineering are first presented in order to provide a background for the present work. Then, the mathematical models proposed in this work for different scenarios are formulated. Also real-world applications of synthesis, design, operation, scheduling, and planning problems are posed and solved. The optimal solutions are analyzed in each case and the advantages and disadvantages of each formulation are discussed. Finally, desirable future work in this area is briefly addressed.

Chapter 2

DEFINITIONS

In this section, some definitions are given in order to introduce the main characteristics of the processes to be modelled.

BATCH AND SEMI-CONTINUOUS UNITS

Batch and semi-continuous processes are essential to the chemical processing industry. Products produced in a batch plant range from simple agricultural bulk chemicals to innovative, complex, and high value pharmaceutical products. In a batch unit no simultaneous removal and addition of material streams are performed. Contrarily to the case of continuous processes, where processing tasks are arranged in a sequence and all tasks occur simultaneously, continuously receiving feed and producing product streams. A batch unit operates in a non-continuous manner, receiving feed at certain times and after a processing time, producing products or intermediates. Semi-continuous units are characterized by a processing rate for each product; they are operated continuously with periodic startups and shutdowns.

Batch processes consist of a collection of processing equipment where batches of the various products are produced by executing a set of processing tasks or operations like reaction, mixing or distillation. Every processing equipment can perform only some particular operations. Thus, it is possible to recognize production paths consisting of a sequence of processing equipment, which indicates potential routes that a batch might follow. Processing equipment that can perform the same operations can be grouped in a production stage.

The major classification of batch processes is based on the consideration of the type of production paths followed by the batches of products in the plant.

SINGLE PRODUCT, MULTIPRODUCT AND MULTIPURPOSE BATCH PLANTS

In a single product batch plant all the units are totally dedicated to the production of one product. It is the simplest plant operation and no product changeovers are necessary. All units can be designed to exactly fit a batch size and no sequencing has to be performed.

In a multiproduct plant, two or more products are produced following the same production path. When the products are produced through different production paths the plant is a multipurpose plant. Voudouris and Grossmann (1996) introduced a special classification for the multipurpose batch plant. More specifically they divided the multipurpose plants in sequential plants and non-sequential plants (Figure 1.1). In a sequential plant it is possible to recognize a specific direction in the plant floor that is followed by the production paths of all the products. Non-sequential plants are all the remaining cases. Multiproduct plants are used when the production recipes are similar to each other. As the similarities decrease, the plant becomes a multipurpose batch plant. Among these, sequential multipurpose plants are common in industry and hence of practical importance.

When two or more plants are nearly located and there are interconnections between them, the integration scenario is called multiplant complex (MC) integration. The model for a MC frequently considers mass and utility balances between the plants, besides the design, operation, scheduling and planning considerations. In some cases, there is a so called “mother plant”, that supplies raw materials and energy to others plants, called “derivative plants”. Figure 1.2 shows a MC scenario, with a mother plant and two derivative plants.

An important characteristic of batch processes is the way in which the batches are transferred from one unit to the following one in the production path. In this work, the Zero-wait (ZW) transfer policy is adopted. In the ZW policy the material at any stage will be transferred immediately to the next stage after finishing its processing. In this case, special timing constraints are required in the model. The ZW transfer is commonly used when no intermediate storage is available or when it cannot be held further inside the processing vessel (e.g., due to chemical reaction). The option when storage tanks with finite capacity are available is the finite intermediate storage (FIS) policy. When the material is allowed to hold inside the vessel, the policy is known as non-intermediate storage (NIS) policy.

In a batch plant, all the stages have their own processing time and their own maximum possible batch size. The actual size of a batch being processed in a plant depends on the capacity of a size limiting stage, and the time elapsed between the processing of consecutive batches cannot be shorter than the required by a time limiting stage. The limiting cycle time for a product corresponds to the longest processing time among all the stages, and determines the time between two successive batches. There are two types of bottlenecks: size and time. Units can be added at a stage in order to debottleneck the plant. These units can be operated in-phase or out-of-phase.

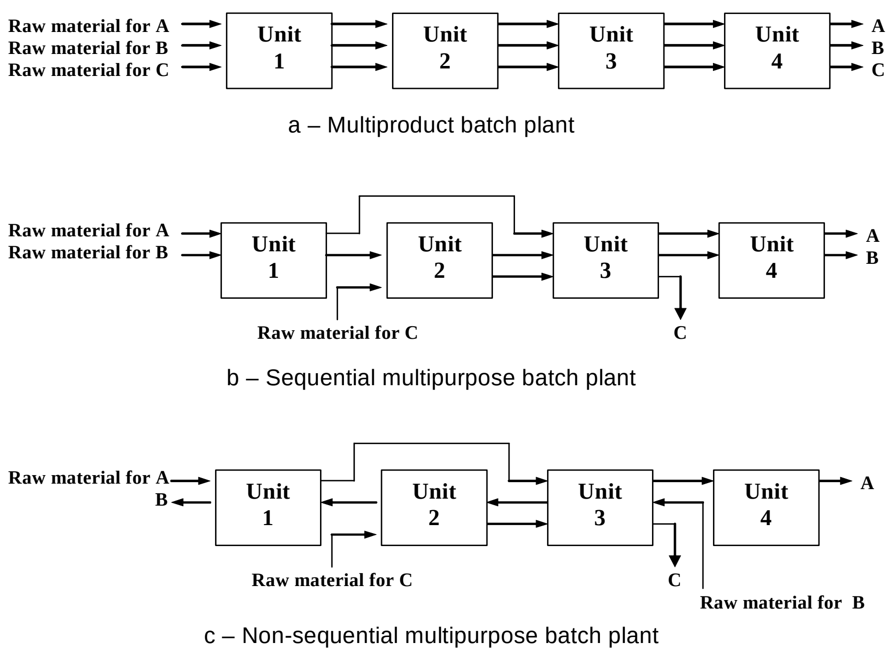


Figure 1.1. Batch plant classification.

Parallel units operating out-of-phase are added to remove a time bottleneck in a series of batch stages. With two units operating out-of-phase the stage cycle time is halved compared with only one unit. If a stage is time limiting, then adding parallel units out-of-phase will reduce the limiting cycle time so that the equipment utilization of the remaining units is increased, and thus the required unit sizes are reduced. Figure 1.3 shows the out-of-phase duplication of a stage.

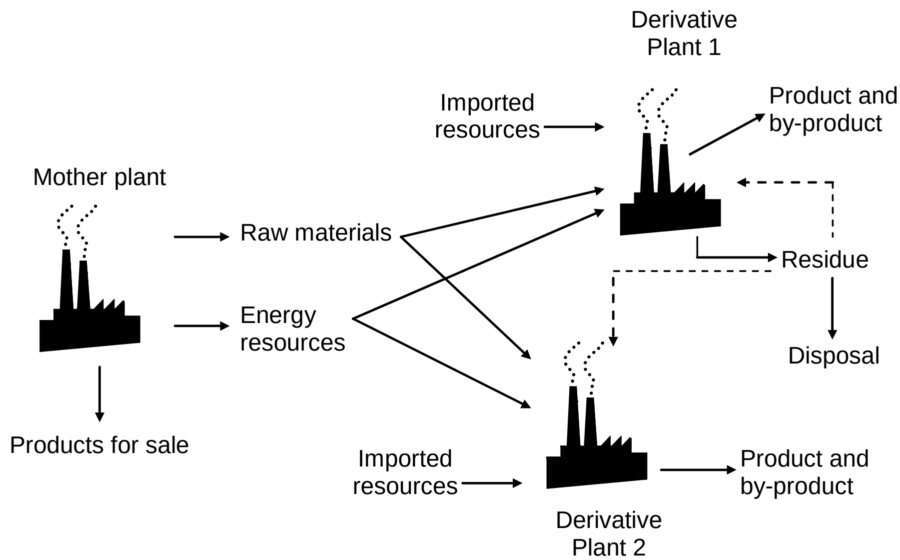


Figure 1.2. Multiplant complex scheme integration.

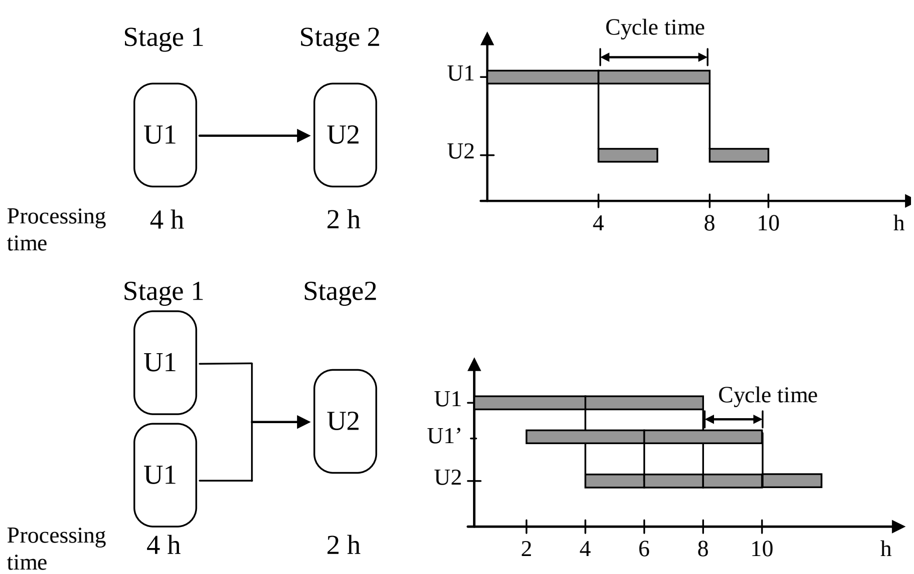


Figure 1.3. Out-of phase duplication. Up, original plant. Bottom, plant with two units in parallel out-of-phase in stage 1.

Parallel units operating in-phase are added to remove capacity bottlenecks. The batch from the previous stage is split and assigned to all the in-phase units of that stage. The units process all the material at the same time and upon completion the batches are mixed together and transferred to the next stage. This does not affect the limiting cycle time but the largest batch size that can be processed in the plant is increased.

A batch unit is fed with the material that arrives from the previous unit. Some batch stages require an extra feeding, e.g. the addition of substrate for fermentation stages. For these cases an interesting optimization option is unit duplication in series, where successive equal or not-equal units operate sequentially in order to fulfil certain final product specification. This type of duplication cannot be generalized since it depends on the processing variables. Duplication in series will be treated in this work as a novel process optimization decision.

OPTIMIZATION MODEL DECISIONS: SYNTHESIS, DESIGN, OPERATION, SCHEDULING AND PLANNING

In an optimization problem (OP), a decision is made aimed at the maximization or the minimization of a related performance criterion such as elapsed time or cost, by exploiting certain available degrees of freedom under a set of constraints. OPs arise in almost all branches of industry, e.g. in product and process design, production, logistics and even strategic planning. While the word optimization, in non-technical language, is often used in the sense of improving, the mathematical optimization community sticks to the original meaning of the word related to finding the best solution either globally or at least in a local neighbourhood. The OPs presented in this work consider decision making in the synthesis, design, operation, scheduling and planning of production plants.

In the process synthesis the structure of the plant is determined, satisfying a set of constraints and specifications. That is, once the problem inputs (feed volume and composition, for example), tasks and desired products have been specified, the synthesis problem determines the optimal selection of equipment and their interconnections that transform the inputs into final products.

The design problem deals with the sizing of equipment and storage units. This optimization can be done with size factors and operating times as constant parameters in the simplest models or as process dependent variables in more detailed models.

The operation decisions deal with finding the optimal value for process variables as operating times, batch sizes, concentrations, yields, etc. In the simplest models these decision variables are involved in linear equations or algebraic models that describe the units performance (Salomone and Iribarren, 1992). In more detailed models, this kind of decisions is described through differential equations (Bhatia and Biegler, 1996; Corsano, et al., 2004).

Production planning determines the optimal allocation of resources within the production facility over a time horizon of a few weeks up to a few months, whereas short-term scheduling provides the feasible production schedules to the plant for day to day operations. Since the boundaries of planning and scheduling problems are not well established and there is an intrinsic integration between these decision making stages, there is a lot of work in the literature addressing the simultaneous consideration of planning and scheduling decisions (Wu and Ierapetritou, 2007).

In multiproduct and multipurpose plant, where two or more products are handled, an important decision to be modelled is the sequence or order in which the products are produced. In single product campaign models all the batches of a product are processed without overlapping with others products. On the other hand, for mixed product campaign models a production sequence has to be determined and the campaign is repeated over the horizon time. From the point of view of the mathematical model, mixed product campaigns raise greater challenges than the formulations for single product campaigns.

Table 1.1 lists the most important synthesis, design, operating and scheduling/planning decisions and the related objective functions in order to have a brief overview of the model complexity and characteristics.

MATHEMATICAL FORMULATIONS

Mathematical models for optimization usually lead to structured problems such as:

- linear programming (LP) problems,
- mixed integer linear programming (MILP) problems,
- nonlinear programming (NLP) problems, and
- mixed integer nonlinear programming (MINLP) problems.

Table 1.1. Problem decisions and objectives

	Synthesis and Design	Operation	Scheduling/Planning
Decisions	Plant configuration Resources utilization Number of units in series Blend and recycle allocation Unit sizes In parallel units duplication Intermediate storage tank allocation Heating and cooling areas Power consumption (vapor and electricity)	Batch blending, batch splitting and batch recycling flow rates Material and energy resources allocation Component concentrations Unit processing times	Cycle time of each production process Units cycle time Units idle time Number of batches Mixed campaign configuration Production
Objectives	Minimizing the investment cost	Minimizing the operative cost Minimizing the utilities costs	Minimizing the makespan Maximizing the profit Minimizing the inventory cost

When the objective function and constraints of the model are linear and the optimization variables are continuous, then the problem is a LP formulation.

If some decision variables are integer, and the model has linear objective function and constraints, then the problem is a MILP formulation.

If the objective function or some constraints are non-linear functions, and the decision variables are continuous, then the problem is a NLP formulation. Finally, if in the last case some variables are integer, the model is formulated through a MINLP programming.

LITERATURE REVIEW

Since the 70s decade, many authors have contributed with new algorithms and formulations for the mathematical modeling of diverse process optimisation decisions. In general each one focused on a different problem, context or structural alternative in such a way that almost all the relevant alternative structures and options in the batch processes design and operation problems can be considered. However, this progress has occurred as extensions of individual works and not as complete reformulations in the sense of including all the possibilities or at least a significant set of alternatives and decisions. There are no models or formulations in the literature that permit consider and select among all the possible structures and alternatives simultaneously. This is so due to the great effort that the simultaneous resolution of the problems involves. However, in this way, the trade-offs among decisions cannot be assessed. Following, the main references about mathematical modeling in batch processes optimization are cited.

There is abundant literature on batch process synthesis and design. The models range from the simplest formulations as “fixed time and size factors” (Knopf et al., 1982; Yeh and Reklaitis, 1987; Ravemark and Rippin, 1998; Montagna et al., 2000) to the more complex as dynamic models (Bhatia and Biegler, 1996; Corsano et al., 2004, 2006a).

The process performance models are additional algebraic equations describing the time and size factors as functions of the units’ process variables. A more detailed description of the performance of batch stages requires that they be modelled with differential equations. First Barrera and Evans (1989) and later Salomone et al. (1994) proposed that this simultaneous optimization should be approached by integrating the batch plant model with dynamic simulation modules for the batch units. Another way of incorporating the units’ dynamic models is to discretize the differential equations to convert them into algebraic constraints of the program. This was the approach used by Bhatia and Biegler (1996) for simple process examples, and by Corsano et al. (2004, 2006) for detailed integrated processes.

Several authors have incorporated scheduling constraints into the synthesis problem of multiproduct and multipurpose batch plants. Again, the simplest models are those that take fixed time and size factors (Birewar and Grossmann, 1989) which are expressed through NLP when structured decision are not considered and MINLP otherwise. More detailed formulations where nonlinear task models (processing time, utility usage, unit availability) and nonlinear capital cost functions are considered, a nonconvex MINLP problem will arise (Zhang and Sargent, 1994, 1996). Therefore, the model is very large in size and difficult to solve. In these cases, decomposition approaches are used in order to find “good solutions” (Barbosa-Povoa and Pantelides, 1999).

Whereas significant development has been made in the design, planning, and scheduling of batch plants with single or multiple production routes, the problem of synthesis, design, and operation in batch multiplant complexes has received much less attention. Previous works have been focused on specific decision levels. Tools and models that solve separately the different aspects of a process have been developed. However, to obtain a good preliminary design of a production process, it is important to consider design, synthesis, operation, and scheduling simultaneously. There are few works in the literature dealing with multiplant complex integration (Lee et al., 2000, Kallrath, 2002, Jackson and Grossmann, 2003).

WORK OUTLINE

In the following sections, three problems are presented, emphasizing the detailed mathematical formulation and results analysis in each case. In Section 2 a superstructure optimization model is presented, that solves the synthesis, design and operation problem for batch plants through a NLP formulation. In Section 3 a heuristic method is presented for finding the optimal mixed product campaign configuration of multiproduct/multipurpose batch plants. The planning problem is simultaneously solved with the design and operation problem. The third problem deals with the optimal processes integration in a multiplant complex. Different aspects of design, operation, scheduling and planning are analyzed according to diverse operational conditions and environmental issues. MC scenario solutions are compared with multiproduct scenario solutions for a specific industrial studied case. Finally, a summary of the contributions of this work are outlined.

Chapter 3

NLP SUPERSTRUCTURE MODELING FOR THE OPTIMAL SYNTHESIS, DESIGN AND OPERATION IN A BATCH PLANT

3.1. INTRODUCTION

The synthesis and design problem of a batch process plant determines the plant structure, the number of units to be used at each stage and the unit sizes. Previously published works on this area resorted to Mixed Integer Non-Linear models (MINLP) to solve these problems. Binary variables allowed contemplating the allocation of units and the different alternatives to organize them at each stage. The various models were characterized by a certain number of operations, which are the necessary steps to elaborate the product according to the previously settled recipe. This problem was initially modelled with this format by Grossmann and Sargent (1979).

All previous works on this area start from a plant where the number of stages is settled by a decision made in a previous step, taking into account that synthesis and design problems are separately solved. Thus, the only structural decision that usually remains is the one related to unit duplication at each previously determined stage. However, there are many operations that pose alternatives as regards the number of stages to be used that cannot be considered with this approach. For example in the case of fermentation, depending on reaction rate, 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. Then these options should be considered in relation to the sizing decisions. As illustrated with this example, a strong relationship exists among the number of stages, the way in which each stage is configured and the operative characteristics of stages (fermentors feeding, processing times, substrate concentration, among others), which has not been posed yet. This is due to the difficulties in solving a problem in which all these elements are optimization variables.

This work intends to solve the aforementioned problem. Firstly, a model with a high level of detail is posed. Operations have been represented through discretized differential equations that describe mass balances. Furthermore, constraints on feeds to each processing unit and equations of interconnections between stages are considered. This level of detail has been posed by few authors. Some exceptions that can be mentioned are Bhatia and Biegler (1996), even though with a simpler model since they work with a predetermined number of stages and they do not admit units duplication.

The option of optimizing the number of stages in series to be considered in this work has not been included in previous general models of batch plants design. The plant structure problems have been solved in previous synthesis 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 (Bhatia and Bieglier, 1996; Barrrera and Evans, 1989) this last option was not even considered. As previously pointed, this formulation leads to difficulties or limits the capacity for solving the model.

This work optimizes the plant superstructure in order to model this problem. This is a systematic method for the synthesis of chemical process networks. For the given raw materials and final products, there are a lot of feasible production paths that can produce the desired products. In a superstructure optimization model, all the possible alternatives for the process are included in the overall model. In order to obtain the optimal solution, the resolution procedure selects the optimal production alternative among the available options.

This work proposes to explicitly include a superstructure that contemplates all possible options for the plant structure with units in series or in parallel. These alternatives can be obtained by means of different mechanisms. Corsano et al. (2004) presented a heuristic procedure through a simplified optimization model that provides an upper bound for the number of stages of each operation. Another option is to pose an exhaustive enumeration of all the alternatives that arise from the upper bounds for the units in series or in parallel. The designer’s criteria and his or her experience are also critical to bound the superstructure size by taking into account only the most expensive units with a significant impact on the process performance.

An original approach is developed to solve the model where discrete alternatives are selected without resorting to binary variables. Taking into account that the model is a non-convex NLP due to the equations that describe the plant operations, difficulties of resolution methodologies for MINLP programs are avoided. This kind of models is usually solved through methods like the outer approximation algorithm (Duran and Grossmann, 1986; Viswanathan and Grossmann, 1990; Varvarezos et al., 1992) where a sequence of NLP and MILP problems is solved. The available MINLP algorithms can miss the optimal solution due to the application of linear cuts to non-convex regions. On the other hand, our optimisation approach finds the optimal solution by modeling a superstructure with as options as proposed by the designer. The optimal solution will eventually eliminate units of the network taking their size to be zero. In this way we solve the model as a NLP problem instead of a MINLP problem. With this approach, the user can provide physically meaningful initializations increasing the robustness and usefulness of the optimization models. Available computer codes for solving MINLP are of general purpose and do not use initial solutions as those proposed in this work. Finally, the major advantage of this strategy is that all the alternatives can be explored explicitly because their number is relatively low. Therefore, the work presents a problem representation which is extremely compact and allows for taking into consideration a significant number of alternatives.

The developed model is presented working on the case of a fermentors network. It is a typical case for a number of reasons. First of all, it is often present in agro-industrial and biotechnological plants. In addition, it is necessary to represent the process with a high level of detail, due to its high economic impact on the plant cost. Taking into account 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 is bounded by operative considerations. It is important to mention that this approach could be easily extended to other kind of reactions. In the next section, a general model for a single product plant is presented. The model can be easily extended to the multiproduct case where many products are made with the same equipment. Then, its application to the case of a fermentors network is described. The resolution of this example allows assessing 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.

3.2. 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.

To complete 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, the number of stages to be considered for each operation can be modified. 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 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 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 becomes more appropriate when the description of the stages operation is explicitly contemplated.

For each operation p, alternatives $a = 1, ..., A_p$ 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 the production process. This cycle time settles down the time between two successive batches. Therefore, all the units that require less operating time have some idle time. Aiming at reducing this time, out-of-phase parallel units can be included 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 units size is reduced as a result of having less idle time.

The other configuration option for units duplication is in-phase, in which duplicated units operate simultaneously. In this case, when the batch enters that stage, it is split among all units belonging to the stage, and when finishing the operation the exiting batches are added together. In this way, the processing capacity of a stage can be increased, which is important when the unit size reaches the upper bound.

Figure 2.1 shows an example. An operation (P = 1) has C_p = 3 stages, which indicates that any alternative being used in this operation can have at most 3 stages. The problem designer has settled that the A= 8 alternatives shown in Figure 2.1 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 additional stages in series. The other alternatives 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 Figure 2.1.

The model looks for 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:

$$Min \sum_{p=1}^{P} \sum_{a_p=1}^{A_p} \sum_{\mathrm{j_{pa}} \in a_p} \alpha_{\mathrm{p}} M_{paj} G_{paj} V_{paj}^{\beta_p} + OC \tag{2.1}$$

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 (Ravemark and Rippin, 1998). 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 and they are provided by the designer. 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 problem formulation, a set of constraints are developed. First of all, the required demand *Q* should be satisfied. For that purpose, the plant production rate *PR* is employed, which is given by:

$$PR = \frac{Q}{H} \tag{2.2}$$

At the last stage of the last operation, the final product is obtained. The sum of the productions of all the defined alternatives must meet the production requirement for the plant:

$$\sum_{a \in p_{last}} PR_{p_{last},aj_{last}} \geq PR \tag{2.3}$$

where p_{last} corresponds to the last operation of the process and j_{last} to the last stage in each option *a*. Therefore, $PR_{p_{last},a}$ represents the production rate achieved at each alternative *a* in the last operation.

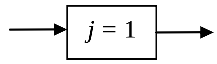
The total amount produced should be at least equal to the plant requirement. Since the model tries to minimize costs, the quantity to be produced will be just *PR*, and will be reached by using only one alternative in operation p_{last}. This will be so because in case of using two alternatives it will 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 describes that operation. Then, considering ZW policy, it should be:

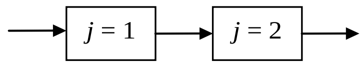
$$TL \geq \frac{T_{paj}}{M_{paj}} \quad \forall p = 1,\ldots,P, a = 1,\ldots,A_p, j = 1,\ldots,C_p \tag{2.4}$$

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

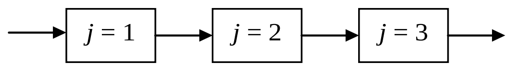
Alternative 1: $a = 1$



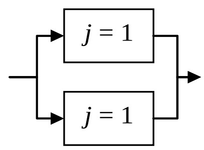
Alternative 2: $a = 2$



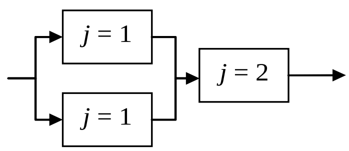
Alternative 3: $a = 3$



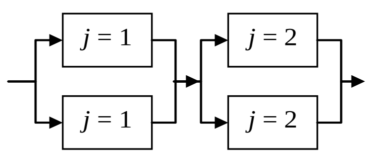
Alternative 4: $a = 4$



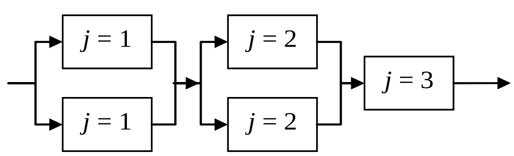
Alternative 5: $a = 5$



Alternative 6: $a = 6$



Alternative 7: $a = 7$



Alternative 8: $a = 8$

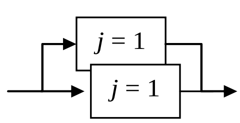


Figure 2.1. Alternatives to be considered for a three-stage operation.

Connection balances should be accounted for between successive stages of each alternative of an operation. Let B_{paj}^{ini} and B_{paj}^{fin} be the batch volume that enters and leaves the unit of stage j in alternative a in operation p; then the balances are:

$$B_{paj}^{ini} = B_{pa,j-1}^{fin} \quad \forall p = 1,...,P, a = 1,...,A_p, j_{pa} \geq 2 \tag{2.5}$$

In case of handling several material streams, this kind of connection constraint should be settled for each of them. As 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 must get in contact with the first stage of the following operation:

$$\sum_{a_p \in p} B_{pa,j_{last}}^{fin} = \sum_{a_{p+1} \in p+1} B_{p+1,a,1}^{ini} \quad \forall p = 1,...,P-1 \tag{2.6}$$

In this case, the total material exiting the last stage j_{last} of all alternatives of operation p, must be equal to all the 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. Also the material streams to be considered could be decomposed into several components (substrate, biomass, product, etc.) as it will be shown in the following example. 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 the involved operation.

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

3.3. 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 describing each unit operation are introduced next.

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 rate 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:

$$\textit{Biomass:}\ \frac{dX_{paj}}{dt} = \mu_{paj} X_{paj} - \upsilon_{paj} X_{paj} \tag{2.7}$$

$$\textit{Substrate:}\ \frac{dS_{paj}}{dt} = -\frac{\mu_{paj} X_{paj}}{Yx_{paj}} \tag{2.8}$$

$$\textit{Non-Active Biomass:}\ \frac{dX_{paj}^{dead}}{dt} = \upsilon_{paj} X_{paj} \tag{2.9}$$

$$\textit{Product:}\ \frac{dE_{paj}}{dt} = \frac{\mu_{paj} X_{paj}}{Ye_{paj}} \tag{2.10}$$

$$\text{where } \mu = \mu_{\max,paj} \frac{S_{paj}}{ks_{paj} + S_{paj}} \tag{2.11}$$

where (2.7) - (2.11) are described for p = 1, 2 (biomass and ethanol fermentation respectively); $\forall a_p \in p;\ \ \forall j_{pa} \in a_p$, X is biomass concentration, S is substrate concentration, X^{dead} is non-active biomass concentration, E is ethanol concentration. For this reason, equation (2.11) is not included in the first operation and μ is growth specific velocity. All these are problem variables. υ represents bacteria death rate, *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 feed composition in biomass fermentors and a constant in the ethanol fermentation operation (Corsano et al., 2004).

These equations have been discretized using the trapezoidal method and included in the global model. This model also contains all the 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 equations (2.5) and (2.6) that is performed for each component: biomass, substrate, non-active biomass and ethanol. For example, substrate balances between successive stages are expressed by:

$$V_{paj} S_{paj}^{ini} = \sum_{f \in Feed_{paj}} SF_f V_{f,paj} + V_{pa,j-1} S_{pa,j-1}^{fin} \quad \forall p = 1,2; \forall a \in A_p; \forall j \geq 2 \qquad (2.12)$$

where S_{paj}^{ini} represents substrate concentration entering stage *j* of alternative *a* of operation *p, f* are the various materials that constitute the feed for stage *j* and those that belong to the set *Feed*. In this example we took *Feed*= {*molass, filter juice, vinasses, water*}, each one of them having a substrate concentration that is equal to SF_f and volume equal to $V_{f,paj}$.

$S_{pa,j-1}^{fin}$ 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 materials from other sources represented by the set *Feed* are 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:

$$V_{paj} = \sum_{f \in Feed_{paj}} V_{f,paj} + V_{pa,j-1} \quad \forall p = 1,2; \forall a \in A_p; \forall j \geq 2 \qquad (2.13)$$

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 (2.1) can be posed as shown by expression (2.14). 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*, then the total annual cost can be computed as:

$$Min \left\{ C_{ann} \sum_{p=1}^{P} \sum_{a_p=1}^{A_p} \sum_{j_{pa} \in a_p} \alpha_p M_{paj} G_{paj} V_{paj}^{\beta_p} + \frac{H}{TL} \sum_{p=1}^{P} \sum_{a_p=1}^{A_p} \sum_{j_{pa} \in a_p} \sum_{f \in Feed} \gamma_f V_{f,paj} \right\} \quad (2.14)$$

3.4. Example Resolution

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

This is a problem with $P=2$ operations. For both first examples, the chosen superstructure is shown in Figure 2.2. This figure includes the diverse alternatives that were selected by the designer for each one of the two operations performed at the plant. It should be noted that this superstructure allows considering the combination of the different alternatives that are chosen for each operation.

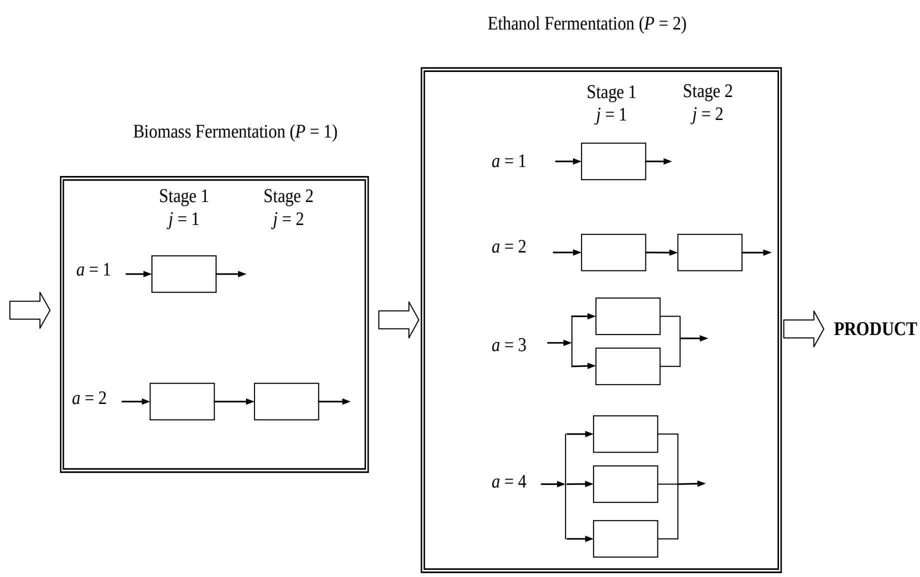


Figure 2.2. Superstructure for the ethanol fermentation model in examples 1 and 2.

In the first operation, there are $C_1=2$ stages, so any alternative can have up to two stages. Figure 2.2 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, $A_2 = 4$ 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. The selection of alternatives for these operations is assumed to be based on the knowledge that the designer has about the problem, regarding its feasibility from an engineering point of view. In this case, as the reaction rate of the biomass fermentation operation is faster than that of the ethanol fermentation operation, the processing time of the first operation is lower than that of the second and therefore the option of in parallel stages duplication in not included for the first operation.

It is necessary to characterize each of the alternatives. Table 2.1 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 of each alternative, and 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.

Table 2.1. Description of the alternatives of ethanol superstructure for the proposed examples

	Operation: Biomass Fermentation			Operation: Ethanol Fermentation		
	Stage 1	Stage 2	Last Stage	Stage 1	Stage 2	Last Stage
Alternative 1	$M_{111} = 1$	$M_{112} = 0$	1	$M_{211} = 1$	$M_{212} = 0$	1
	$G_{111} = 1$	$G_{112} = 0$		$G_{211} = 1$	$G_{212} = 0$	
Alternative 2	$M_{121} = 1$	$M_{122} = 1$	2	$M_{221} = 1$	$M_{222} = 1$	2
	$G_{121} = 1$	$G_{122} = 1$		$G_{221} = 1$	$G_{222} = 1$	
Alternative 3	NO	NO		$M_{231} = 2$	$M_{232} = 0$	1
				$G_{231} = 1$	$G_{232} = 0$	
Alternative 4	NO	NO		$M_{241} = 3$	$M_{242} = 0$	1
				$G_{241} = 1$	$G_{242} = 0$	

The models have been implemented and solved in GAMS (Brooke et al., 1998) 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 2.2.

Table 2.2. 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	115550
υ_{paj}	0.02 h^{-1}
Yx_{2aj}	0.124
Ye_{2aj}	0.23
H	7500 h year^{-1}
ks_{paj}	20 k m^{-3}

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/hr of ethanol corresponds to the first stage of operation 1 and the first stage of operation 2, i.e., alternatives $a = 1$ for $p = 1$ and $a = 1$ for $p = 2$. Figure 2.3 shows the optimal solution. The values of some process and design variables are found in Table 2.3. Sub-index "*final*" of some variables denotes the value of the variable at final time (value corresponding to the last point of discretization). The cycle time of the plant is 16.4 h and the Total Annual Cost is $287,865.

In the second example, the production rate is increased to 500 k/h. The best alternative consists of using a biomass fermentor and two ethanol fermentors in series.

Figure 2.4 shows this solution and Table 2.3 presents the values of some optimal design and process variables. The time cycle is 16 h and the Total Annual Cost is $ 883,732.

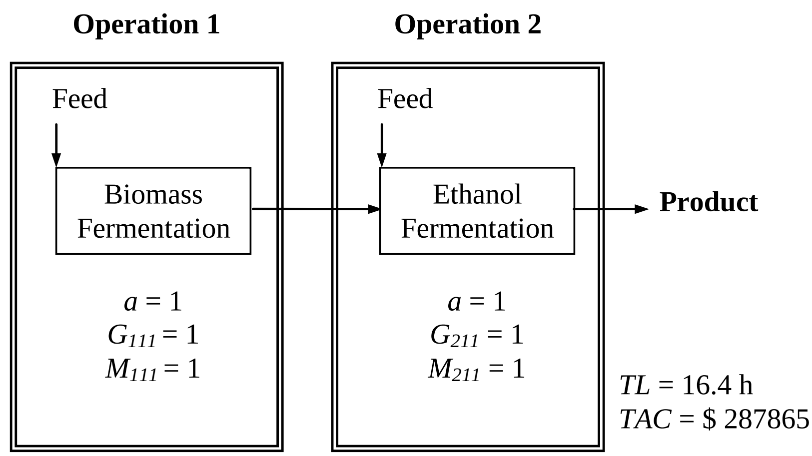


Figure 2.3. Optimal solution for β_p*=0.43 and PR*=100 KH^{-1}.

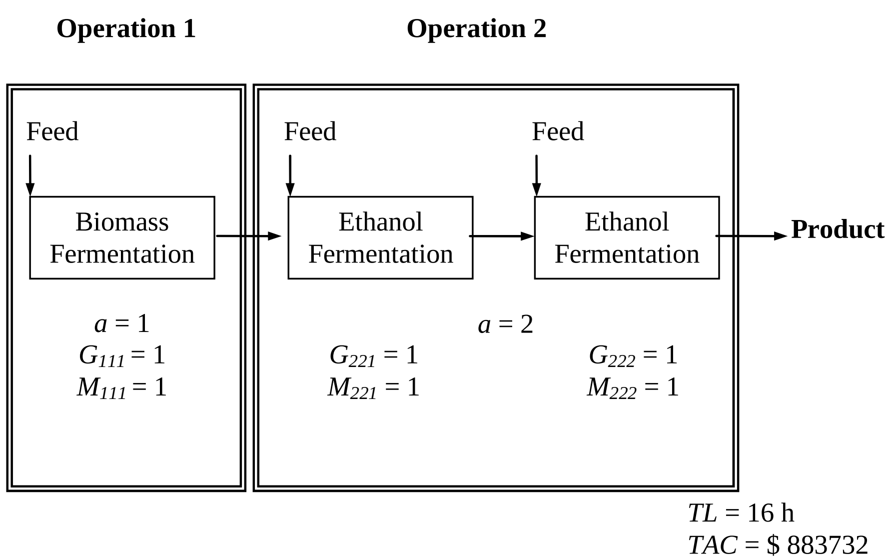


Figure 2.4. Optimal solution for β_p=0.43 and *PR* =500 kh^{-1}.

Table 2.3. 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	16.02	16.02	16.02	10.33	5.16	5.16	5.16
Size (m^3)	6.72	31.89	11.29	57.84	98.09	4.07	4.17	4.67	5.33
$X_{initial}$ (k m^{-3})	0.1	7.45	0.1	6.74	8.6	0.1	5.75	31.86	34.94
X_{final} (k m^{-3})	35.38	15.39	34.53	14.58	16.43	5.88	35.73	39.8	42.83
X_{final}^{dead} (k m^{-3})	2.7	0.57	2.40	3.94	6.6	0.30	2.1	5.65	9.08
S_{final} (k m^{-3})	2.27	4.4	5.22	8.74	2.37	84.36	17.56	5.52	3.1
E_{final} (k m^{-3})	-------	51.54	-------	49.2	81.64	-------	-------	50.94	96.96

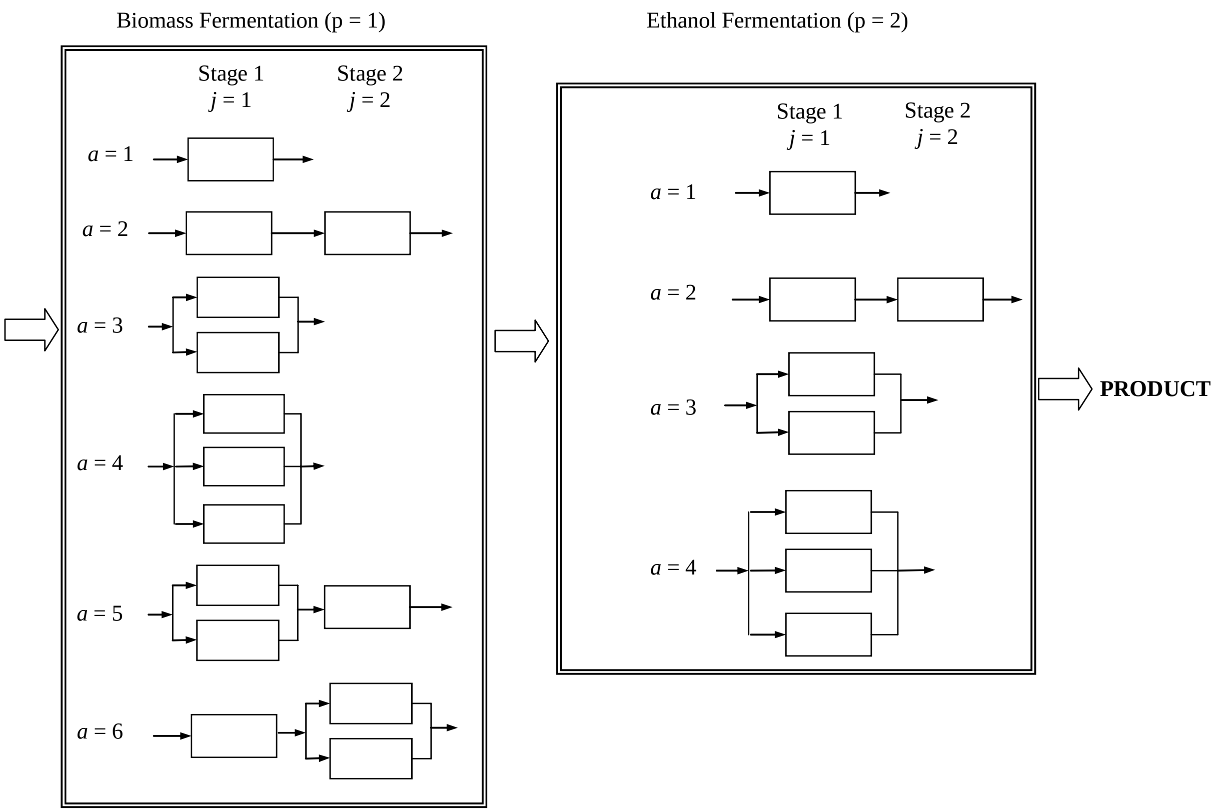


Figure 2.5. Superstructure for the ethanol fermentation model in example 3.

In the third example we decreased the equipment cost exponent of the first operation (β_1) to 0.3 and increased the second ones (β_2) to 1. For this case, we changed the superstructure presented on Table 2.1. Table 2.4 shows the information about the superstructure for both biomass and ethanol fermentation operation, and Figure 2.5 shows this superstructure. 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. Figure 2.6 shows this solution and Table 2.3 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 5.15 h and the Total Annual Cost is $526,822.

3.5. 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 modelled without resorting to binary variables, and the traditional approach, in which the problem is represented through a MINLP program.

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 sensibly simpler than the one presented in this work. Therefore, the only way of comparing both approaches is solving a sequence of MINLP problems that contemplate all the alternatives. This could be made in this example because it includes a small number of operations and stages. In larger 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 at 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, 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 were parameters of each alternative, now become variables M_j and G_j, since it is intended to determine the number of units at each stage. All the previously posed equations remain.

Among the previously solved examples, the third example was chosen. The optimal solution obtained there 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.

Table 2.4. Description of ethanol superstructure alternatives for example 3

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

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

The cases modelled 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 2.5 for each previously mentioned case. On Table 2.6 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 achieve the solution.

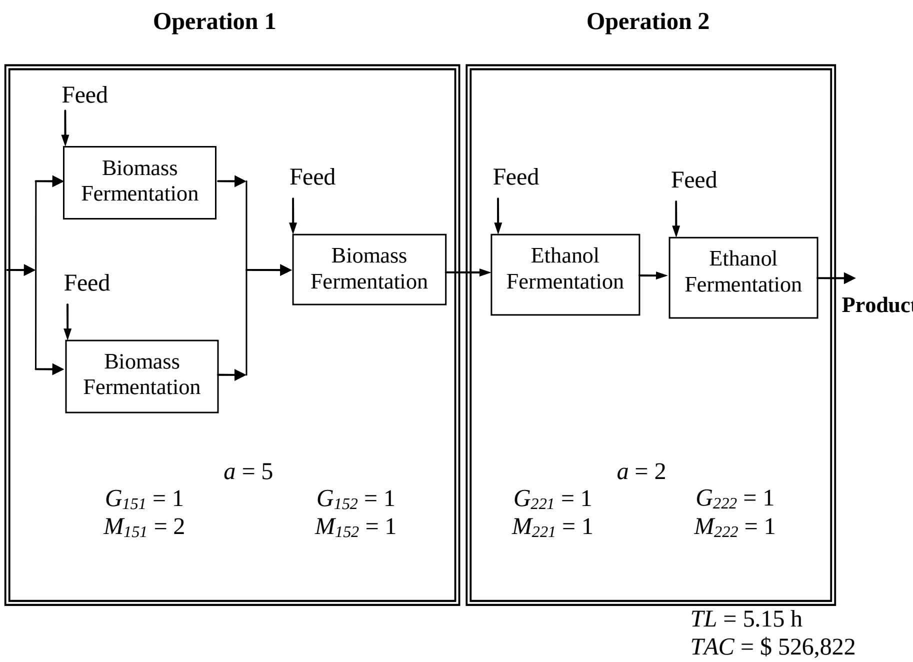


Figure 2.6. Optimal solution for PR = 100 kh^{-1}, β_1=0.3 and β_2=1.

The NLP superstructure model of Example 3 has 1707 continuous variables and 1617 constraints and the solution was achieved in 10.5 CPU seconds. As it can be observed, the solutions of the MINLP cases were obtained 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 comment on the CPU resolution time is that the differences are not so significant (of the same order of magnitude). Anyway this depends strongly on diverse factors, for example the initialization of variables. 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 large, because all possible combinations of alternatives must be accounted for. Another issue to be considered is the need of handling several models with different configurations, which leads to confusions.

Table 2.5. 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

3.6. Conclusions and Outlook on the Proposed Superstructure Modeling

This book section presented a novel NLP model for finding the optimal configuration of plants with several operations. The approach is relevant for cases where units can be duplicated either in series or in parallel (in-phase and out-of-phase). Furthermore, all possible options (or as bounded by the designer) are simultaneously considered. This formulation is most appropriate and useful when detailed operation models are posed. The resulting NLP avoids difficulties arising from resolution methodologies of MINLP problems applied to non convex programs.

The model was described as a set of general constraints, but also admits constraints specific for the operation to be designed and optimized. A detailed description for yeast and ethanol fermentation processes can be found in Corsano et al. (2004, 2006a).

Table 2.6. Optimal solutions of MINLP cases

	Case (i)		Case (ii)			Case (iii)			Case (iv)			
	Bio Fer	Etha Fer	Bio Fer	Etha Fer 1	Etha Fer 2	Bio Fer 1	Bio Fer 2	Etha Fer	Bio Fer 1	Bio Fer 2	Etha Fer 1	Etha Fer 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 (hr)	14.46	7.23	14.2	7.1	7.1	10.64	5.32	5.32	10.32	5.16	5.16	5.16
Size (m^3)	12.6	13.88	5.84	6.39	7.28	7.76	9.15	10.29	4.07	4.17	4.67	5.33
TAC ($)	643,687		583,410			605,692			526,822			
Constraints	252		387			359			494			
Continuous Variables	270		412			384			526			
Discrete Variables	8		12			12			16			
CPU time (sec)	1.28		2.16			3.71			8.10			

For the particular operations on which this modeling technique was applied, the number of alternatives is limited. Indeed, in most cases it is not necessary to consider all the combinations among the various alternatives of each operation because the designer can judge which combinations are feasible for the process that is being optimized.

This model is simple to write, convergence and good solution are guaranteed in reasonable CPU time.

Chapter 4

SYNTHESIS AND DESIGN OF MULTIPRODUCT/MULTIPURPOSE BATCH PLANTS: A HEURISTIC APPROACH FOR DETERMINING MIXED PRODUCT CAMPAIGNS

4.1. INTRODUCTION

In a multiproduct / multipurpose batch plant, several products are manufactured following the same or different production sequences, sharing the equipment, raw materials and other production resources. The inherent operational flexibility of multiproduct / multipurpose plants gives rise to considerable complexity in the design and synthesis of such plants. In many published case studies, scheduling strategies are not incorporated or well integrated. Usually the simplest scheduling sequence, single product campaign, is considered, which may lead to over-design.

In order to ensure that any resource incorporated in the design can be used as efficiently as possible, detailed consideration of plant scheduling must be taken into account at the design stage. Therefore, in this section, the synthesis, design and operational issues for a sequential multipurpose batch plant are considered simultaneously in an NLP model.

In a sequential multipurpose plant a specific direction in the plant floor is recognized that is followed by the production paths of all the products (Voudouris and Grossmann, 1996). However some processing units are used only by some products. Obviously, the model presented is also valid for the multiproduct batch plant where all the products use all the stages. Besides, alternatives for the number of units in series are introduced. The configuration options are explicitly considered in terms of a superstructure as was presented in the previous section.

The simultaneous optimization of several problems is not an usual approach in the chemical engineering literature. In general, these problems are treated in separate form: first the plant configuration problem, then the sizing problem and lastly the campaign determination problem. This leads to sub-optimal solutions.

The proposed methodology in this work solves in first place a relaxed model where scheduling constraints for mixed campaigns are not considered, with the purpose of obtaining the ratios among the number of batches of the different products considered. With these ratios, it is possible to envisage different campaign configurations. Then, different structures for the mixed campaign are proposed. Taking into account that the approach is applied to problems with a moderate number of products and stages where the model detail is emphasized, the number of campaigns to be planned is manageable.

Once the campaign is defined, the appropriate sequence constraints are added to the relaxed model and thus the design and operation integrated problem of a sequential multipurpose plant is solved. The plant configuration obtained in the relaxed model solution is adopted for the mixed product campaign model, therefore the alternative plant configurations remaining are deactivated in this later model.

An extra plant, or mother plant, is considered in this work to provide the material and power streams that the multipurpose plant requires, so that these resources are bounded. Also, the multipurpose batch plant can produce a by-product, which is a product that is obtained by splitting a batch or processing it in a different manner.

The objective function employed in this formulation is the maximization of the net annual profit as given by the earnings of selling products and savings due to unused resources (those produced and available in the mother plant and not used in the multipurpose plant), minus the annualized investment and operating costs.

Several examples of different mixed campaigns are stated for a Torula Yeast, Brandy and Bakery Yeast production plant to assess the approach proposed.

4.2. MODEL ASSUMPTIONS

The problem considered here has the following characteristics:

(i) The plant has batch and semi-continuous units.
(ii) N_p products are processed in the plant.

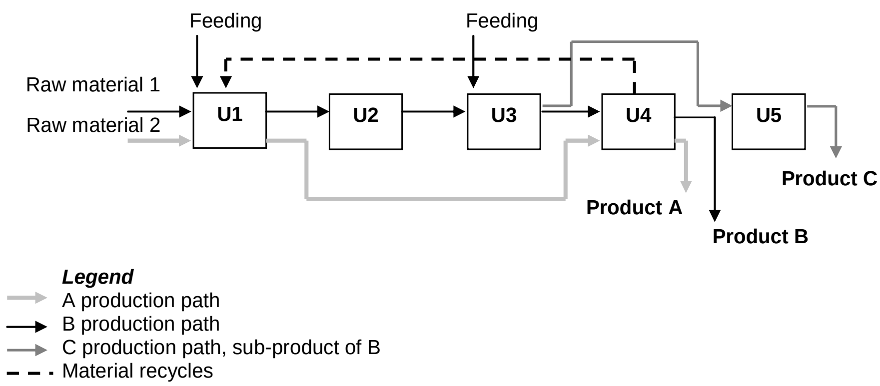


Figure 3.1. Flowsheet of a sequential multipurpose batch plant.

(iii) Not all the products follow the same production path, i.e. a sequential multipurpose batch plant is considered (Figure 3.1).
(iv) The production path for each product is known.
(v) The product demands are upper and lower bounded.
(vi) The processing times are continuous variables and the horizon time is given.
(vii) The mixing, splitting and recycle of batches are allowed.
(viii) The production of by-products is also considered.
(ix) The material and energy resources are bounded.
(x) The unit sizes are continuous variables

The objective is to determine the optimal plant design and operation to meet a specified economic criterion.

Figure 3.1 shows a sequential multipurpose plant where two products, A and B, and a by-product of B, product C are produced. Product A follows the production path U1→ U4 and U1 receives an extra feed (blend of batches) and a recycled batch from U4. Product B follows the path U1→ U2→ U3→ U4. At U3 batches are split to produce product C through U5. U3 also has an extra feed.

4.3. SOLUTION PROCEDURE

The simultaneous optimization of the synthesis, design, operation and scheduling of a sequential multipurpose batch plant, results in a very large size problem, difficult to solve as was pointed in the introduction section. So, a heuristic procedure is proposed in order to solve this simultaneous optimization. The main idea lies in solving first a model without mixed product campaign constraints and then, according to the optimal number of batches of each product obtained in the first model solution, determining the possible campaign configurations. For each campaign configuration proposed, an NLP model is formulated for the optimal plant configuration obtained in the first model solution. The heuristic approach is resumed in the following steps:

(i) First, a model whose constraints consider the design and operation of a multipurpose plant without considering the tasks scheduling constraints is solved. This model is a relaxation of the mixed campaigns problem and is solved as an NLP problem. The model has an embedded superstructure that considers different configuration options for the plant synthesis. The solution of the relaxed model provides the estimated number of batches of each product and the plant configuration.
(ii) Relationships between the number of batches of each product, which are obtained from the relaxed model are established, and the possible sequences of the multiproduct campaigns are selected for the plant synthesis obtained in the relaxed model solution.
(iii) For each proposed campaign configuration, an NLP problem is modelled and solved. In this model, a novel set of tasks scheduling constraints are added to the relaxed model in order to ensure that the production processes of two different products do not overlap in the same unit. In this way, a model for each mixed product campaign is formulated and solved, with the optimal plant configuration obtained from the relaxed model solution. At this step, the plant configuration is fixed and the sizing problem is solved.
(iv) The campaign with the best objective function value is chosen as the optimal solution.

(v) The first model represents a relaxation for the second one. Therefore, the objective function value of the relaxed model solution represents an upper bound for the objective value of the mixed product campaign model. In the studied cases presented below, the gap between these values is very tight, which ensures that the solution obtained for the mixed product campaign is the optimal.

4.4. MATHEMATICAL MODELING

A plant with N_j batch units and N_k semi-continuous units is considered. N_p products are manufactured in the plant, which do not necessarily follow the same production path.

Both problems (the relaxed one and the problem with scheduling constraints) include a detailed modeling for all the products and the batch and semi-continuous units.

4.4.1. Relaxed Model

The components and total mass balances at each stage, the connection constraints between stages and the design equations for each stage for each product are considered as a detailed model. If there are recycles or interconnections between the production processes, as it really happens in the study cases, also the balances that correspond to these connections are considered. Mass balances for some units are given by differential equations such as

$$\frac{dC_{xij}}{dt} = h(t, x) \qquad \forall x \tag{3.1}$$

where C_{xij} is the concentration of component x (biomass, substrate, product, etc.), at stage j of the production process of product i. These dynamic equations are discretized and included in the overall model. Note that the discretized equations involve the processing time of the batch item and the time integration step, all of which are considered variables. The number of grid points is a problem data, but as the final processing time is variable, the discretization step length is also an optimization variable determined according to the final time for each unit. For these models, the trapezoidal method was adopted (Atkinson, 1989). For example, if the biomass balance is

$$\frac{dX_{ij}}{dt} = \left(\mu_{ij} - \upsilon_{ij}\right) X_{ij} \tag{3.2}$$

where X represents the biomass concentration, μ the specific growth rate of biomass, and υ the biomass death rate, the corresponding set of algebraic equations is

$$X_{ij}^{(p+1)} = X_{ij}^{(p)} + \frac{l_{ij}}{2}\left(\left(\mu_{ij}^{(p+1)} - \upsilon_{ij}\right) X_{ij}^{(p+1)} + \left(\mu_{ij}^{(p)} - \upsilon_{ij}\right) X_{ij}^{(p)}\right) \tag{3.3}$$

where l is the step length and p = 1, …, P are the grid points.

In addition, for the stages that are shared by several products, the following constraints are considered.

For batch item j and product i:

$$V_j \geq V_{ij} \qquad \forall i = 1,\ldots, N_p, \forall j \in EB_i \tag{3.4}$$

For semi-continuous item k and product i:

$$V_k \geq V_{ik} \qquad \forall i = 1,\ldots, N_p, \forall k \in ES_i \tag{3.5}$$

where V are the batch and semi-continuous unit sizes and EB_i and ES_i represent the set of batch and semi-continuous units in the production path of product i. In both cases the unit size, V_j or V_k, assures to process the required volume V_{ij} or V_{ik}, for all products.

Let t_{ij} be the processing time for product i at stage j, θ_{ik} the processing time for product i at semi-continuous stage k, CT_i the cycle time for the production of product i and Nb_i the number of batches of product i over the horizon time HT, then

$$T_{ij} = \theta_{ik'} + t_{ij} + \theta_{ik''} \qquad \forall i = 1,\ldots, N_p, \forall j \in EB_i \tag{3.6}$$

$$CT_i \geq T_{ij} \qquad \forall i = 1,...,N_p \quad \forall j \in EB_i \tag{3.7}$$

Note that Eq. (3.6) defines the time that the batch unit *j* will be occupied with product *i*, which contemplates the material loading ($\theta_{ik'}$) and unloading ($\theta_{ik''}$) time if this unit is located between semi-continuous units. In this approach variables t_{ij} and $\theta_{ik'}$ are assumed to be involved in detailed sub-models, some of them written as differential equations and included in the actual model as was presented in equations (3.1)-(3.3).

Several consecutive semi-continuous units give rise to a semi-continuous sub-train. In this paper, only perfectly synchronized semi-continuous sub-trains are considered, then:

$$\theta_{ik} = \theta_{i,k+1} \qquad \forall i = 1,...,N_p \tag{3.8}$$

where *k* and *k*+1 belong to the same sub-train.

For products *i* that share the unit *j* ($i \in I_j$) the following constraints are considered:

$$\sum_{i \in I_j} Nb_i T_{ij} \leq HT \quad \forall j = 1,...,N_j \tag{3.9}$$

In the same way, for all the products *i* that share the unit *k* ($k \in I_k$)

$$\sum_{i \in I_k} Nb_i \theta_{ik} \leq HT \quad \forall k = 1,...,N_k \tag{3.10}$$

In this way the available time is not exceeded.

If all the products follow the same production path, then Eq. (3.10) becomes redundant because the batch processing time considers the semi-continuous processing times upstream and downstream of the batch unit.

A characteristic of this model is that, for certain batch stages, the number of units in series is a priori unknown. For these stages, a superstructure that contemplates all the possible configurations (or those chosen by the designer as feasible) is modelled and embedded in the global model, as was described in Section 2. Then, if the stage is preceded by a semi-continuous unit, the first unit in the series must include the filling time in its operating time, or the emptying time if this stage has a downstream semi continuous unit (see Figure 3.2).

In this case, the cycle time of stage j is given by

$$T_{ij} = \max_{u}\left\{T_{ij}^{u}\right\} \text{ for each } u \in Nu_j \tag{3.11}$$

or in a continuous formulation:

$$T_{ij} \geq T_{ij}^{u} \text{ for each } u \in Nu_j \tag{3.12}$$

where Nu_j is the set of units in series at stage j.

In order to simplify the results analysis, in this work only units in series are considered as possible configurations for the plant stages. The incorporation of units in parallel on the superstructure model can also be done as proposed in Corsano et al. (2004) and it does not represent a model limitation.

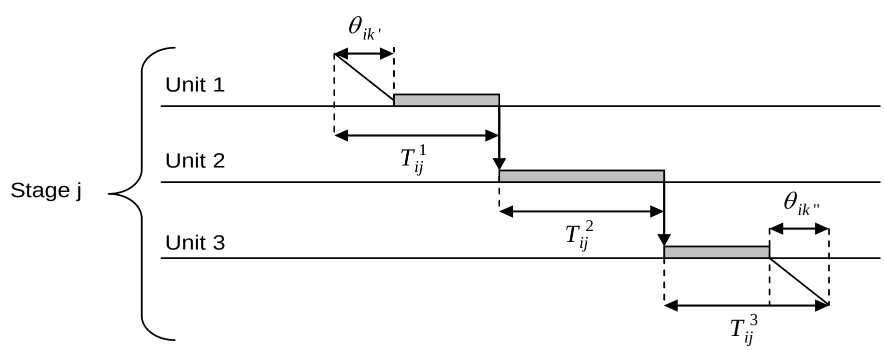


Figure 3.2. In series units configuration for a batch stage.

The material and energy resources s required for each production process can be obtained from another plant that belongs to the same industrial complex called “mother plant” or can be imported from another plant. The unused amount of resource s, i.e. the amount of s that is not consumed by the multipurpose plant, can be sold to other complexes. Let F_s^{prod}, F_s^{imp} and F_s^{ex} be the amounts per hour of produced, imported and exported resource s respectively, and let f_{sij} and f_{sik} be the amount of s consumed for producing product i at the stage j or k respectively, then

$$F_s + F_s^{imp} = \sum_{i=1}^{N_p} \left(\sum_{j=1}^{N_j} \frac{f_{sij}}{CT_i} + \sum_{k=1}^{N_k} \frac{f_{sik}}{CT_i} \right) + F_s^{ex} \quad (3.13)$$

The production rate constraints for each product are

$$Nb_i B_i = Q_i \qquad \forall i = 1,..,N_p \quad (3.14)$$

$$Q_i^{\min} \le Q_i \le Q_i^{\max} \qquad \forall\, i = 1,..,N_p \quad (3.15)$$

where Q_i is the total production of product i which is bounded by $Q_i^{\min}$ and $Q_i^{\max}$, and B_i is the batch size of product i.

The selected objective function is the maximization of the net annual profit (*NAP*), given by the sum of the earnings from products sales and the exported resources (*Sl*) minus the total annualized cost (*TAC*) given by investment (*CInv*) and operating (*CO*) costs. The considered operating costs are the raw material, power resources and disposal costs. Then:

$$NAP = Sl - TAC \quad (3.16)$$

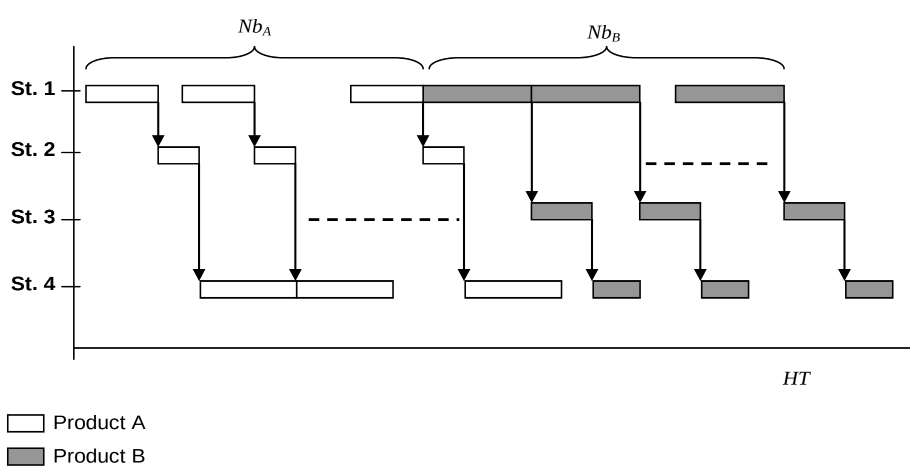


Figure 3.3. Gantt chart for multipurpose plant relaxed model.

$$Sl = \sum_{i=1}^{N_p} G_i Q_i + \sum_{s} G_s F_s^{\exp} \; HT \tag{3.17}$$

where G_i represents the product i sale price (\$ ton^{-1}), G_s the resource price of s (\$ ton^{-1}) and $F_s^{\exp}$ the amount of unused resource s (ton).

$$TAC \; = \; CInv \; + \; CO \tag{3.18}$$

$$CInv = C_{ann} \left(\sum_{j} \alpha_j V_j^{\beta_j} + \sum_{k} \alpha_k V_k^{\beta_k} \right) \tag{3.19}$$

$$CO = \sum_{i=1}^{N_p} Nb_i Res_i + HT \left(\sum_{s} C_s^{prod} F_s^{prod} + \sum_{s} C_s^{imp} F_s^{imp} \right) \tag{3.20}$$

α_j, β_j, α_k, and β_k are cost coefficients for units, C_s is the cost of resource s, and Res_i the disposal cost of product process i that varies according to the effluent.

The relaxed model solution provides the optimal plant configuration and design and the number of batches of each product to be produced.

It is worth noting that the relaxed model resembles a single product campaign one, in which all the batches of a product are processed without overlapping with others products. The difference is that in the relaxed model, the scheduling constraint of a single campaign model

$$\sum_{i=1}^{N_p} CT_i Nb_i \leq HT$$

is not necessarily satisfied because of Eq. (3.9).

Figure 3.3 schematizes the relaxed model solution of a plant that processes two products with different production paths. Product *A* follows the path Stage 1 → Stage 2 → Stage 4, while product *B* follows the path Stage 1 → Stage 3 → Stage 4.

4.4.2. Multiproduct Campaign Model

In many cases, a stream in the production of a product can be recycled to a previous stage in the processing of the same or another product. In such cases the single product campaign is impracticable because the material to be recycled should be stored. In addition single product campaigns require high inventory levels. Furthermore many products cannot be stored because they are degraded. From the point of view of the mathematical model, greater challenges arise than in the formulations for single campaigns. The first decision to be considered is how the multiproduct campaign will be configured. In this work this decision is imposed by the designer from the estimation of the ratio of number of batches of the different products elaborated in the plant.

Let *i'* be the product with the small number of batches in the relaxed model solution. Let $r_i = round\left(\frac{Nb_i}{Nb_{i'}}\right)$ be the rounding of the relation between the number of batches of each product *i* and product *i'*, obtained in the relaxed model solution, so that r_i is a model parameter.

Let *Nb* be the number of times that the mixed campaign is repeated. For the mixed campaign model, the following constraints are imposed:

$$Nb = Nb_{i'} \tag{3.21}$$

$$Nb = Nb_i \; r_i^{-1} \quad \forall i = 1,\ldots, N_p \tag{3.22}$$

Nb is an optimization variable since Nb_i is an optimization variable for each product *i*.

For example, if three products *A*, *B* and *C* are processed in the sequential multipurpose plant with N_A = 100, N_B = 120 y N_C = 310 in the relaxed model solution, then:

$Nb = N_A$, $r_B = 1$ y $r_C = 3$, i.e. the campaign *A-B-C-C-C* or some of its permutations is established.

Given that this strategy is here applied to detailed models with a reduced number of products, this is an affordable approach. Therefore, this procedure estimates the proportion among the number of batches of all products. Different campaigns can be proposed by the designer.

Now, new constraints have to be developed to formulate the different conditions that arise when mixed campaigns are used. All the following constraints are posed for a determined mixed campaign.

Let SL_{ij} be the idle time at unit j after processing a batch of product i and before processing the next batch and CT_j be the cycle time for unit j defined by:

$$CT_j = \sum_{i \in I_j} \left(T_{ij} + SL_{ij} \right) \quad \forall j = 1,..., N_j \tag{3.23a}$$

By the same token for semi-continuous units:

$$CT_k = \sum_{i \in I_k} \left(\theta_{ik} + SL_{ik} \right) \quad \forall k = 1,..., N_k \tag{3.24}$$

If there is more than one batch of some product in the campaign, the processing time and idle time for that product must be added as many times as repetitions occur.

If a stage j has more than one unit in series as a result of the superstructure optimization model performed in the relaxed model, the following constraints have to be added:

$$CT_j^u = \sum_{i \in I_j} \left(T_{ij}^u + SL_{ij}^u \right) \quad \forall u \in Nu_j \tag{3.23b}$$

The modeller must establish for each unit the order in which products will be processed, using the relationship between the number of batches previously determined. Next the constraints that must be implemented according to the production path that each product follows are settled down. These constraints are established for two consecutive products, in order to assure that the production processes of two different products do not overlap in a same unit.

Due to the ZW transfer policy adopted,

$$CT_j = CT_{j+1} \quad \forall j = 1,..., N_j \tag{3.25}$$

$$CT_k = CT_{k+1} \quad \forall k = 1,..., N_k \tag{3.26}$$

$$CT_j = CT_k \text{ for some } j = 1, \ldots, N_j \text{ and } k = 1, \ldots, N_k \tag{3.27}$$

Suppose that in the production path, the product $i + 1$ is processed in unit j immediately after product i and both follow the path $j \rightarrow j+1$. Three cases are presented.

Case i

if all the products follow the same production path, the following constraints are added to the model with the objective of avoiding tasks superposition at the same processing unit.

$$T_{i+1,j} + SL_{ij} = T_{i,,j+1} + SL_{i,,j+1} \quad \forall i = 1,\ldots,N_p - 1, \forall j = 1,\ldots,N_j - 1 \tag{3.28}$$

$$CT_j Nb \leq HT \quad \text{for some } j \tag{3.29}$$

Constraints (3.28) were used by Birewar and Grossmann (1990) but with a different definition of the idle time at stage j. In their work they defined SL_{ijk} as the idle time between the batches of products i and k in processing unit j. In that model the processing times and size factors are fixed, the campaign configuration is obtained as a result of the model solution and the model is solved as an MINLP problem.

As Eqns. (3.25) – (3.27) establish that the unit cycle times are equal, the constraint (3.29) written for some j means that it will hold for every unit j.

This first case is shown on Figure 3.4.

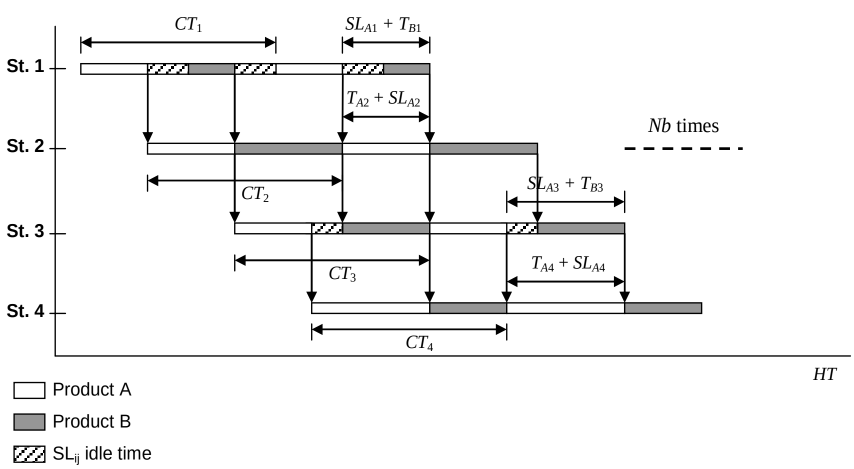


Figure 3.4. Gantt chart for product productions that follow the same path - Case *i*.

It is worth noting that if stage j has more than one unit in series (as a result of the superstructure model optimization), for each of these units the constraints (28) must be satisfied and CT_j is defined by equation (3.23b).

Case ii

If a production path is different, the following constraints are imposed for two consecutive products with different production paths. Let A and B be two consecutive products in the production campaign such that A follows the path $l \rightarrow s$ and B the path $m \rightarrow s$ and let J_A and J_B be the set of processing units that are utilized in the process production of A and B respectively, then:

(a) If the processing order is kept at stage s, the following constraint is added in order to avoid the tasks superposition at stage s:

$$T_{Ap} + SL_{Ap} + \sum_{\substack{j \in J_B \\ p \le j \le m}} T_{Bj} - \sum_{\substack{j \in J_A \\ p \le j \le s}} T_{Aj} \ge 0 \tag{3.30}$$

p represent the first stage shared by both products. The two first terms indicate that the B process production at stage p begins after the time T_{Ap} + SL_{Ap}.

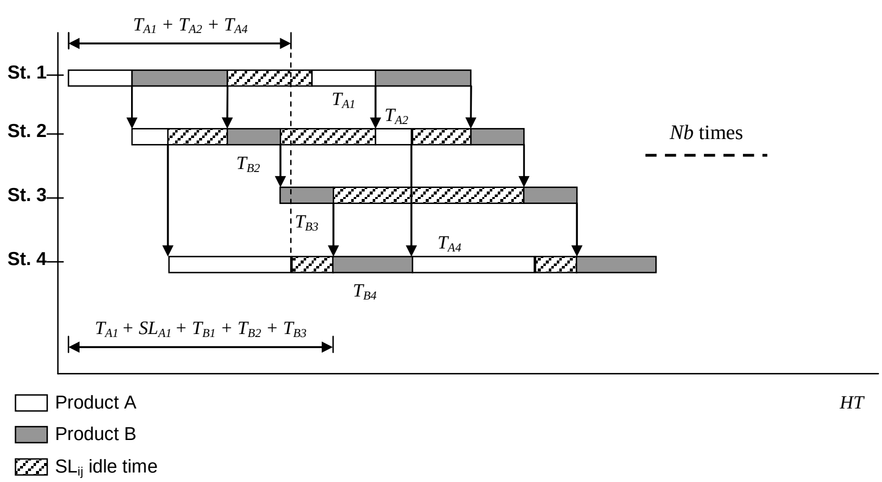


Figure 3.5. Gantt chart for case *ii - a)* without changing the production sequence.

Figure 3.5 shows this situation for the processing of two products, *A* and *B*, where the production path of *A* is $J_A = \{1, 2, 4\}$ and that of *B* is $J_B = \{1, 2, 3, 4\}$, i.e. $l = 2$, $s = 4$, $m = 3$ and $p = 1$, so the equation that must be added is

$$T_{A1} + SL_{A1} + \sum_{\substack{j \in J_B \\ j \le 3}} T_{Bj} - \sum_{\substack{j \in J_A \\ j \le 4}} T_{Aj} \ge 0$$

Figure 3.6 shows another case where the sequence order is conserved but the first processed product has more stages than the second one and $p \neq 1$. The production path for *A* is $J_A = \{1, 2, 3, 4\}$ and for *B* is $J_B = \{2, 4\}$, i.e. $l = 3$, $s = 4$, $m = 2$, $p = 2$ and the constraint added is

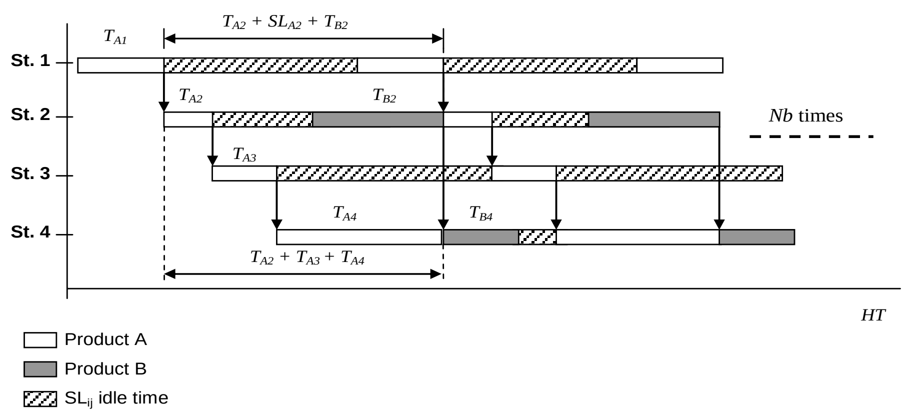


Figure 3.6. Gantt chart for case *ii - a)* with $p \neq 1$.

$$T_{A2} + SL_{A2} + \sum_{\substack{j \in J_B \\ 2 \le j \le 2}} T_{Bj} - \sum_{\substack{j \in J_A \\ 2 \le j \le 4}} T_{Aj} \ge 0 \,.$$

(b) If the designer chooses to change the production order at stage *s* the constraint that must be added instead of (3.30) is:

$$\sum_{\substack{j \in J_A \\ p \le j \le l}} T_{Aj} - \left(T_{Ap} + SL_{Ap} + \sum_{\substack{j \in J_B \\ j \le s}} T_{Bj} \right) \ge 0 \tag{3.31}$$

In this way, as the processing times are variables, the distribution of them will be different. The designer can evaluate both solutions and choose the best economical solution as the optimal solution.

Figure 3.7 shows the scheduling production for two products that change the production order. A follows the production path $J_A = \{1, 2, 3, 4\}$, while for B $J_B = \{1, 2, 4\}$, i.e. $l = 3$, $s = 4$, $m = 2$ and $p = 1$. In stage 1 and 2, product A is processed before product B, while in stage 4 this order is changed.

If stage s is a semi-continuous unit, Eq. (3.30) and (3.31) are valid in each case, taking into account that T_{ij} represents the batch processing time with the loading and unloading times, and therefore the operating times of the semi-continuous units must not be added because they are contemplated on T_{ij}.

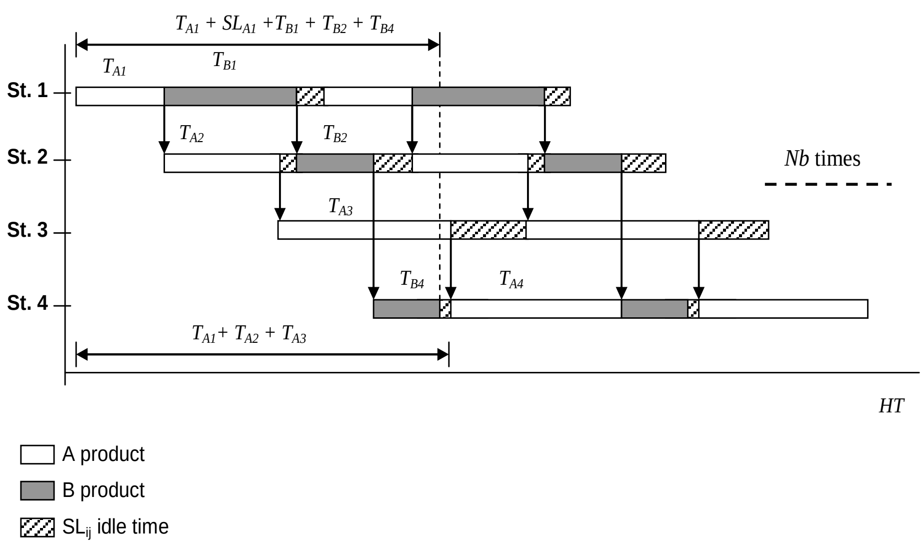


Figure 3.7. Gantt chart for case *ii - b)* changing the production sequence.

For all the situations described for *case ii*, the constraints (3.28) and (3.29) must be added for those products that follow the same path in two consecutive units. For example, for Figure 3.5 the following constraint must be added:

$$SL_{A1} + T_{B1} = T_{A2} + SL_{A2}$$

Case iii

If two consecutive products A and B in the production campaign are such that A follows the path $s \to l$ and B the path $s \to m$ no constraints are added, because they follow independent paths.

All the constraints considered in the different cases are added to the previous relaxed model where only the optimal plant configuration is active, that is, the plant structure is fixed.

4.5. STUDY CASE

Sequential Multipurpose Plant: Torula Yeast, Brandy and Bakery Yeast Production Integrated to a Sugar Plant

The integration of several processes into a Sugar Cane Complex is considered. The Sugar plant produces sugar and bagasse for sale and molasses, filter juices, vapor and electricity that are used in the derivatives plant. The derivatives plant is a sequential multipurpose plant with batch and semi-continuous units to produce Torula Yeast, Brandy and Bakery Yeast. The Bakery Yeast is a by-product of the Brandy production that is obtained by the evaporation and drying of the centrifugation residue of this process. Figure 3.8 shows the integration scheme.

The molasses and filter juices produced in the sugar plant serve as sugaring substrates for the biomass and alcohol fermentations. In addition, water and vinasses are added to the fermentation feed. The vinasses are a non-distilled waste of Brandy production. The electricity generated in the sugar plant is used in the centrifuges of the derivatives plant, whereas the fermentors, the evaporator, the spray dryer and the distillation column consume the steam. In addition, if it is necessary, steam can be imported from other power stations with operative cost imputed on the total annual cost. The vapor and the electricity that are not consumed by the derivatives plant can be sold. For the fermentation stages, the superstructure optimization model proposed in the previous section integrated to the overall model is adopted. For a detailed description of the Brandy process model see Corsano et al.(2006b). Therefore, a synthesis, design, operation, and scheduling problem is solved for the sequential multipurpose plant integrated to the Sugar plant as an NLP model.

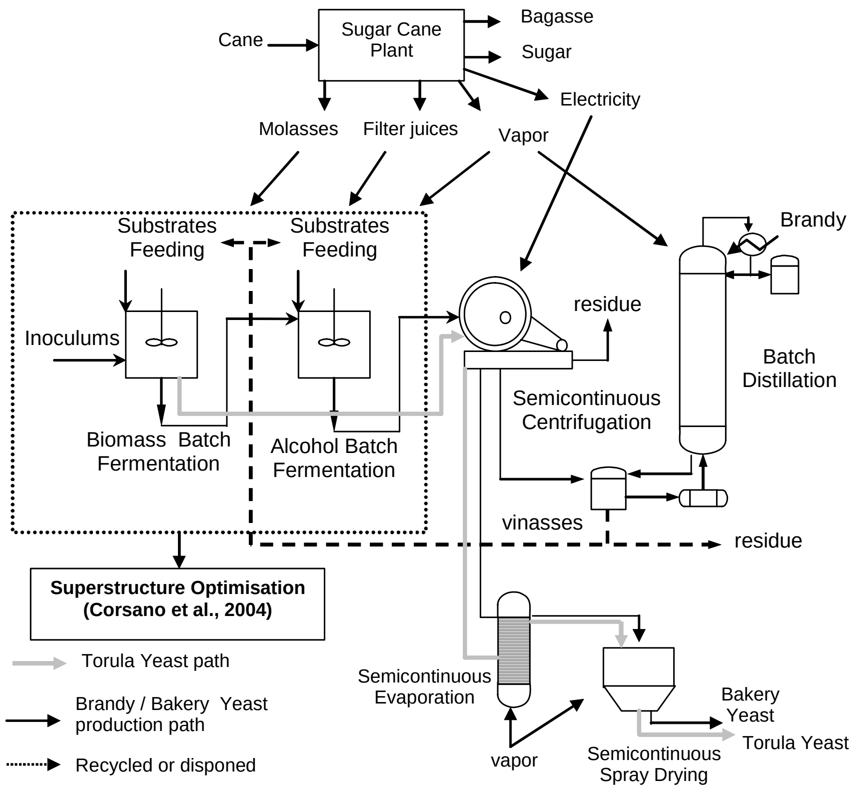


Figure 3.8. Flow sheet for Sugar Cane Complex Integration.

Table 3.1. Decision variables description

Synthesis and Design	Operation	Scheduling
Plant configuration. Number of units in series. Blend and recycle allocation. Unit sizes Heating and cooling areas Power consumption (vapor and electricity) Stage number of distillation column	Batch blending, batch splitting and batch recycling flow rates within the same production process Flow rate recycles from one process to another Material and energy resources allocation from mother plant to the different production processes Production rates Component concentrations Unit processing times for each product	Cycle time of each production process Units cycle time Units idle time Number of batches Mixed campaign configuration

For the Sugar plant, the model optimizes the amount of extracted filter juices. The sugar plant is considered as an existing mother plant, and the amount of extracted filter juices is a process variable. The production of sugar, molasses, vapor and electricity depends on the amount of filter juice extraction. If more filter juices are extracted, molasses and sugar productions are reduced, so the consumption of vapor and electricity in the Sugar production process is also decreased and therefore the amount of electricity and vapor available for derivatives, and bagasse for sale is increased.

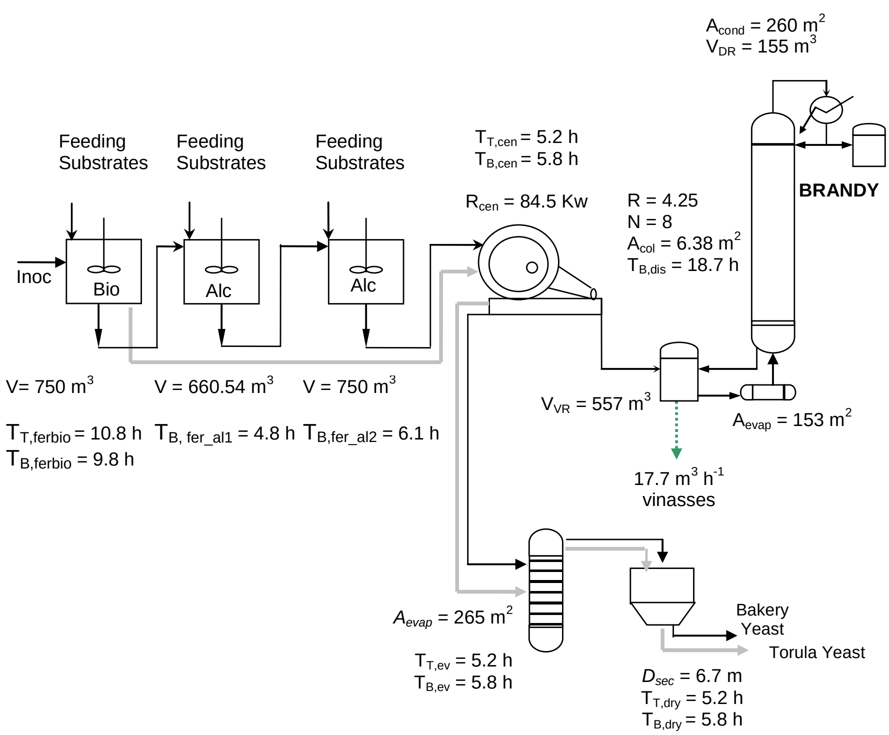


Figure 3.9. Optimal flowsheet for relaxed model plant design.

Table 3.1 lists the most important synthesis, design, operating and scheduling decisions considered in this study case in order to have a grasp of the model complexity, but in the results only some of these variables are reported since the objective of this work is to focus on the heuristic approach and the mathematical models involved.

The models were implemented and solved in GAMS (Brooke, 1998) in a Pentium IV, 1.60 Ghz. The code CONOPT2 was employed for solving the NLP problems.

Firstly the relaxed model is solved. Table 3.2 shows the description and optimal values for some optimization variables. Minimum and maximum productions were fixed for each product at $Q_i^{\min}$ = 7500 ton and $Q_i^{\max}$ = 37500 ton, while the time horizon was fixed at 7500 h. Figure 3.9 shows the optimal plant synthesis. The fermentation stage configuration consists of one biomass fermentor and two alcohol fermentors in series. The fermentors size is upper bounded by 750 m^3.

As can be observed in Table 3.2, the number of Torula batches is 281 while for Brandy and Bakery Yeast is 305. So, for the mixed campaign model the campaign Brandy-Torula (*B*-*T*) is proposed, that means, one batch of each product. This is a reasonable campaign in the sense that the vinasses produced in Brandy production would be used in Torula fermentation. The vinasses cannot be stored for long periods of time because of the degradation and inventory considerations, so the campaign *B*-*T* seems a good option.

Table 3.2. Optimal variables for sequential multipurpose plant relaxed model

Variable	Description	Optimal Value
Q_T	Torula production rate[ton]	14025
Q_{BY}	Bakery Yeast production rate[ton]	10200
Q_B	Brandy production rate[ton]	37500
Nb_T	Torula batches number	281
Nb_B	Brandy and Bakery Yeast batches number	305
CT_T	Cycle time for Torula production [h]	16.0
CT_B	Cycle time for Brandy production [h]	24.5
CT_{BY}	Cycle time for Bakery Yeast production [h]	11.9
NAP	Net Annual Profit [$]	51772500.

Besides this campaign, other alternatives can be assessed adding the corresponding constraints to the relaxed problem, as it is shown below.

According to the proposed methodology, the mixed product campaign model adopts the plant configuration obtained in the relaxed model optimal solution.

Figure 3.10 shows the Gantt chart for the relaxed model solution.

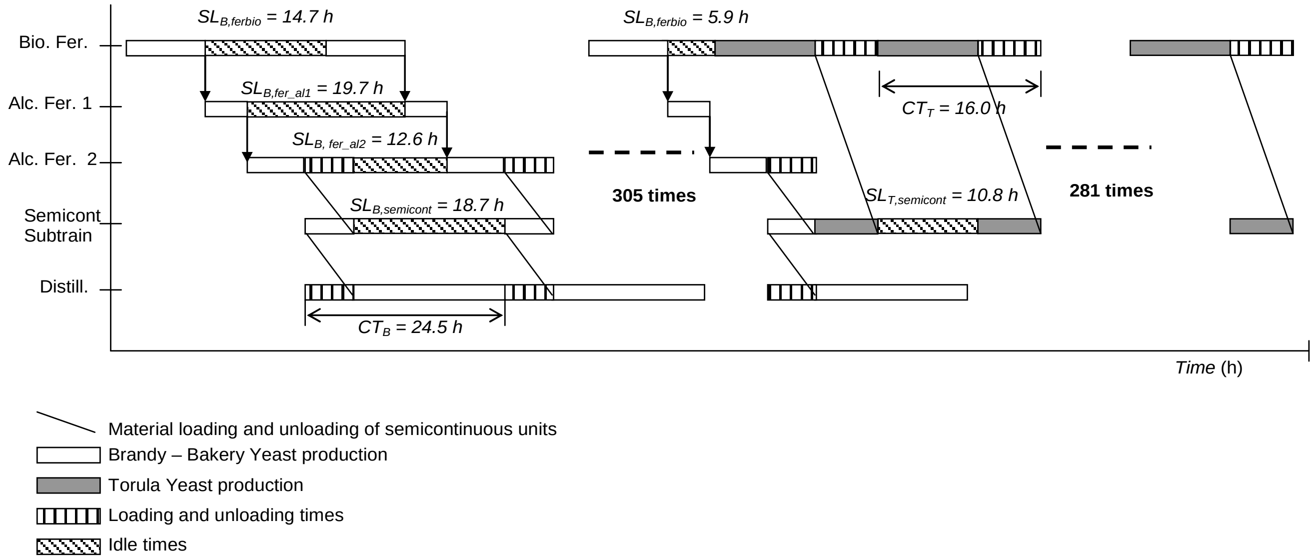


Figure 3.10. Gantt chart for Torula Yeast, Bakery Yeast and Brandy production relaxed model.

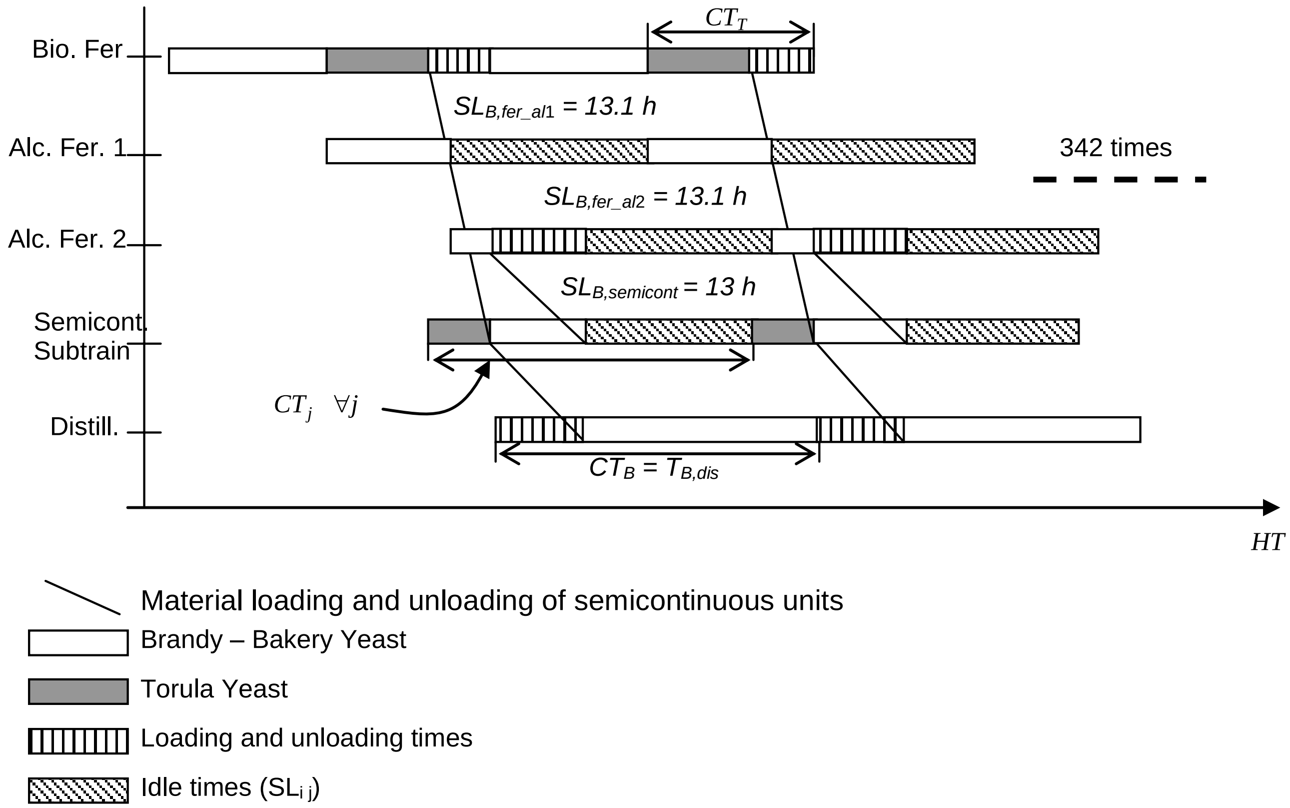


Figure 3.11. Gantt chart for *B-T/T-B* mixed product campaign.

4.5.1. B-T Sequence Campaign for Fermentation Stage and T-B for Semi-continuous Stages (B-T / T-B)

The mixed campaign model consists of the relaxed model plus the constraints corresponding to the *B-T* campaign for the plant synthesis obtained in the relaxed model solution. The sizing problem is solved in this stage. As the Brandy production uses alcohol fermentors that the Torula production does not use, the sequence campaign at the semi-continuous sub-train (centrifuge, evaporator and dryer) is changed. This campaign is denoted by *B-T/T-B*. Then, the following constraints are added to the relaxed model with the plant configuration fixed:

Campaign definition: The number of batches of *B* and *T* must be the same

$$Nb = Nb_B = Nb_T$$

To avoid the task overlapping at the semi-continuous train:

$$(T_{B,ferbio} + T_{B,fer\_al1} + T_{B,fer\_al2} - T_{B,cen}) - (T_{B,ferbio} + SL_{B,ferbio} + T_{T,ferbio}) \geq 0$$

Table 3.3. Optimal variables for *B-T / T-B* model

Variable	Description	Optimal Value
Q_T	Torula production rate [ton]	16500
Q_{BY}	Bakery Yeast production rate [ton]	10350
Q_B	Brandy production [ton]	37500
Nb	Number of times that the mixed campaign is repeated	342
CT_T	Cycle time for Torula production [h]	12.4
CT_B	Cycle time for Brandy production [h]	22.0
CT_{BY}	Cycle time for Bakery Yeast production [h]	9.6
NAP	Net Annual Profit[$]	51675000.

The subscripts *B* and *T* referrer to the Brandy and Torula production respectively, while *ferbio*, *fer_al*1 and *fer_al*2 represent the biomass fermentor and alcohol fermentors 1 and 2 respectively. The first term in brackets represents the time needed to process the brandy batch up to the alcohol fermentation second unit, while the second parenthesis represents the time at which the Torula batch finished processing on the centrifuge. T_{B,fer_al2} and $T_{T,ferbio}$ consider the centrifuge loading time, so in the first case $T_{B,cen}$ must be subtracted. The units that share both productions are the biomass fermentor and the semi-continuous sub-train, so no additional constraints are added.

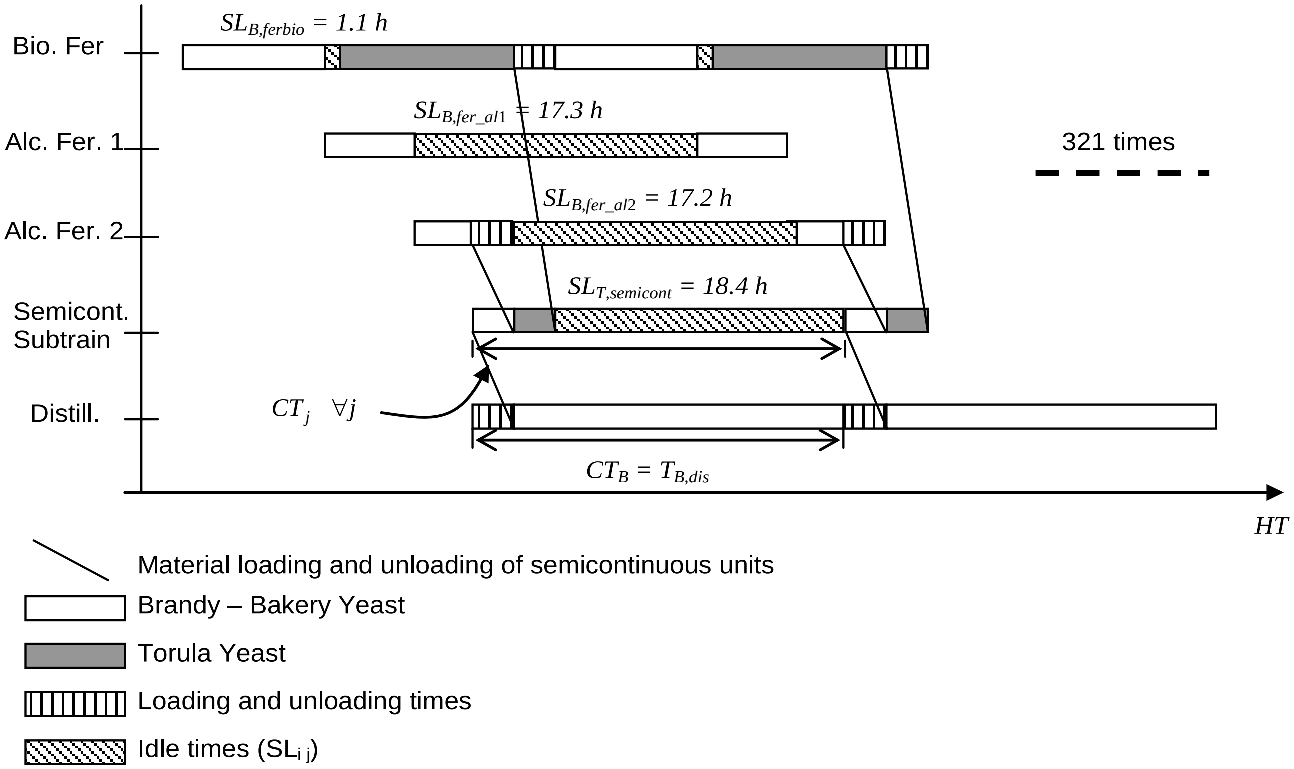


Figure 3.12. Gantt chart for *B*-*T* mixed product campaign.

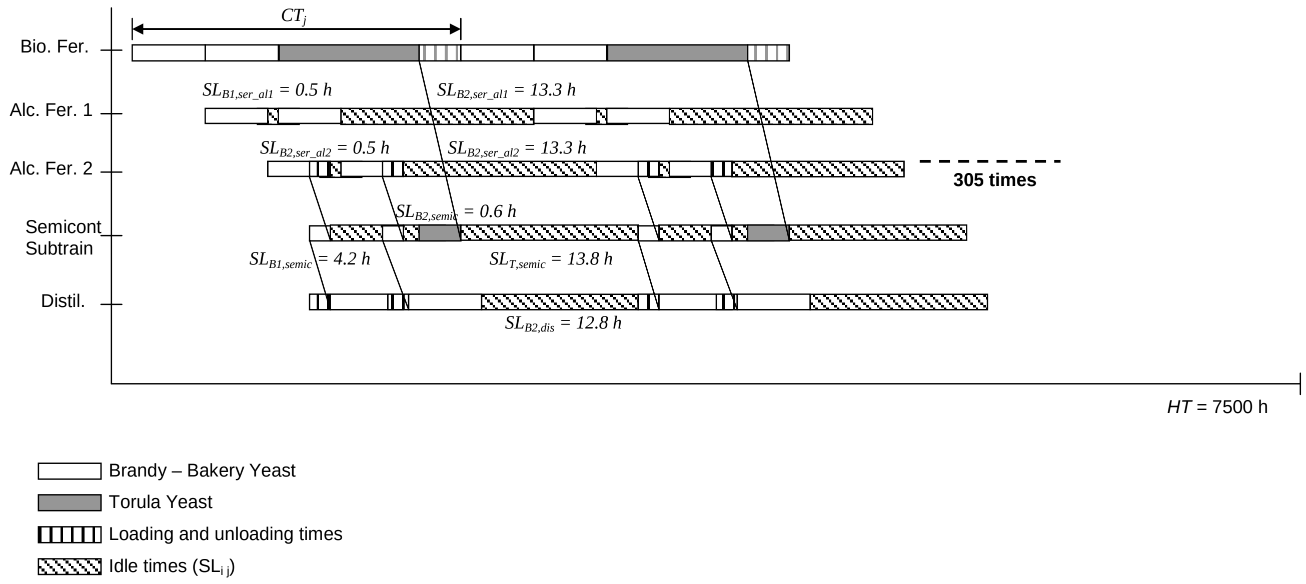


Figure 3.13. Gantt chart for *B-B-T* mixed product campaign.

The results for some optimal variables are presented in Table 3.3 and the production schedule is displayed in a Gantt chart on Figure 3.11. The optimal design variables are displayed in Table 3.7.

A novel result of this sequential multipurpose plant model with the mixed-product campaign is the fact that, because some units are not used by all products, the operating times of such stages are larger, and therefore, the operating and investment costs of these stages are reduced. This means that a better use of equipment is achieved, as it occurs at the distillation stage. This would not happen if the process adopted a single-product campaign, which is usually the case.

The objective functions of relaxed and mixed product campaign models are not comparable because of the satisfaction of constraints (3.9) and (3.10) in the relaxed model do not imply that the total production of Torula Yeast, Brandy and Bakery Yeast hold in the time horizon. In this case, for the relaxed model solution

$$CT_B\,Nb_B + CT_T\,Nb_T = 24.5 \cdot 305 + 16 \cdot 281 = 11968.5 \geq 7500 = HT$$

However, the total production of Torula Yeast, Brandy and Bakery Yeast is completed in the mixed product campaign model in 7500 hours (*HT*), since for all the stages the cycle time is 22 hours and the campaign is repeated 342 times.

Table 3.4 shows the processing and idle times.

Table 3.4. Processing and idle times for B-T / T-B campaign

	Brandy		Torula	
	Processing Time (h)	**Idle Time (h)**	**Processing Time (h)**	**Idle Time (h)**
Biomass Fermentor	9.6	0	8.7*	0
Alcohol Fermentor 1	8.9	13.1		
Alcohol Fermentor 2	3.6*	13.1		
Semicont. Subtrain	5.3	13.0	3.7	0
Distillation	16.7*	0		

* without considering loading and unloading times.

4.5.2. B-T Sequence Campaign for all the Stages

In this example a change is introduced with respect to the previous one. In the semi-continuous sub-train the same sequence as in the other stages is employed.

For this campaign the following constraints are added to the relaxed model:

Campaign definition:

$Nb = Nb_B = Nb_T$

Nb_B and Nb_T are variables.

To avoid the task overlapping at the semi-continuous train:

$$(T_{B,ferbio} + SL_{B,ferbio} + T_{T,ferbio} - T_{T,cen}) - (T_{B,ferbio} + T_{B,fer\_al1} + T_{B,fer\_al2}) \geq 0$$

The first term in brackets represents the time at which the Brandy batch arrives to the centrifuge, while the second one is the time at which the Torula batch leaves the centrifuge.

Table 3.5. Processing and idle times for B-T campaign

	Brandy		Torula	
	Processing Time (h)	**Idle Time (h)**	**Processing Time (h)**	**Idle Time (h)**
Biomass Fermentor	8.9	1.1	10.8*	0
Alcohol Fermentor 1	5.9	17.3		
Alcohol Fermentor 2	3.6*	17.2		
Semicont. Subtrain	2.4	0	2.4	18.4
Distillation	20.8*	0		

* without considering loading and unloading times.

Table 3.6. Processing and idle times for *B-B-T* campaign

	Torula		Brandy		
	Processing Time (h)	**Idle Time (h)**	**Processing Time (h)**	**Idle Time 1 (h)***	**Idle time 2 (h)****
Biomass Ferm.	10.2	0	5.6	0	0
Alcohol Ferm. 1			5.1	0.5	13.3
Alcohol Ferm. 2			3.7	0.5	13.3
Semicont. Subtrain	2.6	13.8	1.4	4.2	0.6
Distillation			4.2	0	12.8

*, ** means idle time after first and second batches in the campaign respectively

Table 3.7. Optimal design variables for sequential multipurpose plant models

Unit	*B-T / T-B* campaign	*B-T* campaign	*B-B-T* campaign
Biomass Fermentor (m^3)	750	750	750
Alcohol Fermentor 1 (m^3)	631.8	655.7	344.4
Alcohol Fermentor 2 (m^3)	724.8	750	391.5
Centrifuge (Kwh)	118.3	184.5	172
Evaporator (m^2)	389	571.4	539.61
Dryer (m of diameter)	7.2	13.	11.3
Distillation			
Condenser Area (m^2)	305.6	272.3	715.7
Evaporator Area (m^2)	180.8	161.1	423.4
Stages Number	9	10	9
Reflux Ratio	5.18	5.5	5.66
Transversal Column Area (m^2)	7.53	6.71	17.64

The model is solved for the same production as for the *B-T / T-B* campaign in order to establish a comparison. The optimal solution for this sequence campaign increases the investment cost in 7% and the idle times in 30%. Table 3.5 shows the processing and idle times and Figure 3.12 the Gantt chart for the *B-T* campaign. The optimal design variables values are displayed on Table 3.7 and economic results on Table 3.8.

As can be seen from comparing Table 3.4 and Table 3.5 the semi-continuous sub-train processing time is shorter than in the previous case, so the equipment sizes are increased and then the investment cost is increased too. The negative terms in Table 3.8 mean that there is unused electricity that is sold in order to increase the profit.

Table 3.8. Economical comparison between different campaigns

	B-T / T-B campaign	*B-T* campaign	*B-B-T* campaign
Investment costs, ($):			
Biomass Fermentors	512025	512025	512025
Alcohol Fermentors	219150	222675	166425
Centrifuge	154650	209550	199575
Evaporator	172050	210975	204675
Dryer	436950	576750	539850
Distillation	878325	881700	1105125
Operating Costs, ($)			
Inoculums	585825	487800	1125000
Water (fresh and cooling)	234975	249225	251700
Vinasses disposal	124875	130050	190875
Profit for sales of unused electricity, ($)	-80250	- 33000	- 43050
Total ($)	3238575	3447750	4252200

Table 3.9. Studied cases - Computational results

	Relaxed model	*B-T/T-B* campaign	*B-T* campaign	*B-B-T* campaign
Number of variables	2398	761	761	772
Number of constraints	2244	704	705	729
CPU [sec.]	161.4	42.9	60.6	69.9

4.5.3. B-B-T Sequence Campaign for all the Stages

This mixed product campaign does not adjust to the ratio between the number of batches of Torula and Brandy products previously determined. However it is solved in order to assess the effectiveness of the proposed strategy.

For this campaign two consecutive Brandy batches are processed and one Torula batch. Then the superposition of tasks must be avoided in the alcohol fermentors and distillation stage between the two Brandy batches and in the semi-continuous sub-train between Brandy and Torula batches. The following constraints are added to the relaxed model with the plant configuration fixed to the optimal configuration obtained in the relaxed model solution:

To define the campaign:

$Nb = Nb_T$

$Nb = ½\ Nb_B$

Nb_B and Nb_T are variables.

To avoid the task overlapping at the first alcohol fermentation stage of Brandy:

$T_{B,ferbio} + SL_{B1,ferbio} = T_{B,fer\_al1} + SL_{B1,fer\_al1}$

To avoid the task overlapping at the second alcohol fermentation stage of Brandy:

$$T_{B,fer\_al1} + SL_{B1,fer\_al1} = T_{B,fer\_al2} + SL_{B1,fer\_al2} \tag{3.32}$$

To avoid the task overlapping at the distillation stage of Brandy:

$T_{B,fer\_al2} + SL_{B1,fer\_al2} = T_{B,dis} + SL_{B,dis}$

To avoid the task overlapping between the second Brandy batch and the Torula batch at the semi-continuous train:

$$\left(2T_{B,\,ferbio} + SL_{B1,\,ferbio} + SL_{B2,\,ferbio} + T_{T,\,ferbio} - T_{T,cen}\right) - \left(2T_{B,\,ferbio} + SL_{B1,\,ferbio} + T_{B,\,fer\_al1} + T_{B,\,fer\_al2}\right) \geq 0$$

$SL_{B1,unit}$ and $SL_{B2,unit}$ corresponds to the idle time after the first and second Brandy batches in this campaign respectively at that unit.

It is not necessary to add constraints to avoid task overlapping between the two consecutive Brandy batches at the semi-continuous sub-train because the second alcohol fermentor considers the centrifugation time that represents the fermentor unloading time. Therefore Eq. (3.32) ensures that there will not be task overlapping at the semi-continuous sub-train.

For the *B-B-T* campaign, the optimal solution is about a 31% worse than the objective function obtained in example 3.5.1 for the same production. Table 3.6 shows the processing and idle times for this campaign. As can be observed, the distillation processing time is reduced more than three times, so the investment cost is also incremented (Table 3.8). The unit sizes for this campaign can be observed on Table 3.7. The total idle time is increased in 26%. Figure 3.13 shows the Gantt chart for this example.

As the earnings from sales are the same in all cases since the productions are fixed, Table 3.8 compares the investment and operation costs of the first campaign analyzed and this last campaign. In both cases, there is unused electricity that is considered as benefit.

Another disadvantage of this campaign is that the biomass fermentor is sub-occupied in Brandy production (Brandy batch size in biomass fermentor is 308.64 m^3, while the biomass fermentor size is 750 m^3 because it reaches this value for Torula production). This occurs because the same production that was first reached in one batch is now reached after two batches.

Only the alcohol fermentation stage is cheaper in this case because the unit sizes are smaller. This occurs because each Brandy batch size is smaller since two batches are processed.

Table 3.7 shows the unit sizes for the different examples studied.

Table 3.9 presents the solutions times and number of variables and constraints of each studied case. The reduction of the number of variables and constraints in mixed product campaign models is because these models the plant configuration is fixed and therefore the superstructure model is not considered.

4.6. Conclusions and Outlook on the Proposed Heuristic Approach for Mixed Product Campaign Model

In this book section a detailed model for the optimal synthesis, design, operation and scheduling of a sequential multipurpose non-continuous plant was developed. The resolution strategy considers two steps. Firstly, a relaxed model is solved to obtain the number of batches of each product and the plant synthesis. Then the designer chooses the mixed campaign based on the ratio between the number of batches. A novel set of tasks scheduling constraints was proposed in order to avoid tasks superposition at processing units.

The problem was formulated as an NLP model and a superstructure model presented in section 2 was embedded in order to solve the synthesis problem. There are not previous published works dealing with the synthesis, design and scheduling problem simultaneously solved as an NLP model.

Another characteristic of these models is the high level of detail reached in the processing unit description, some of them by means of ordinary differentials equations. Batch blending, batch splitting and recycles are allowed as novel components for the multipurpose plant model, decisions taken in this work as optimization variables.

The model was implemented for a Torula Yeast, Brandy and Bakery Yeast production plant. The model was formulated and solved according to the proposed strategy. The optimal solution was compared with different campaign sequences. In all the cases, the investment and operative costs and the idle times were increased. Economic as well as synthesis, design and operational results are also reported. The gap between the objective function value of the relaxed model solution and the objective value of the mixed product campaign model is very tight, which ensures that the solution obtained for the mixed product campaign is the optimal and serves to validate the proposed heuristic methodology.

Chapter 5

PROCESS INTEGRATION: MATHEMATICAL MODELING FOR THE OPTIMAL SYNTHESIS, DESIGN, OPERATION AND PLANNING OF A MULTIPLANT COMPLEX

5.1. INTRODUCTION

The constant shift towards production of higher-added value products in chemical processing industries has encouraged modeling and optimization studies of batch processes. Whereas significant development has been made in designing, planning and scheduling of batch plants with single or multiple production routes, the problem of synthesis, design, operation, and planning in batch multiplant complexes has received much less attention.

In a multiplant complex (MC), there are two or more interconnected plants that are supplied with raw materials and energy by a mother plant and by external plants. The mother plant produces raw materials and energy resources r ($r = 1, \ldots, N_r$) that are considered as "produced resources". The derivative plants l ($l = 1, \ldots, L$) can also receive resources from other not nearby plants (external plants). This type of resources is called "supplied resources". The unused resources, those produced by the mother plant and not used in the derivative plants, can be sold and they are called "exported resources".

The MC considered in this work includes plants that can produce only one product and the production of a by-product is allowed. A by-product is a product which is obtained by splitting a batch or processing it in a different manner.

The derivative plants have batch and semi-continuous units, and mixing, splitting, and recycling batches are allowed. The residue of a derivative plant may become raw material of the same plant or of another derivative plant. If the residue is discarded, a disposal cost is allocated. Recycles amount and concentration are process variables and the allocation or not of a recycled flow to processing unit is also an optimization variable.

In this section a detailed NLP model is developed in order to obtain the optimal synthesis, design, and operation of a MC. The structure of the plant is decided on simultaneously with the design, operating, and scheduling issues. The objective function employed is the maximization of annualized net profit given by the total expected sales price minus the total investment and operation cost, as was presented in the previous section.

The work is focused on providing a tool for generating and evaluating different alternatives of product production. The importance of this approach lies in the integration of synthesis, design, operation, and scheduling decisions working on a multiplant complex where trade-offs must be contemplated among the different processes. When simultaneously approached, these decisions allow considering the relationships and effects between critical elements of the problem that are usually analyzed sequentially.

The example in Figure 1.2 shows that with only two derivative plants, there are interconnections between the derivative plants given by residue recycles and intermediate productions. In our approach, both derivative plants can produce a product and a by-product. Besides producing material and energy resources for derivative plants, the mother plant produces final products to be sold.

The synthesis, design and operation problem for multiplant complex production is defined as follows:

Given N_p derivative products to be processed, their production targets, selling prices, and the production routes for each product, determine the plant configuration for each product including unit sizes, material and energy streams among the plants and the involved processing variables in order to obtain the best economical and environmental solution.

5.2. Model Formulation

In a MC, each product is produced in a different plant and some plants can also produce by-products. Given N_p different derivative products and by-products to be processed in L different plants, the model considers:

Mass balances at every unit of each plant: some of them are given by differential equations which are discretized and included in the global model as algebraic equations, for example

$$\frac{dC_{xlj}}{dt} = h(t, x) \qquad x = 1, ..., N_x, \; l = 1, \; .., L, \; j \in E_l \tag{4.1}$$

where C_{xlj} is the concentration of component x (biomass, substrate, product, etc.), at stage j of plant l. E_l represents the set of units of plant l. These dynamic equations are discretized and included in the overall model as algebraic equations in the same way as it was posed in the previous section.

Mass balances between units of the same plant:

$$VS_{lj} = \sum_{r=1}^{N_r} F_{ljr} + VS_{l,j-1} \qquad \forall l = 1, .., L, \; \forall j \in E_l \tag{4.2}$$

$$VS_{lj} C_{xlj}^{ini} = \sum_{r=1}^{N_r} C_{xlj}^{r} F_{ljr} + C_{xl,j-1}^{fin} VS_{l,j-1} \qquad \forall l = 1, .., L, \; \forall j \in E_l \tag{4.3}$$

where superscripts *ini* and *fin* represent the initial and final concentration respectively and VS_{lj} represents the batch volume at stage j in plant l, and F_{ljr} is the amount of resource r used in unit j at plant l.

Interconnection constraints between the mother plant and derivative plants:

The material and energy required resources for each process production can be obtained from the mother plant (F_r^{prod}) or can be supplied for another plant outside the complex (F_r^{s}). The unused amount of resource r, i.e. the amount of r that is not consumed by the derivative plants (F_r^{ex}), can be sold to market. The constraints for the consumed resources are:

$$F_r^{prod} + F_r^{s} = \sum_{l=1}^{L} \sum_{j=1}^{N_l} \frac{f_{rlj}}{CT_l} + F_r^{ex} \quad \text{for each resource } r \tag{4.4}$$

where f_{rlj} is the amount of r consumed at stage j in the derivative plant l. CT_l represents the cycle time of plant l defined by

$$CT_{lt} \geq T_j \quad j \in E_l, l = 1, ..., L \tag{4.5}$$

where T_j is the time for processing a batch at stage *j* of plant *l* in time period *t*. Let θ_k be the processing time at semi-continuous stage *k* of plant *l*, then

$$T_j = \theta_{k'} + t_j + \theta_{k''} \qquad for\, j, k', k'' \in E_l \tag{4.6}$$

Note that Eq. (4.6) defines the time that unit *j* will be occupied is the processing time of the batch (t_j), plus the material loading ($\theta_{k'}$) and unloading ($\theta_{k''}$) time if this unit is located between semi-continuous units. It is worth noting that in this approach it is assumed that variables t_j and θ_k are involved in detailed sub-models some of them written as differential equations and included in the actual model (Corsano et al., 2004).

If a product and a by-product are produced in a plant *l*, then CT_l defined as (4.5) is the maximum of all processing time of units *j* used for the production of the product and by-product.

All products must be produced within the production time horizon. In this work, the time horizon is the same for all plants (*HT*); so:

$$Nb_l\, CT_l \leq HT \text{ for each } l = 1, \ldots, L \tag{4.7}$$

If a product and a by-product are produced in plant *l*, then

$$Nb_i\, CT_l \leq HT \text{ for each } i \text{ product produced in plant } l = 1, \ldots, L \tag{4.7'}$$

The interconnection constraints between derivative plants: mass and energy balances and the recycle equations between two different plants and/or from one stage to another in the same production process.

$$F_{lj}^e \geq \sum_{l \in L_e} \sum_{j \in EB_e} f_{lj}^e \qquad \forall\ e \tag{4.8}$$

where F_{lj}^e is the amount of recycle *e* produced at stage *j* in plant *l*, and f_{lj}^e is the amount of recycle *e* consumed at stage *j* in plant *l*. L_e and EB_e represent the set of plants and units that consume *e* respectively. For model simplification purposes, the store cost of raw materials and effluents is not considered in this work.

The design equations for each batch and semi-continuous unit depend on process variables as follows:

$$V_{lj} \geq S_{ij}^{l} B_i \qquad \forall i \text{ produced in } l,\ \forall j \in E_l, \forall l = 1,..,L \tag{4.9}$$

$$V_{lk} \geq S_{ik}^{l} \frac{B_i}{\theta_{ik}} \qquad \forall i \text{ produced in } l,\ \forall k \in E_l, \forall l = 1,..,L \tag{4.10}$$

where S represents size or duty factor of batch and semi-continuous units respectively. These factors are computed as a function of the process variables. In the last two equations, product i and plant l appear simultaneously because of some plants can produce a by-product, and thus they manufacture more than one product. B_i is the batch size of product i, and V_{lj} and V_{lk} are the batch and semi-continuous unit size respectively.

The production constraints of each plant:

For each product i produced in plant l, the required demand has to be satisfied

$$B_i Nb_i = Q_i \quad \forall i \text{ produced in } l, \forall l = 1,..,L \tag{4.11}$$

$$Q_i^{\min} \leq Q_i \leq Q_i^{\max} \tag{4.12}$$

where Q_i is the production of product i which is bounded by $Q_i^{\min}$ and $Q_i^{\max}$.

Just like in the multipurpose plant model, a superstructure model that considers a set of different alternatives configurations is embedded in the overall model so that the model keeps the NLP nature.

The objective function: the maximization of annualized net profits given by the total expected total sales minus the investment and operative costs:

$$Max \sum_{i=1}^{N_p} p_i Q_i + HT \sum_{r=1}^{N_r} q_r F_r^{ex} - \left(\sum_{l=1}^{L} \left(\sum_{j \in E_l} \alpha_{lj} V_{lj}^{\beta_{lj}} + \sum_{k \in E_l} \alpha_{lk} V_{lk}^{\beta_{lk}} + \mathrm{Res}_l \right) + HT \sum_{r=1}^{N_r} \left(c_r F_r^{imp} + c_r^{'} F_r^{prod} \right) \right) \tag{4.13}$$

where Res_l represents the disposal cost for each plant l, p_i and q_r are the selling price of product i and resource r respectively, while c_r and $c_r^{'}$ are the imported and produced resource costs respectively.

The MC model considers constraints (4.1)-(4.13), which are simultaneously optimized and no heuristic or decomposition strategy is applied.

5.3. MULTIPLANT COMPLEX TO PRODUCE DERIVATIVES FROM SUGAR CANE

The Cane Sugar Complex consists of three plants interconnected by material and energy flows. The plants that constitute the complex are a Sugar plant (mother plant) and two derivative plants: Torula Yeast and Brandy/Bakery Yeast.

Production processes were described in Section 3.5, with the only difference that in this scenario each product is manufactured in a different plant. Bakery Yeast is a by-product of Brandy plant.

For both derivative plants, the configuration of the fermentation stage is obtained using the superstructure model presented in Section 2 of this chapter embedded in the global integration model, considering only in series units duplication.

The derivatives plants are connected by the vinasses recycles, and the connections between Sugar and derivatives plants are given by material (molasses and filter juices) and energy (vapor and electricity) resources.

For the vinasses recycle equation (4.8) is rewritten as:

$$F^{DV}_{brandy,dist} Nb_{brandy} + Res_{brandy} = \sum_{j \in \{fermentors\}} f^{DV}_{torula,j} Nb_{torula} + \sum_{j \in \{fermentors\}} f^{DV}_{brandy,j} Nb_{brandy}$$

where *DV* means distillery vinasses and Res_{brandy} represent the residual vinasses.

For the electricity integration between the mother plant and derivative plants, for instance, equation (4.4) is rewritten as

$$F^{prod}_{elec} + F^{s}_{elec} = F_{torula,cent,elec} + F_{brany,centr,elec} + F^{ex}_{elec}$$

where *cent* means centrifuge, the only stage that consumes electricity.

In Table 4.1 the different simultaneous decisions made in this model are described.

Figure 4.1 shows the Sugar Complex integration. This figure shows that the model considers blending, recycling and splitting batches.

Table 4.1. Simultaneous decisions made for each model

Synthesis and Design	Operation	Scheduling
Plant Configuration	Batch blending, batch splitting and batch recycling flow rates within the same production process	Units idle time of units in each plant
Number of units in series for batch stages in each plant	Flow rate recycles from one process to another	Plant cycle time
Blend and recycle allocation	Material and energy resources allocation from mother plant to the different process production	Number of batches of each product
Unit sizes	Component concentrations	
Heating and cooling areas	Processing times of each unit in each plant	
Stage number of distillation column	Power consumption (vapor and electricity)	

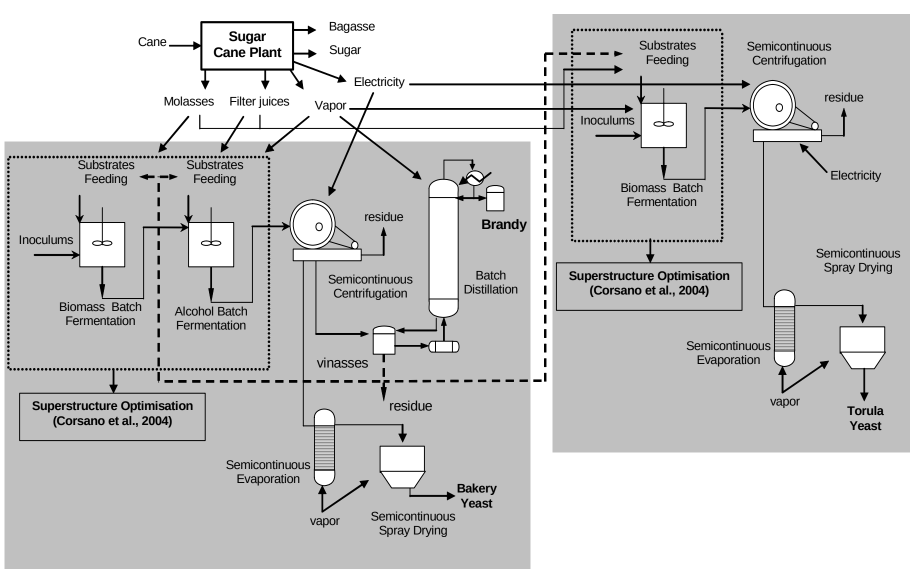


Figure 4.1. Flowsheet for Sugar Cane Complex Integration.

5.4. RESULTS AND ANALYSIS

The presented model for optimal synthesis, design, operation and scheduling of MC provide a tool for the analysis of different alternative configurations. In addition, the economical tradeoffs among the different contemplated elements can be established and assessed. In this section, the results of the optimization of the model under different operative conditions and their analysis are shown for the Torula Yeast, Brandy and Bakery Yeast processes integrated to a Sugar plant as it was presented in the previous section. This study is based on specific data of product profits, equipment and resources costs, etc. These values can be modified by the manager or the designer, taking into account different contexts or scenarios. In particular, this work tries to show the advantages of considering all these elements simultaneously so as to assess the effects or relationships between them. Regardless of the attained results, which depend on several factors, the analytic capability of this approach is emphasized.

Due to a matter of limited space, only one example is presented here. For more examples and detailed analysis, review the work of Corsano et al. (2006c).

All models were implemented and solved in GAMS (Brooke et al., 1998) in a Pentium IV, 1.60 Ghz. The code CONOPT2 was employed to solve the NLP problems. The MC model has about 1100 equations 1200 variables, and CPU time for its resolution is about 160 sec.

In this section, we show the optimal solution for the MC model with the same model parameters employed in the previous section for Multiproduct Plant (MP) scenario. Then, taking into account the example analyzed in section 3, the both scenarios are compared. Therefore, through two different models, two possible production options are assessed and compared. Thus, we prove the versatility of mathematical models in order to make decisions in different contexts. Not only different options in a specific scenario can be evaluated, but also different scenarios can be compared.

EXAMPLE

In order to evaluate different production alternatives, the MC model is solved for the same operative condition presented for the case of multiproduct plant model of Section 3, that is, $Q_i^{\min}$ = 7500 ton and $Q_i^{\max}$ = 37500 ton for Torula and Brandy production, while for Bakery Yeast production no bounds are imposed since this production depends on Brandy production. The time horizon is equal to 7500 h. Table 4.2 shows the optimal design variables. The optimal fermentation configuration for the Torula plant is three units in series while for the Brandy/Bakery Yeast plant is one biomass fermentor and two alcohol fermentors in series. Processing times and unit sizes are displayed in Table 4.3. The ZW transfer policy avoids idle times as shown in Figure 4.2 for both productions. Anyway, it is worth noting that the second alcohol fermentor in the Brandy plant has idle time and this is due to the trade-off that exists between the processing time of this unit and the substrate concentration of vinasses. Longer processing time implies smaller substrate concentration because the substrate is consumed at this stage.

Table 4.2. Processing time and unit sizes of MC model solution

	Torula Plant		Brandy/Bakery Yeast Plant	
	Processing Time (h)	Unit Sizes	Processing Time (h)	Unit Sizes
Biomass Fermentor 1	7.5	9.2 m^3	15.0	140 m^3
Biomass Fermentor 2	7.5	107.2 m^3	-	-
Biomass Fermentor 3	2.8	295.5 m^3	-	-
Alcohol Fermentor 1	-		15.0	518.3 m^3
Alcohol Fermentor 2	-		5.3	593.1 m^3
Centrifuge	4.7	37.1 Kwh	5.8	55.1 Kwh
Evaporator	4.7	124.2 m^2	5.8	152.6 m^2
Dryer (diameter)	4.7	2.5 m	5.8	1.8 m
Distillation				
Stage number				10
Reflux ratio				5.1
Distillate tank				94.6 m^3
Still vessel	-	-	9.2	442.4 m^3
Condenser				373.5 m^2
Evaporator				221 m^2
Column area				9.2 m^2

The optimal productions for this scenario are 10,350 t for Torula, 37,500 t for Brandy, and 4,500 t for Bakery Yeast production. As Brandy is the most profitable production, it is produced up to this upper bound; and Torula and Bakery Yeast are produced according to the available resources: molasses, vapor and electricity.

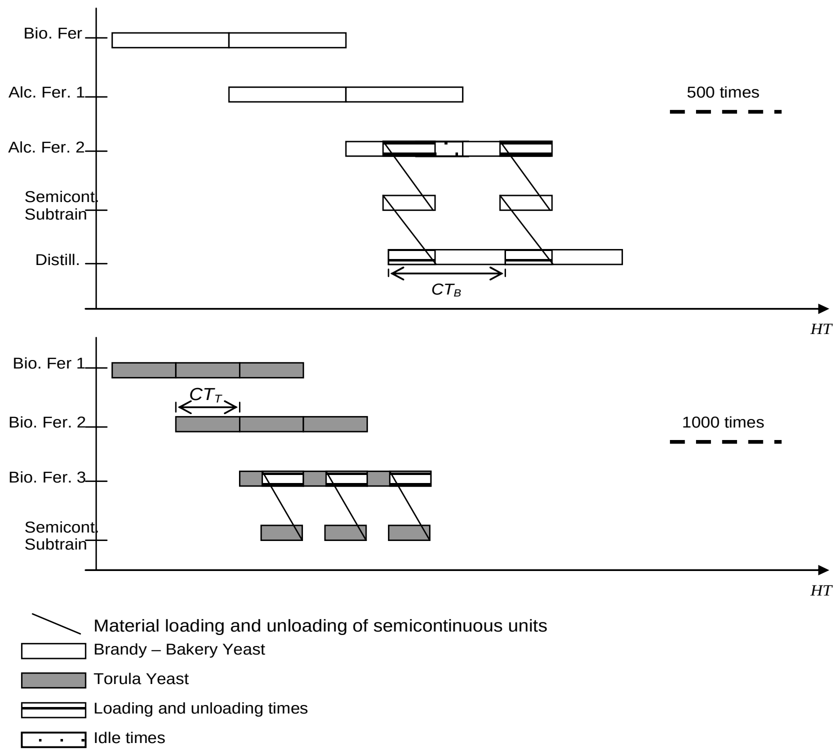


Figure 4.2. Gantt chart for MC scenario.

The Net Annual Profit is 51,622,500 $, which is similar to the Net Annual Profits of multiproduct plant. But, since the incomes for Sugar, Bagasse, and Brandy sales are the same in both cases, only the benefits for Torula, Bakery Yeast and electricity sales and the total annualized cost for both scenarios are compared and displayed in Table 4.3 for a detailed analysis. The "partial benefits" means the incomes for Torula, Bakery Yeast and unused electricity sales minus the investment and operative costs. The difference between both total partial benefits is not significant, but the investment cost for the MP plant is 19% smaller than MC. If the operative costs, such as inoculums cost, are not considered, the optimal solution may change. In this case, the operative costs are higher for the MP plant because productions are mutually dependent since all products are produced in the same plant; while at MC plant scenario, processes performances are good and there is an efficient use of units because each product is produced in a separate plant. Therefore, it is very important to simultaneously consider all these characteristics in order to perform a real comparison.

In addition, human resource demand is higher for the MC scenario than in MP plant. If we assume that one worker is needed for the fermentation stages, one for the semi-continuous units and one for the distillation stage, and considering three work shifts a day, 9 workers will be needed for the MP plant against 15 for MC plant. Human resources demand is not considered in the model.

Since each product is produced in a separate plant in MC scenario, each process production is performed optimally under the integration conditions because the units in each plant are exclusively used for only one product. The biomass fermentation stage performance is better in MC because a good use of units is achieved since there are no idle times and no underused units. The investment cost for this stage is about 30% higher for the MC because the total number of units used in this case is greater than in the MP scenario as a result of production in separate plants. The same difference occurs for semi-continuous units. It can be noted that the inoculums cost is lower for the MC plant due to the good use of fermentative units. The investment cost of alcohol fermentation is lower in the MC plant because unit sizes of this stage are smaller than those in the MP plant solution due to a better yield of biomass fermentation.

The increment of distillation investment cost is a consequence of the processing time of this stage. A reduction on the processing time implies bigger sizes of transference areas and column diameter of this stage.

The increment of vinasses disposal cost is due to a higher volume and substrate concentration of discarded vinasses. If more vinasses were used in fermentation stages, the unit sizes would be increased and therefore the investment cost of fermentation stages would be also increased. So, there is a trade-off between vinasses use and fermentation investment cost.

Therefore, by means of a detailed analysis of economic results (Table 4.3) it can be concluded that both scenarios solutions are similar. If the synthesis, design and operation items are not taken into account simultaneously, as it is usually the case in the literature, solutions and conclusions might be erroneous. Also, the different achieved conclusions in the last paragraphs emphasize the trade-offs among the involved elements of the problem.

Table 4.3. Economic comparison between MC and MP plant models solutions

	MC Plant Model	MP Plant Model
Profit for Torula Yeast sale, ($)	6216000	5152500
Profit for Bakery Yeast sale, ($)	898500	1805250
Profit for electricity sale, ($)	109500	81750
Total profit for sales ($)	7224000	7039500
Investment cost, ($)		
Biomass Fermentors	675750	477000
Alcohol Fermentors	200250	214500
Centrifuge	162000	135750
Evaporator	198750	151500
Dryer	472500	418500
Distillation	901500	791250
Total investment cost	2610750	2188500
Operative cost, ($)		
Inoculums	35250	438750
Water (cooling and diluted)	234000	203250
Vinasses Disposal	0	28500
Imported Vapor	690000	544500
Total operative cost	959250	1215000
Total partial benefits ($)	3654000	3636000

5.5. Conclusions and Outlook on the Proposed Multiplant Integration Model

Detailed models for optimal process synthesis, design and operation were proposed in this work in order to evaluate different production alternatives for a multiplant complex.

One of these models' characteristics is the high level of detail reached in the processing unit description, some of them being attained by means of ordinary differential equations. Batch blending, batch splitting and recycles are allowed as novel components for this type of models, and these decisions are considered as optimization variables in this work. Also, the recycles streams have been considered in order to reduce the environmental impact. All these options are very challenging taking into account the MC scenario, where the connections among all the plants must be assessed.

For a rigorous analysis, several decisions must be considered simultaneously. The proposed models integrate synthesis, design, operating and scheduling decisions.

This formulation was implemented for a Torula Yeast, Brandy and Bakery Yeast productions integrated to a Sugar plant. With the aim of evaluating different production scenarios, the solution of MC model was compared with that obtained in the previous section for a MP model. For the study case, several results were analyzed; some tradeoffs between process and design variables were presented together with the economic impact in each case. Finally the conclusions for each comparison were reported.

Further on these specific results, this work emphasizes the significant value of formulations that take into account all involved decisions simultaneously so as to reach effective solutions.

The idea presented in this work can be applied to other process productions, and the analysis can be performed according to different variations on the operative conditions.

Chapter 6

GENERAL SUMMARY AND SUGGESTIONS FOR FURTHER READING

This chapter has been prepared in order to present different applications of mathematical modeling in chemical engineering. Really it is a powerful tool to solve significant problems in the different stages of the chemical process lifecycle. We have chosen a particular context, and modelled different problems related to batch processes. The obtained conclusions have allowed us to present the valuable results that can be attained when complete and comprehensive models have been developed.

The detailed models provided in this chapter have been focused on the simultaneous optimization of the synthesis, design, operation, and scheduling of chemical processes. These models include decisions of plant configuration, material and energy balances, design equations, product and by-products specifications constraints, environmental considerations, integration processes decisions, blending and recycles constraints, economics objective functions, among others. Thus, we have posed models that show one of the main advantages of mathematical modeling: decisions can be made taking into account all the elements involved and the trade-offs among them. Usually, different actors, areas, stages, etc. may have different and opposite goals that must be related and coordinated in order to achieve the optimal results for the global system.

In the first section, a concise overview of basic concepts and definitions was provided, in order that the reader can be introduced in process engineering models and some methodologies used in this area. For further reading, a classic text of this area is due to Biegler, Grossmann, and Westerberg (1997).

In the second section, a novel superstructure model is presented in order to obtain the optimal plant configuration simultaneously with the optimal plant design and operation. The main characteristic of this approach remains in the fact that discrete decisions are taken without resort to integer optimization variables. The details of this approach and more examples can be found in Corsano et al. (2004, 2006a).

In the third section a heuristic procedure for finding the optimal mixed product campaign for a multipurpose/multiproduct plant is presented. The approach consists in two steps: first a relaxed model is solved in order to obtain the plant configuration and the relationship between the numbers of batch of each product. Then, according to that relationship, a mixed product campaign model is proposed and solved. Sometimes, in this model, the designer criteria or knowledge can influence in the campaign sequence selection and it can be taken into account. For further details of this methodology see Corsano et al. (2007). For others approaches for mixed product campaign models see Birewar and Grossmann (1989, 1990), Xia and Macchietto (1997), Lin and Floudas (2001), and Ierapetritou et al. (1999).

In the fourth section a model for the processes integration in a multiplant complex is developed. The model stresses the optimization of all the production processes embedded in an overall model, emphasizing the relations among all them. The use of recycles streams in order to reduce the environmental impact is considered. The presented model for optimal synthesis, design, operation and scheduling of MC provide a tool for the alternatives analysis of different configurations. In addition, the economical tradeoffs between each production scheme were established and assessed as well as a comparison with a multiproduct plant configuration.

In all the sections, numerical examples corresponding to the Sugar Cane industry and its derivative productions were posed. Although the Sugar Cane example serves as good case of processes integration, the proposed models can be modified to other industrial and engineering examples where several decisions and different alternatives can be analyzed.

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