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Simultaneous design and scheduling of a semicontinuous/batch plant for ethanol and derivatives production

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ABSTRACT

The interest on renewable fuels has greatly increased in the last years. Particularly, ethanol production arises as a good solution to many current economic-environmental problems. Yeast production from the ethanol residuals constitutes a sustainable alternative. Usually, this kind of plants is designed using single product campaigns. However, since yeast degradation is fast and a continuous supply must be assured, the mixed product campaign policy is the most appropriate. Besides, a stable context can be assumed to justify this approach that takes advantage of the special structure of the plant. Therefore, in this paper, a mixed integer linear programming model is formulated for simultaneous design and scheduling of a semicontinuous/batch plant for ethanol and derivatives production. The optimal plant configuration, unit sizes, number of batches of each product in the campaign and its sequencing is obtained in order to fulfill the ethanol and yeast demands minimizing the investment cost.

1. Introduction

Ethanol production is motivated by the use of renewable energy and, among bio-fuels, it is considered the most appropriate solution for short-term gasoline substitution (Zamboni, Shah, & Bezzo, 2009). Several countries are promoting the production of ethanol for fuel blending, but the implementation of this policy entails the expansion of existing plants and construction of new facilities.

Ethanol production generates residuals (Mele, Kostin, Guillén-Gosálbez, & Jiménez, 2011) that must be treated or reutilized in order to minimize the environmental impact caused by their disposals. Producing yeast from the ethanol residuals constitutes a sustainable alternative. Two kind of yeast are possible derivatives from ethanol: torula yeast for cattle feeding produced with the non-distilled remainder called vinasses, and bakery yeast obtained by evaporating and drying the wet solids from the centrifugation operation. Nevertheless, due to yeast degradation, these products cannot be stored and therefore the approach using single product campaign (SPC) is not appropriate to plan the production over the time horizon.

The inherent operational flexibility of multiproduct batch plants gives rise to considerable complexity in their design. Many times, scheduling strategies are not incorporated or well integrated to the formulation. Even though SPCs are not appropriate, for example when perishable products must be supplied during the entire time horizon, they were widely used in the literature since the model resolution is simplified, focusing on the sizing problem (Grossmann & Sargent, 1979; Patel, Mah, & Karimi, 1991; Pinto, Montagna, Vecchietti, Iribarren, & Asenjo, 2001; Salomone, Montagna, & Iribarren, 1994; van den Heever & Grossmann, 1999). Barbosa-Póvoa (2007) presented a complete review where the characterization of design problem is made and the key decisions and elements involved are identified. She emphasized that the design with detailed structural and operational aspects is not yet fully explored. The joint resolution of both problems, design and scheduling using mixed product campaigns (MPC), is very difficult since the plant configuration must be usually known for a suitable process scheduling.

Many times, forecasting cannot assure appropriate demand values. However, in the considered problem, a stable context allows to forecast demands and scheduling decisions can be incorporated to the design problem.

Batch process scheduling has been extensively researched over the past decades and, nowadays, it attracts the interest of both academic and practitioners' communities. Interesting reviews on short-term scheduling of batch processes have been reported by Pinto and Grossmann (1998), Kallrath (2002), Floudas and Lin (2004, 2005), Méndez, Cerdá, Grossmann, Harjunkoski, and Fahl (2006), and Pan, Li, and Qian (2009). In particular, Méndez et al. (2006) have presented a very detailed review of numerous modeling and optimization approaches based in Mixed Integer Linear Programming (MILP) methods, considering the computational

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performance, capabilities and limitations of the resulting optimization models. Also, other modeling and solution paradigms, including Meta-Heuristics (Genetic Algorithms, Simulated Annealing, Tabu Search, etc.), Constraint Programming, and Artificial Intelligence techniques, among others, have been discussed by these authors.

There have been some attempts for incorporating scheduling in design models. A particular approach for ethanol and yeast productions was presented by Corsano, Montagna, Iribarren, and Aguirre (2007). They formulated a heuristic strategy for the design of a special type of multiproduct plant with semicontinuous and batch stages, where the production scheduling is considered through MPCs. They addressed a two stage methodology, where non linear programming (NLP) models were solved at each stage. In the first stage, a detailed NLP model for the simultaneous solution of the synthesis and design problems considering SPC is solved. Then, taking into account the ratios among the numbers of batches of the different products obtained in the first stage, different MPC configurations are recommended by the designer in the second stage. Next, using the optimal plant configuration obtained from the previous model and for each proposed MPC, a new NLP model allows solving the sizing problem. The best solution is determined after solving several models, comparing them and selecting among the proposed MPCs. In this way, the number of batches of each product and the batches sequencing in each campaign are predetermined.

Despite the importance of integrating design and scheduling decisions, there are few published works that jointly consider these issues. Birewar and Grossmann (1989) considered scheduling constraints for simple plants with only one unit per processing stage in order to determine the cycle time of the campaign. They presented formulations for Unlimited Intermediate Storage (UIS) and Zero wait (ZW) storage policies. In a later work they considered simultaneous synthesis, design and scheduling in a Mixed Integer Non Linear Programming (MINLP) formulation (Birewar & Grossmann, 1990). However, unit duplication was not considered for the ZW policy formulation. Then, Voudouris and Grossmann (1992) simplified this approach considering a set of available discrete sizes for the potential equipment to be installed in order to obtain linear formulations. Later, these authors extended that approach in order to incorporate parallel units. However, this last proposal was limited with an approximation for the cycle time (Voudouris & Grossmann, 1993). Pinto, Barbosa-Póvoa, and Novais (2005) presented a mathematical approach for the design of all equipment structures, network circuits and the associated plant operation scheduling, applying the Resource-Task Network (RTN) methodology. The authors analyzed the tradeoffs between capital and production costs, revenues and operational flexibility, for the design and retrofit of periodic multipurpose batch plants problems.

Voudouris and Grossmann (1996) defined a special class of multipurpose batch pants: sequential multipurpose batch plants. These are plants where all batches follow the same direction throughout the stages although some of them might be skipped. In this work, in particular, the design problem is considered for this kind of plants where scheduling aspects are tightly coupled. As will be shown through examples, the utilization of MPCs avoids relatively long idle times and significant overdesign of the plant.

This approach is formulated for a plant that produces ethanol and two type of yeast: for cattle feed sharing with ethanol production some of the processing units, and yeast from the wet solid of the centrifuge residue in ethanol production. Due to yeast degradation is fast and a continuous supply must be assured, the MPC policy is the most appropriate for these productions. Also, this policy allows reducing the idle times, caused by the difference among processing time and different processing routes for products, and avoids unit sizes overestimation.

The number of parallel units out of phase for batch stages, unit sizes, product batch sizes, the number of batches for each product in the campaign and production sequence on each unit is determined in order to fulfill the product demands in the time horizon. The model involves fixed processing times and size factors.

The objective function minimizes the investment cost. In order to avoid non linear formulations, the assumption of discrete sizes for semicontinuous and batch units (which is the usual commercial procurement policy), and a maximum number of batches of each product in the campaign are adopted.

The proposed MILP model is a novel approach where the simultaneous optimization of design and scheduling considering MPCs, for a multiproduct semicontinuous/batch plant, can be solved to global optimality with reasonable computational effort. Although the proposed formulation is focused on ethanol and yeast productions, this approach can be extended to similar industries, for example food and pharmaceuticals, with similar conditions and contexts.

The remaining of the paper is organized as follows. Section 2 presents the definition of the problem under study. In Section 3, the mathematical formulation is posed for a general semicontinuous/batch plant while in Section 4 a particular case study is addressed and solved. Finally, the main contributions and conclusions of the work are drawn in Section 5.

2. Ethanol and derivatives plant: process description

The plant under study is a sequential multipurpose plant (Voudouris & Grossmann, 1996), involving semicontinuous and batch stages, dedicated to ethanol, torula yeast, and bakery yeast productions. Fig. 1 shows the plant flowsheet. It is worth mentioning that the plant operates in two different modes: to simultaneously produce ethanol and bakery yeast, and to produce torula yeast.

The processing stages for ethanol production are the inoculation preparation (biomass fermentation), alcohol fermentation, centrifugation and distillation. For alcohol fermentation, two units in series are used in order to obtain higher alcohol yields according to Corsano et al. (2007). The batch distillation is a combination of two batch items: the distiller feed vessel and the distillate tank; and three semicontinuous items: the evaporator, the condenser and the column itself. Bakery yeast is a by-product of ethanol production which is obtained through evaporation and drying of the centrifugation residue of this process. In other words, the ethanol fermented broth is centrifuged, separating solids and liquids. The solids are evaporated and dried for producing bakery yeast while the liquids are distillated for producing ethanol. Torula yeast is used for cattle feed and it is obtained through biomass fermentation, centrifugation, evaporation and drying stages. The batch stages are biomass and alcohol fermentations, and distillation, while centrifugation, evaporation and drying make a semicontinuous subtrain. The number of parallel units for each batch stage is a decision variable, while only one unit is used for semicontinuous stages.

In this work, fixed size factors and processing times are adopted. The value for each model parameter was estimated from Corsano et al. (2007) for a similar plant where no scheduling constraints were considered, in such way that the production stages are decoupled among them. From the optimal solution of that approach, the size and duty factors, as well as the processing times were obtained. That formulation involved detailed units performance models, where batch blending is allowed, operating variables are considered through differential equations, and the process synthesis, design, and operation are simultaneously optimized in such way that different tradeoffs among decision variables are assessed. Therefore, the process recipe for the model proposed in this paper is obtained from the optimization of a detailed formulation.

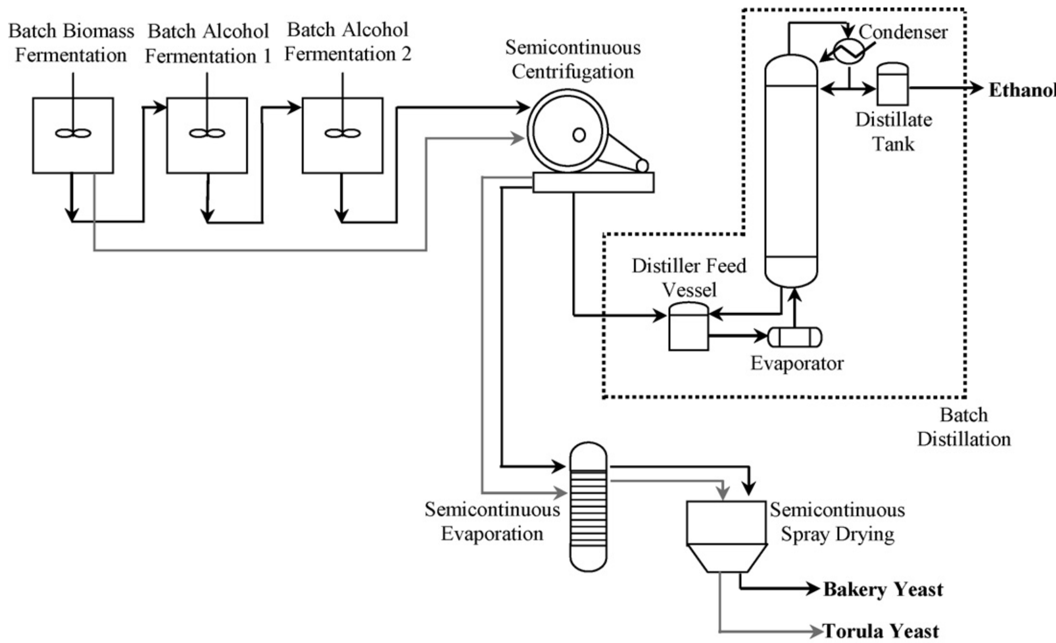

Fig. 1. Ethanol plant flowsheet.

From the design point of view, the units of batch and semicontinuous stages have to be sized and the number of parallel units operating out-of-phase for each batch stage must be determined. Taking into account that batch distillation stage consists of five different units, for their sizing, these units are treated as individual stages. However, if distillation stage is duplicated, then all the distillation items are duplicated with identical sizes. On the other hand, from the scheduling point of view, the considered stages are five because two reasons: centrifugation, evaporation and drying form a semicontinuous subtrain and therefore they have the same processing time; and distillation processing time is unique for all the items involved in it.

3. Model formulation

In this section, a general model for simultaneous design and scheduling of a semicontinuous/batch plant is formulated. Then, in Section 4, the model is applied to the ethanol plant defined in the previous section.

The considered plant is composed by J processing stages, and a set of I products is elaborated in the plant. Taking into account that not all products follow the same production path, the sets EB_i and ES_i represent the batch and semicontinuous processing stages, respectively, utilized for the manufacturing of product i.

For each batch stage j, $j \in EB_i$, unit duplication is admitted and a maximum number K_j of parallel units can be allocated in stage j. It is assumed that the parallel units in each stage are identical and that the unit sizes are restricted to take discrete values. Following the usual procurement policy in this industry, a set $SV_j = \{VF_{j1}, VF_{j2}, \ldots, VF_{jP_j}\}$ is provided, where VF_{jp} represents the discrete size p for batch equipment of stage j and P_j is the given number of available standard sizes for stage j. In a similar way, for each semicontinuous stage j, $j \in ES_i$, the semicontinuous unit sizes are restricted to take values from the set $SR_j = \{RF_{j1}, RF_{j2}, \ldots, RF_{jM_j}\}$, where RF_{jm} represents the discrete size m for semicontinuous equipment of stage j and M_j is the given number of available standard sizes for stage j. From the mathematical point of view, these assumptions allow a MILP formulation for the design model and has been used by authors as Voudouris and Grossmann (1992, 1993, 1996), Ierapetritou and Pistikopoulos (1996), Tan and Mah (1998), Maruejouls, Azzaro-Pantel, Schirlin, Pibouleau, & Domenech (2002), and Dietz, Azzaro-Pantel, Pibouleau, and Domenech (2005). In this way, a realistic design case is posed, which can be solved to global optimality with reasonable computational effort.

In this paper, consecutive semicontinuous equipment items constitute a semicontinuous subtrain, i.e. a series of semicontinuous units with no batch unit or intermediate storage among them. All the units belonging to the subtrain must operate for the same length of time to avoid accumulation of material. Due to material degradation, no intermediate storage tanks are allocated between stages and the material processed in a unit of a stage is immediately transferred to a unit of the next stage. Therefore, the ZW transfer policy between stages is adopted. For the studied plant, the stages shared by both products process similar material. Then, sequence-dependent changeover times can be the same for all possible sequences. Therefore, the changeover time can be included in the processing time.

The processing time of product i at stage j, t_{ij}; the size factor of product i in batch stage j, SF_{ij}, for $j \in EB_i$; the duty factor of product i in semicontinuous stage j, D_{ij}, for $j \in ES_i$; and the demand of each product i, Q_i, over the time horizon H, are model parameters. As the plant is multipurpose, if a product is not processed in a specific stage, then its processing time and size/duty factor are zero at that stage.

During the time horizon H the plant operates in MPC mode, i.e. the production campaign, composed by a set of batches of the different involved products, is cyclically repeated over H. Taking into account that the number of batches of each product i is a decision variable, the composition of the campaign is unknown a priori. Only upper bounds for the number of batches of each product i in the campaign are proposed. If BI_i denotes the set of batches proposed of product i in the campaign, and I_j represents the set of products that stage j can process, then, the maximum number of batches of product i in the campaign, NBC_i^{UP}, is $|BI_i|$ and, the maximum number of batches that can be processed in stage j is $\sum_{i \in I_j} |BI_i|$, i.e. $\sum_{i \in I_j} NBC_i^{UP}$.

Production scheduling in sequential multipurpose plants is both a complex and critically important optimization problem. In this work, taking into account that it is considered through MPCs, the number of times that the campaign is repeated over the time horizon also must be determined. In order to eliminate idle time between campaigns as much as possible and taking into account that units can be duplicated in each stage, the simultaneous production of batches of consecutive campaigns is allowed. Therefore, the number of times that the same production sequence can be executed during the available time horizon is determined considering the cycle time of the campaign. Hence, the initial and final times of the campaign in each unit must be calculated and consequently, the units of each stage must be treated as individual units.

An asynchronous slot-based continuous-time representation for modeling the assignment of batches to units is appropriate for dealing with sequential batch processes (Erdirik-Dogan & Grossmann, 2008; Méndez et al., 2006; Pan et al., 2009; Prasad & Maravelias, 2008). This representation requires postulating a priori an appropriate number of production slots for each unit that integrates the plant (Lim & Karimi, 2003; Susarla, Li, & Karimi, 2010). In this case, this is a not trivial decision because the number of batches of each product in the campaign composition is a model variable. Then, a novel expression for the number of slots postulated for each unit, which guarantee the optimality of the solution and significantly reduce the computational effort, is presented below.

In summary, the problem consists of determining:

(1) The configuration of the sequential multipurpose plant, i.e. the number of parallel units in each stage, and batch and semicontinuous unit sizes.
(2) The number and size of the batches for each product.
(3) The composition of the MPC, i.e. the number of batches for each product in a campaign.
(4) The assignment of batches to units in each stage, production sequence on each unit, and initial and final processing times for the batches that compose the MPC in each processing unit.
(5) The number of times that the campaign is cyclically repeated over the time horizon.

The problem goal is to minimize the plant investment cost while fulfilling the product demands in the available time horizon.

Following, a MILP mathematical formulation to simultaneously solve the design and scheduling problems of a sequential multipurpose plant, considering MPCs, is described.

3.1. Design constraints

In this section, design constraints are posed. As the number of allocated units to each batch stage is a design decision, the following binary variable is defined:

$$z_{jk} = \begin{cases} 1 & \text{if unit } k \text{ of stage } j \text{ is employed} \\ 0 & \text{otherwise} \end{cases}$$

Without loss of generality and in order to reduce the search space, it is assumed that available units for each batch stage are utilized in ascending order. Then, the following constraint establishes that unit $k+1$ is only used if unit k has been already allocated:

$$z_{jk} \geq z_{jk+1} \quad \forall j, \quad 1 \leq k \leq K_j - 1 \tag{1}$$

Given that the binary variable z_{jk} determines if unit k is allocated in batch stage j, then, their sum over k gives the number of units assigned to stage j.

The sizing equation described in the general literature on batch process design (Biegler, Grossmann, & Westerberg, 1997) defines the batch unit size at stage j, V_j, in terms of the size factor, SF_{ij}, and the batch size, B_i, for each product i processed at this stage, namely:

$$V_j \geq SF_{ij} B_i, \quad \forall i, \quad j \in EB_i \tag{2}$$

As size factor SF_{ij} represents the required size in stage j to produce a unit of mass of final product i, the right-hand side represents the minimum capacity required at stage j for production of product i. Then, Eq. (2) guarantees that the unit sizes of stage j will be large enough to process all products.

For each semicontinuous stage j, the unit size is a processing rate, R_j, defined in terms of the duty factor, D_{ij}, a constant equivalent to the size factor, the processing time, t_{ij}, and the batch size, B_i, for each product i processed at this stage, that is:

$$R_j \geq \frac{D_{ij}}{t_{ij}} B_i, \quad \forall i, \quad j \in ES_i \tag{3}$$

The total number of batches of product i in the time horizon H, symbolized by NB_i, depends on the product demand Q_i and the batch size B_i, and is defined by:

$$NB_i = \frac{Q_i}{B_i}, \quad \forall i \tag{4}$$

Let NC and NBC_i be the decision variables corresponding to the number of times that the mixed campaign will be cyclically repeated over the time horizon H and the number of batches of product i included in the campaign, respectively. Then, NC is related with the variables NB_i and NBC_i by the following expression:

$$NBC_i NC = NB_i, \quad \forall i \tag{5}$$

By substituting Eqs. (4) and (5) into Eqs. (2) and (3), the following nonlinear inequalities are obtained:

$$V_j \geq \frac{SF_{ij} Q_i}{NBC_i NC}, \quad \forall i, \quad j \in EB_i \tag{6}$$

$$R_j \geq \frac{D_{ij} Q_i}{t_{ij} NBC_i NC}, \quad \forall i, \quad j \in ES_i \tag{7}$$

In order to determine the number of batches of product i that composes the production campaign, the following binary variable is defined:

$$x_{in} = \begin{cases} 1 & \text{if } n \text{ batches of product } i \text{ are processed in the campaign} \\ 0 & \text{otherwise} \end{cases}$$

The following constraint is posed to ensure that exactly one option is selected:

$$\sum_{n=1}^{NBC_i^{UP}} x_{in} = 1, \quad \forall i \tag{8}$$

Therefore,

$$\sum_{n=1}^{NBC_i^{UP}} n x_{in} = NBC_i, \quad \forall i \tag{9}$$

As it was pointed out at the beginning of this section, the unit sizes V_j and R_j are available in discrete sizes, which correspond to the usual commercial procurement of equipment. Then, the following binary variables are introduced to select a discrete value for each variable:

$$v_{jp} = \begin{cases} 1 & \text{if units of batch stage } j \text{ have size } p \\ 0 & \text{otherwise} \end{cases}$$

$$r_{jm} = \begin{cases} 1 & \text{if units of semicontinuous stage } j \text{ have size } m \\ 0 & \text{otherwise} \end{cases}$$

Then, the size of equipment in batch stage j is given by:

$$V_j = \sum_p v_{jp} VF_{jp}, \quad \forall j \in \underset{i}{\cup} EB_i \tag{10}$$

whereas in semicontinuous stage j is given by:

$$R_j = \sum_m r_{jm} RF_{jm}, \quad \forall j \in \underset{i}{\cup} ES_i \tag{11}$$

where

$$\sum_p v_{jp} = 1, \quad \forall j \in \underset{i}{\cup} EB_i \tag{12}$$

and

$$\sum_m r_{jm} = 1, \quad \forall j \in \underset{i}{\cup} ES_i \tag{13}$$

In this way, by substituting Eqs. (9)–(11) into Eqs. (6) and (7), the following constraints are obtained:

$$NC \geq \sum_p \sum_{n=1}^{NBC_i^{UP}} \frac{SF_{ij} Q_i}{VF_{jp} n} v_{jp} x_{in}, \quad \forall i, j \in EB_i \tag{14}$$

$$NC \geq \sum_m \sum_{n=1}^{NBC_i^{UP}} \frac{D_{ij} Q_i}{t_{ij} RF_{jm} n} r_{jm} x_{in}, \quad \forall i, j \in ES_i \tag{15}$$

These constraints are nonlinear due to the bilinear products $v_{jp}x_{in}$ and $r_{jm}x_{in}$. Then, in order to eliminate these nonlinearities, new binary variables are defined:

$$w_{ijpn} = \begin{cases} 1 & \text{if both } v_{jp} \text{ and } x_{in} \text{ are 1} \\ 0 & \text{otherwise} \end{cases}$$

$$u_{ijmn} = \begin{cases} 1 & \text{if both } r_{jm} \text{ and } x_{in} \text{ are 1} \\ 0 & \text{otherwise} \end{cases}$$

In order to enforce its values, the following conditions are added:

$$w_{ijpn} \geq v_{jp} + x_{in} - 1, \quad \forall i, j \in EB_i, p, 1 \leq n \leq NBC_i^{UP} \tag{16}$$

$$u_{ijmn} \geq r_{jm} + x_{in} - 1, \quad \forall i, j \in ES_i, m, 1 \leq n \leq NBC_i^{UP} \tag{17}$$

and taking into account Eqs. (8), (12) and (13), the following constraints must be satisfied:

$$\sum_p \sum_{n=1}^{NBC_i^{UP}} w_{ijpn} = 1, \quad \forall i, j \in EB_i \tag{18}$$

$$\sum_m \sum_{n=1}^{NBC_i^{UP}} u_{ijmn} = 1, \quad \forall i, j \in ES_i \tag{19}$$

Consequently, Eqs. (14) and (15) are reduced to the linear inequalities:

$$NC \geq \sum_p \sum_{n=1}^{NBC_i^{UP}} \frac{SF_{ij} Q_i}{VF_{jp} n} w_{ijpn}, \quad \forall i, j \in EB_i \tag{20}$$

$$NC \geq \sum_m \sum_{n=1}^{NBC_i^{up}} \frac{D_{ij} Q_i}{t_{ij} RF_{jm} n} u_{ijmn}, \quad \forall i, \ j \in ES_i \tag{21}$$

As the campaign is cyclically repeated over the time horizon H, then the campaign cycle time, CTC, multiplied by the number of times that it is repeated cannot exceed the available time horizon. Therefore, using Eqs. (20) and (21):

$$CTC \sum_p \sum_{n=1}^{NBC_i^{UP}} \frac{SF_{ij} Q_i}{VF_{jp} n} w_{ijpn} \leq H, \quad \forall i, j \in EB_i \tag{22}$$

$$CTC \sum_m \sum_{n=1}^{NBC_i^{UP}} \frac{D_{ij} Q_i}{t_{ij} RF_{jm} n} u_{ijmn} \leq H, \quad \forall i, j \in ES_i \tag{23}$$

In order to avoid the nonlinearities in Eqs. (22) and (23), new non-negative continuous variables ww_{ijpn} and uu_{ijmn} are considered to represent the bilineal terms $w_{ijpn}CTC$ and $u_{ijmn}CTC$, respectively (Voudouris & Grossmann, 1992). Substituting in Eqs. (22) and (23), the following expressions are obtained:

$$\sum_p \sum_{n=1}^{NBC_i^{UP}} \frac{SF_{ij} Q_i}{VF_{jp} n} ww_{ijpn} \leq H, \quad \forall i, j \in EB_i \tag{24}$$

$$\sum_m \sum_{n=1}^{NBC_i^{UP}} \frac{D_{ij} Q_i}{t_{ij} RF_{jm} n} uu_{ijmn} \leq H, \quad \forall i, j \in ES_i \tag{25}$$

where the following constraints must be also considered:

$$\sum_p \sum_{n=1}^{NBC_i^{UP}} ww_{ijpn} = CTC, \quad \forall i, j \in EB_i \tag{26}$$

$$\sum_m \sum_{n=1}^{NBC_i^{UP}} uu_{ijmn} = CTC, \quad \forall i, j \in ES_i \tag{27}$$

$$ww_{ijpn} \leq CTC^{UP} w_{ijpn}, \quad \forall i, j \in EB_i, p, 1 \leq n \leq NBC_i^{UP} \tag{28}$$

$$uu_{ijmn} \leq CTC^{UP} u_{ijmn}, \quad \forall i, j \in ES_i, m, 1 \leq n \leq NBC_i^{UP} \tag{29}$$

where CTC^{UP} represents an upper bound for the variable CTC.

3.2. Scheduling constraints

3.2.1. Slot-based representation

An asynchronous slot-based continuous-time representation for modeling the assignment of batches to units is employed. The slots correspond to time intervals of variable length where batches will be assigned, and in this case, the set of postulated slots can differ from one unit to another. In each slot l of a specific unit k at most one batch can be processed, and, if no product is assigned to slot l, its length will be zero. Taking into account that the cycle time must be determined, the initial and final operation times of the first slot and last slot assigned to each unit, respectively, must be calculated.

In order to reduce the search space, it is assumed that slots of each unit are utilized in ascending order, that is, slot $l+1$ is only used if slot l has been already allocated. Hence, the slots of zero length take place at the end of each unit. Moreover, taking into account that for each stage all parallel units are identical, it is assumed that the number of processed slots in a unit is greater than or equal to the number of processed slots in the following unit (Fig. 2). Since computational performance of model strongly depends on the number of slots postulated for each unit, the previous assumptions allow proposing a tighter number of slots for each unit, without lead to suboptimal or unfeasible solutions.

As previously mentioned, the slots of each unit are utilized in ascending order. Besides, between two consecutive units of a same stage, it is established that the number of processed slots in the first unit is greater than or equal to the number of processed slots in the

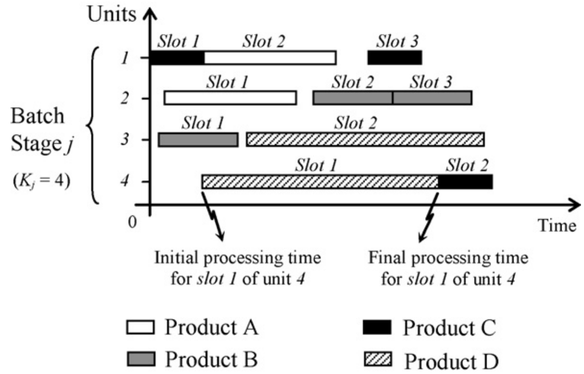

Fig. 2. Asynchronous slot-based, continuous-time representation.

next unit. Then, the tighter maximum number of slots postulated for unit k of stage j, L_{kj}, is specified by the following expression:

$$L_{kj} = \left\lfloor \frac{\sum_{i \in I_j} NBC_i^{UP}}{k} \right\rfloor, \quad \forall j, 1 \leq k \leq K_j \tag{30}$$

where $\lfloor \cdot \rfloor$ is integer part operator, i.e. the greatest integer not exceeding the argument.

This novel rule, based on the number of batches admitted to be processed in stage j and the order of unit k of that stage, allows solving the model in reasonable time, keeping its global optimality. For each stage j, the number of slots considered for the first unit coincides with the maximum number of batches that can be processed in this stage. In fact, if the optimal plant configuration consists of exactly one unit in stage j, i.e. $z_{1j} = 1$ and $z_{kj} = 0$ for $2 \leq k \leq K_j$, and if the number of batches processed for all products is the maximum one, then, $\sum_{i \in I_j} NBC_i^{UP}$ slots must be utilized in this unit. Similarly, if the optimal plant configuration consists of exactly two units in stage j, i.e. $z_{1j} = z_{2j} = 1$, and $z_{kj} = 0$ for $3 \leq k \leq K_j$, and if the number of processed batches for all products is the maximum one, then, altogether $\sum_{i \in I_j} NBC_i^{UP}$ slots are utilized in these units. So, taking into account that the number of occupied slots in the first unit must be greater than or equal to the number of occupied slots in the second unit, the maximum number of slots proposed for the 2nd-unit is $L_{2j} = \left\lfloor \sum_{i \in I_j} NBC_i^{UP}/2 \right\rfloor$. In general, if the optimal plant configuration consists of exactly k units in stage j, $k \leq K_j$, and if the number of batches processed for all products is the maximum one, according to previous assumptions, the number of slots considered for the kth-unit is given by expression (30).

As an example, consider a plant where the maximum number of batches in the composition of a campaign is 2 for products A and C, 3 for product B, and 4 for product D. Let j be a stage of the plant where a maximum of $K_j = 4$ identical parallel units can be allocated in this stage. Then, taking into account that $\sum_{i \in I_j} NBC_i^{UP} = 2 + 3 + 2 + 4 = 11$, the number of slots postulated for each unit at stage j is illustrated in Fig. 3.

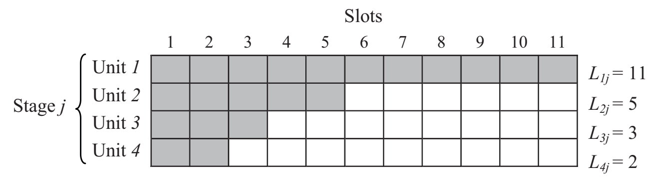

Fig. 3. Slots postulated for each unit of stage j.

3.2.2. Assignment of batches to specific slots of units

One of the decisions that involve the posed problem is the assignment of batches to specific slots of units in each stage. In order to represent this decision the following binary variable is introduced:

$$Y_{bjkl} = \begin{cases} 1 & \text{if batch } b \text{ is assigned to slot } l \text{ and processed in unit } k \text{ of stage } j \\ 0 & \text{otherwise} \end{cases}$$

Taking into account that the number of batches of each product is a model variable, each batch of product i that composes the campaign and that is processed at stage j, must be assigned to a slot of a unit of this stage:

$$\sum_{1 \leq l \leq L_{kj}} \sum_{1 \leq k \leq K_j} Y_{bjkl} \leq 1, \quad \forall j, i \in I_j, \quad b \in BI_i \tag{31}$$

Moreover, each slot l of unit k at stage j is only employed for processing at most one batch. Then, the following inequality must be added:

$$\sum_{b \in \bigcup_{i \in I_j} BI_i} Y_{bjkl} \leq 1, \quad \forall j, 1 \leq k \leq K_j, 1 \leq l \leq L_{kj} \tag{32}$$

Note that, taking into account that the number of slots proposed in each unit was overestimated, some of them may be empty.

Besides, the following constraint is imposed:

$$\sum_{1 \leq l \leq L_{kj}} \sum_{1 \leq k \leq K_j} Y_{bjkl} = \sum_{1 \leq l \leq L_{kj'}} \sum_{1 \leq k \leq K_{j'}} Y_{bj'kl}, \quad \forall j, j', j < j', b \in \bigcup_{\substack{i \\ i \in (I_j \cap I_{j'})}} BI_i \tag{33}$$

$$\sum_{1 \leq k \leq K_j} \sum_{1 \leq l \leq L_{kj}} Y_{bjkl} \geq \sum_{1 \leq k \leq K_j} \sum_{1 \leq l \leq L_{kj}} Y_{b+1jkl}, \quad \forall j, i \in I_j, b \in BI_i, b+1 \in BI_i \tag{34}$$

Constraint (33) ensures that for each product i the set of batches to be processed in the stages that form part of the production path of this product should be the same. Besides, in order to reduce the number of alternative solutions, Eq. (34) guarantees that the batches of a same product that compose the campaign are used in ascending order.

As it will be shown below, the computational performance can be improved by introducing the following assignment variable:

$$X_{jkl} = \begin{cases} 1 & \text{if slot } l \text{ of unit } k \text{ at stage } j \text{ is employed} \\ 0 & \text{otherwise} \end{cases}$$

Taking into account Eqs. (31) and (32), the following constraint must be satisfied for each stage j:

$$\sum_{1 \leq k \leq K_j} \sum_{1 \leq l \leq L_{kj}} X_{jkl} \leq \left| \bigcup_{i \in I_j} BI_i \right|, \quad \forall j \tag{35}$$

Without loss of generality and in order to reduce the search space, it is assumed that in each stage the slots of each unit are utilized in ascending order. Then, the following constraint establishes that for each unit k, slot $l+1$ is only used if slot l has been already allocated:

$$X_{jkl} \geq X_{jkl+1}, \quad \forall j, 1 \leq k \leq K_j, 1 \leq l < L_{kj} \tag{36}$$

Also, in order to eliminate alternative optimal solutions and to reduce the number of postulated slots for each unit of a stage, the following constraint is used:

$$\sum_{1 \leq l \leq L_{kj}} X_{jkl} \geq \sum_{1 \leq l \leq L_{k+1j}} X_{jk+1l}, \quad \forall j, 1 \leq k \leq K_j \tag{37}$$

Eq. (37) establishes that for each stage, the number of processed slots in a unit is greater than or equal to the number of processed slots in the following unit.

Lastly, the decision variable Y_{bjkl} allows defining a linear expression for the number of batches of product i included in the campaign. So, for each product i:

$$NBC_i = \sum_{b \in BI_i} \sum_{1 \leq k \leq K_j} \sum_{1 \leq l \leq L_{kj}} Y_{bjkl}, \quad \forall j, i \in I_j \tag{38}$$

3.2.3. Relation among assignment variables z_{jk}, Y_{bjkl} and X_{jkl}

From the logical point of view, relations among variables Y_{bjkl} and X_{jkl} can be defined. In fact, if slot l of unit k at stage j is not utilized, then none batch is processed in it. This implication is enforced by the following linear inequality:

$$Y_{bjkl} \leq X_{jkl}, \quad \forall j, b \in \bigcup_{i \in I_j} BI_i, 1 \leq k \leq K_j, 1 \leq l \leq L_{kj} \tag{39}$$

On the contrary, if slot l of unit k at stage j is utilized, then only one batch is assigned to it. The reciprocal implication is also true, therefore, the following constraint must be satisfied:

$$\sum_{b \in \bigcup_{i \in I_j} BI_i} Y_{bjkl} = X_{jkl}, \quad \forall j, 1 \leq k \leq K_j, 1 \leq l \leq L_{kj} \tag{40}$$

The following constraints link assignment variables X_{jkl}, Y_{bjkl} and z_{jk}:

$$Y_{bjkl} \leq z_{jk}, \quad \forall j, b \in \bigcup_{i \in I_j} BI_i, 1 \leq l \leq L_{kj}, 1 \leq k \leq K_j \tag{41}$$

$$X_{jkl} \leq z_{jk}, \quad \forall j, 1 \leq l \leq L_{kj}, 1 \leq k \leq K_j \tag{42}$$

Following Eqs. (41) and (42), if unit k of stage j is not allocated, then none of their slots is used to process batches. Taking into account Eqs. (39) and (42), Eq. (41) becomes redundant.

Also, when unit k of stage j is employed, then, at least one batch of a product in a slot must be processed in that unit. Then,

$$\sum_{b \in \bigcup_{i \in I_j} BI_i} \sum_{1 \leq l \leq L_{kj}} Y_{bjkl} \geq z_{jk}, \quad \forall j, 1 \leq k \leq K_j \tag{43}$$

3.2.4. Timing constraints

3.2.4.1. Initial and final times of slots. A batch unit is periodically operated through the basic cycle of filling, processing and emptying, and possibly waiting. Then, for each batch stage j involved in the production path of product i, filling and emptying times may be part of the time required to process a batch of product i in this stage, depending on whether adjacent semicontinuous units exist or not. If t_{ij} denote the processing time of product i at batch stage j, $t_{ij'}$ the processing time of product i at upstream semicontinuous stage j' and $t_{ij''}$ the processing time of product i at downstream semicontinuous stage j'', the time that a unit of stage j will be occupied to process a batch of product i, T_{ij}, is given by the following expression:

$$T_{ij} = t_{ij'} + t_{ij} + t_{ij''}, \quad \forall i \in I_{j'}, i \in I_j, i \in I_{j''}, j \in EB_i, \ j', j'' \in ES_i \tag{44}$$

as is illustrated in Fig. 4.

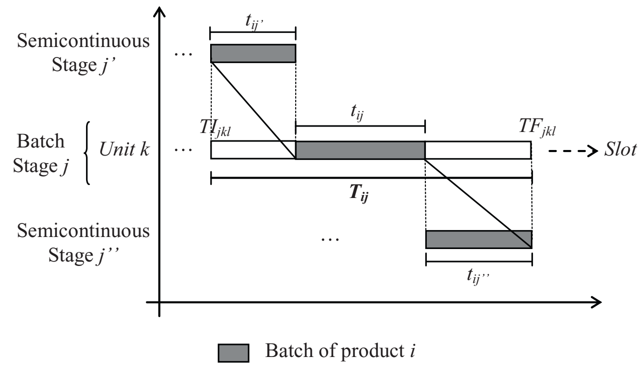

Fig. 4. Required time to process a batch of product i assigned to slot l of unit k at batch stage j.

If batch stage j is preceded by semicontinuous stage j', $t_{ij'}$ represents the material loading time from semicontinuous unit of stage j' to the unit of stage j where the batch of product i is processed, while if stage j is followed by semicontinuous stage j'', $t_{ij''}$ is the material unloading time to semicontinuous unit of stage j''. Therefore, while a semicontinuous unit connected to two batch units is operating, these units cannot be used for any other type of operation.On the other hand, if j and j' are stages whose units constitute a semicontinuous subtrain, then:

$$T_{ij} = T_{ij'} = t_{ij} = t_{ij'}, \quad \forall i \in I_j, i \in I_{j'}, j \in ES_i \tag{45}$$

As already mentioned, the slots correspond to time intervals of variable length where batches will be assigned. Let TI_{jkl} and TF_{jkl} be the initial and final times, respectively, of slot l in unit k of stage j.Thus, the relation between variables TI_{jkl}, TF_{jkl} and Y_{bjkl} is established by the following equation:

$$TF_{jkl} = TI_{jkl} + \sum_{i} \sum_{b \in BI_i} T_{ij} Y_{bjkl}, \quad \forall j, 1 \leq k \leq K_j, 1 \leq l \leq L_{kj} \tag{46}$$

Taking into account that a slot must not be necessarily occupied, when no product batch is assigned to slot l in unit k of stage j (i.e. $Y_{bjkl} = 0, \forall b \in \bigcup_{i \in I_j} BI_i$), the initial and final times of this slot are equal, i.e. $TI_{jkl} = TF_{jkl}$.In order to avoid the overlapping between the processing times of different slots in a unit, the following constraint is added:

$$TF_{jkl} \leq TI_{jkl+1}, \quad \forall j, 1 \leq k \leq K_j, 1 \leq l < L_{kj} \tag{47}$$

Besides, if no batch is assigned to slot $l+1$ of unit k at stage j ($X_{jkl+1} = 0$), then the initial time of this slot is enforced to be equal to the finishing time of slot l. Then, taking into account that Eq. (47) is satisfied for successive slots in a unit, this new condition is represented by:

$$TF_{jkl} - TI_{jkl+1} \geq -M_1 X_{jkl+1}, \quad \forall j, 1 \leq k \leq K_j, 1 \leq l < L_{kj} \tag{48}$$

where M_1 is a sufficiently large number that makes the constraint redundant when a product is assigned to slot $l+1$.

3.2.4.2. Zero-wait transfer policy. The ZW transfer policy assumes that a batch, after finishing its processing at a stage, must be transferred immediately to the next processing stage. Three cases must be considered taking into account the type of adjacent stages involved in the production path of a batch: consecutive batch stages, a batch stage followed by a semicontinuous stage and vice versa.

If batch b is assigned to slot l of unit k in stage j and to slot l' of unit k' in stage j', where j precedes to j' in the production path of batch b, then:

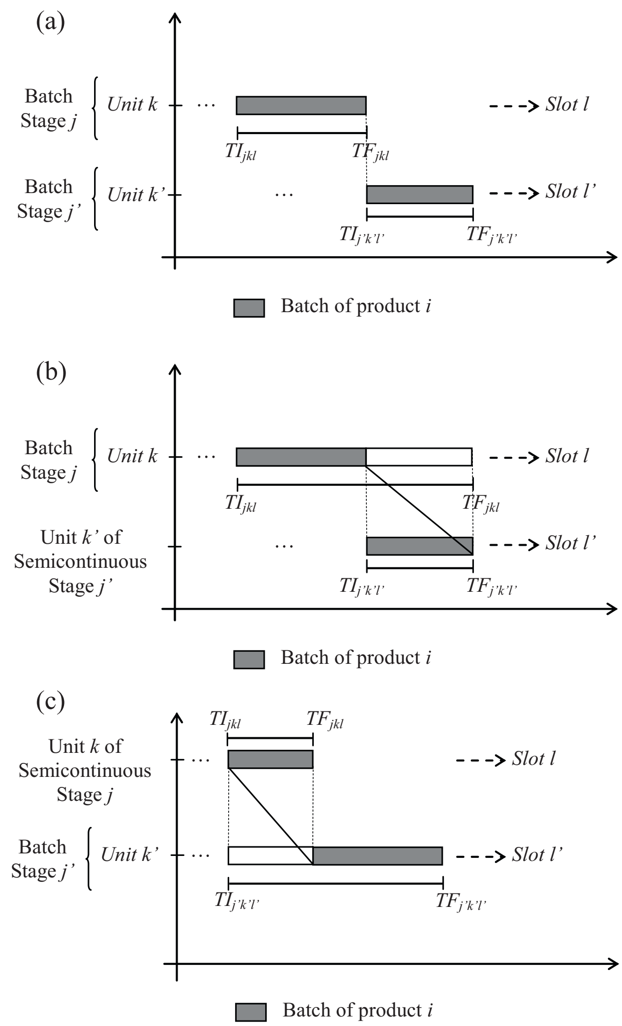

Fig. 5. (a) Consecutive batch stages j and j', (b) batch stage j followed by semicontinuous stage j', (c) semicontinuous stage j followed by batch stage j'.

Case a. If both stages are batch, observing Fig. 5a, the following constraint is imposed:

$$TF_{jkl} = TI_{j'k'l'}, \quad \forall j, j' \in \bigcup_i EB_i, \quad j < j', \quad 1 \le k \le K_j, \quad 1 \le k' \le K_{j'}, \quad k/Y_{bjkl} = 1,$$
$$k'/Y_{bj'k'l'} = 1, \quad i/i \in I_j \cap I_{j'}, \quad b \in \bigcup_i BI_i, \quad 1 \le l \le L_{kj}, \quad 1 \le l' \le L_{k'j'} \tag{49}$$

As this constraint must be only satisfied when a batch is assigned to those units and slots, then the condition can be expressed through constraints of Big-M type, as:

$$TF_{jkl} - TI_{j'k'l'} \ge M_2(Y_{bjkl} + Y_{bj'k'l'} - 2) \quad \forall j, j' \in \bigcup_i EB_i, \quad j < j', \quad 1 \le k \le K_j,$$
$$1 \le k' \le K_{j'}, \quad i/i \in I_j \cap I_{j'}, \quad b \in \bigcup_i BI_i, \quad 1 \le l \le L_{kj}, \quad 1 \le l' \le L_{k'j'} \tag{50a}$$

$$-TF_{jkl} + TI_{j'k'l'} \ge M_2(Y_{bjkl} + Y_{bj'k'l'} - 2) \quad \forall j, j' \in \bigcup_i EB_i, \quad j < j', \quad 1 \le k \le K_j,$$
$$1 \le k' \le K_{j'}, \quad i/i \in I_j \cap I_{j'}, \quad b \in \bigcup_i BI_i, \quad 1 \le l \le L_{kj}, \quad 1 \le l' \le L_{k'j'} \tag{50b}$$

where M_2 is a sufficiently large number that relaxes these constraints when batch b is not processed in slot l of unit k at stage j or in slot l' of unit k' at stage j'.

Case b. If stage j is a batch stage and stage j' is a semicontinuous one, then as is illustrated in Fig. 5b:

$$TF_{jkl} = TF_{j'k'l'}, \quad \forall j \in \bigcup_i EB_i, j' \in \bigcup_i ES_i, j < j', \ 1 \le k \le K_j, 1 \le k' \le K_{j'},$$
$$k/Y_{bjkl} = 1, k'/Y_{bj'k'l'} = 1, i \in I_j \cap I_{j'}, b \in \bigcup_i BI_{i'}, 1 \le l \le L_{kj}, 1 \le l' \le L_{k'j'} \tag{51}$$

Case c. Finally, as is drawn in Fig. 5c, if stage j is a semicontinuous stage and stage j' is a batch one, then:

$$TI_{jkl} = TI_{j'k'l'}, \quad \forall j \in \bigcup_i ES_i, \quad j' \in \bigcup_i EB_i, \quad j < j', \quad 1 \le k \le K_j, 1 \le k' \le K_{j'}, \quad k/Y_{bjkl} = 1,$$
$$k'/Y_{bj'k'l'} = 1, i \in I_j \cap I_{j'}, b \in \bigcup_i BI_{i'}, 1 \le l \le L_{kj}, 1 \le l' \le L_{k'j'} \tag{52}$$

Analogously to Case a, the last two conditions can be expressed through Big-M constraints.

3.2.4.3. Cycle time of the campaign. As it was mentioned in Section 3.1, the number of times that the campaign is repeated over the time horizon must be determined taking into account the cycle time of the campaign, CTC, which is defined by the following expression:

$$CTC \ge TF_{jkL_{kj}} - TI_{jkl_1}, \quad \forall j, 1 \le k \le K_j \tag{53}$$

For each unit k, the production cycle time represents the time that the unit is occupied with the processing of batches that compose the campaign, and is calculated by the difference between the initial and final operation times of the first slot and last slot assigned to that unit. Then, CTC is the maximum of all these values.

Significant savings in computational time have been achieved by establishing a good lower bound on the cycle time of the campaign. In fact, if there are no idle times in the production campaign at each unit, then:

$$CTC \ge \sum_{1 \le l \le L_{kj}} \sum_{i \in I_j} \sum_{b \in BI_i} T_{ij} Y_{bjkl}, \quad \forall j, 1 \le k \le K_j \tag{54}$$

3.3. Objective function

The objective function is the minimization of the annual investment cost of the batch plant, IC, given by:

$$IC = CCF \sum_j \sum_k z_{jk} \alpha_j V_j^{\beta_j} \tag{55}$$

where α_j and β_j are appropriate cost coefficients for units of stage j and CCF is a capital charge factor on the time horizon, which includes an amortization term.

Considering Eqs. (11)–(13), Eq. (55) can be re-written as:

$$IC = CCF \left(\sum_{j \in \bigcup_i EB_i} \sum_k \sum_p \alpha_j VF_{jp}^{\beta_j} z_{jk} \upsilon_{jp} + \sum_{j \in \bigcup_i ES_i} \sum_k \sum_m \alpha_j RF_{jm}^{\beta_j} z_{jk} r_{jm} \right) \tag{56}$$

The first term corresponds to batch units cost whereas the second one to semicontinuous units cost.

In order to avoid nonlinearities in Eq. (56), binary variables e_{jkp} and ee_{jkm} are defined. Variable e_{jkp} links decision variables υ_{jp} and z_{jk} such that e_{jkp} takes value 1 if both are 1 and 0 otherwise, whereas variable ee_{jkm} links decision variables r_{jm} and z_{jk} such that ee_{jkm} takes value 1 if both are 1 and 0 otherwise. As it has been posed in analogous cases, the following constraints enforce these logic relations:

$$e_{jkp} \ge \upsilon_{jp} + z_{jk} - 1, \quad \forall j \in \bigcup_i EB_i, 1 \le k \le K_j, 1 \le p \le P_j \tag{57}$$

$$ee_{jkm} \ge r_{jm} + z_{jk} - 1, \quad \forall j \in \bigcup_i ES_i, 1 \le k \le K_j, 1 \le m \le M_j \tag{58}$$

Nevertheless, these new variables do not need to be declared as binary if the following upper and lower bounds are incorporated:

$$0 \le e_{jkp} \le 1, \quad \forall j \in \bigcup_i EB_i, 1 \le k \le K_j, 1 \le p \le P_j \tag{59}$$

$$0 \leq ee_{jkm} \leq 1, \quad \forall j \in \bigcup_i ES_i, 1 \leq k \leq K_j, 1 \leq m \leq M_j \tag{60}$$

Thus, a lineal objective function is obtained:

$$IC = CCF \left(\sum_{j \in \bigcup_i EB_i} \sum_k \sum_p \alpha_j VF_{jp}^{\beta_j} e_{jkp} + \sum_{j \in \bigcup_i ES_i} \sum_k \sum_m \alpha_j RF_{jm}^{\beta_j} ee_{jkm} \right) \tag{61}$$

Therefore, the proposed model simultaneously determines the optimal plant design, batch sizes, composition of the MPC, and production sequence of batches in each processing unit, satisfying the demand in the available time horizon. Taking into account that different MPCs can correspond to the same optimal plant configuration, a penalty term that involves the cycle time of the campaign is included in the objective function with the aim of reducing alternative solutions. This new term is the product of the variable *CTC* with a weighting factor λ, which is appropriately selected taking into account the involved model parameters Thus, the computational performance is improved. Therefore, the following objective function is proposed:

$$f = IC + \lambda CTC \tag{62}$$

4. Examples

In this section the proposed approach is applied to the ethanol plant described in Section 2. All the examples were implemented and solved in GAMS (Brooke, Kendrick, Meeraus, & Raman, 1998) on an Intel Core i7, 2.8 GHz. The CPLEX 12.1 solver was employed for solving the MILP problems, with a 0% optimality gap. The number of continuous and binary variables and constraints strongly depend on the maximum number of admitted units in each stage, the maximum number of batches allowed for each product in the campaign, the number of slots postulated for each unit, and the number of discrete options considered for the unit sizes.

The production recipe was obtained from a detailed model for similar productions (Corsano et al., 2007), and size and duty factors as well as processing times are shown in Tables 1 and 2, respectively.

For Examples 1 and 2, the product demands, Q_i, are: 8,400,000 kg for torula yeast, 45,000,000 kg for ethanol and 11,000,000 kg for bakery yeast. The maximum number of batches of product *i* in a campaign, NBC_i^{UP}, is 3 for torula and 4 for ethanol/bakery yeast, while the time horizon *H* is equal to 7500 h. For each stage, five discrete sizes are available, that are shown in Table 3. In the same table, cost coefficients are depicted and the *CCF* factor is considered equal to 0.225 (Petrides, Sapidou, & Calandranis, 1995). As was previously mentioned, units of batch stages can be duplicated. For biomass fermentation up to three units are allowed, while for alcohol fermentation and distillation stages up to two units can be assigned. Therefore, using the expression (30) and taking into account biomass fermentation units are used for producing ethanol and torula yeast, the number of postulated slots for this stage is 7, 3, 2 for units 1, 2 and 3 respectively, while for alcohol fermentation and distillation the number of postulated slots are 4 and 2 for units 1 and 2 respectively, since these stages are used only for ethanol production.

4.1. Example 1

The model for the simultaneous optimization of plant design and scheduling is solved for the ethanol/yeast plant presented in Section 2. The proposed MILP model for this example comprises 3623 constraints, 593 binary variables and 1068 continuous variables and it was solved in a CPU time of 33.02 s. The optimal solution corresponds to a total investment cost of $11,525,588.

The optimal plant structure includes duplicated units out of phase at biomass fermentation and distillation stages, and one unit at remaining stages, as shown in Fig. 6. The optimal unit sizes are also depicted in the figure.

The optimal campaign configuration involves two batches of each product with the batch sequencing shown in Fig. 7. The campaign cycle time, *CTC*, is equal to 24.54 h and the campaign is repeated 305 times over the time horizon.

It is worth mentioning that the simultaneous design and scheduling allow selecting the units to be used in each stage in order to reduce the investment cost, the cycle time and complete the product demands in the settled time horizon. In this case, distillation stage is limiting time for ethanol production, therefore, this stage is duplicated and there are not idle times in these units. On the other hand, biomass fermentor is used for both productions: ethanol and torula. Also, for torula production the biomass fermentor remains occupied during material unload to semicontinuous subtrain, increasing the biomass fermentor processing time. Therefore, unit duplication at biomass fermentation stage reduces the campaign cycle time. For this stage, three units out of phase are used and they have idle times. But if fewer units are selected for this stage, the campaign cycle time is increased and bigger unit sizes are needed to fulfill the required demands over the time horizon with a higher investment cost.

Batch sequencing that composes the campaign is a model decision. It is remarkable mentioning that no heuristic rule is imposed for this task and therefore, the model selects the best campaign configuration without batch preordering. Note that at stage 1, ethanol production is firstly processed, while at semicontinuous subtrain, the first processed batch corresponds to torula production. For sequential multipurpose batch plants, where some products do not use some stages, this type of campaign is very appropriate since batch swapping is allowed. This means that batches can alter the processing order from a stage to another stage, with the objective of reducing idle times and, consequently, the cycle time. Also, this batch exchange permits to accommodate the product batch sizes in a suitable manner in order to minimize the number of used units and their sizes.

The same example was performed for different maximum number of batches of each product in the production campaign. Also, in order to highlight the capabilities of the proposed formula given by Eq. (30), each instance is also implemented considering the number of postulated slots for all unit of each stage equal to the maximum number of batches allowed in the campaign. In this way, for biomass fermentation and semicontinuous subtrain, the number of slots postulated for each unit is equal to $NBC_{\text{torula}}^{UP} + NBC_{\text{ethanol}}^{UP}$, while the number of slots postulated for each unit of alcohol fermentation and distillation stages is $NBC_{\text{ethanol}}^{UP}$. Table 4 shows the different instances, model characteristics and computational performance. In all instances, the optimal solution coincides with that reported for $NBC_{\text{torula}}^{UP} = 3$ and $NBC_{\text{ethanol}}^{UP} = 4$.

4.2. Example 2

In this example, the scheduling constraints of the proposed model are adapted for considering SPC policy. This instance is posed with the objective of comparing MPC vs. SPC optimal solutions. In SPC, each campaign is devoted to produce only one product until fulfill its demand. Thus, the campaign is characterized through a unique scheduling constraint to identify the product cycle time. From the commercial point of view, this approach is inappropriate. In plants where perishable products are produced, this type of

Table 1
Size and duty factors for ethanol plant.

	Size and duty factors: SF_{ij} and D_{ij} ($\times 10^{-2}$)										
	Fermentation			Semicontinuous subtrain			Distillation				
	1	2	3	4	5	6	7	8	9	10	11
Torula yeast	2.5	0	0	58.8	1.14	22	0	0	0	0	0
Ethanol/bakery yeast	0.473	0.54	0.612	58.8	1.14	22	0.45	2.33	0.0972	3.94	0.127

References: 1: biomass fermentor, 2: alcohol fermentor 1, 3: alcohol fermentor 2, 4: centrifuge, 5: evaporator, 6: dryer, 7: distiller feed vessel, 8: distiller evaporator, 9: column, 10: condenser, 11: distillate tank.

Table 2
Processing times for stages of ethanol plant.

	Processing time: t_{ij}				
	Biomass fermentation	Alcohol fermentation 1	Alcohol fermentation 2	Semicontinuous subtrain	Distillation
Torula yeast	10.74	0	0	5.22	0
Ethanol/bakery yeast	9.83	4.83	6.14	5.85	18.69

Table 3
Available discrete sizes and cost coefficients for plant stages.

Units	Discrete unit sizes: VF_{jp} and RF_{jm}					Cost coefficient (α_j)	Cost exponent (β_j)
	1	2	3	4	5		
1	150	350	550	700	1100	40,020	0.60
2	200	350	400	700	1400	24,200	0.45
3	235	470	800	940	1600	24,200	0.45
4	40	50	80	100	160	25,000	0.68
5	7	15	30	60	120	30,300	0.53
6	65	130	200	260	400	59,600	0.60
7	175	350	600	700	1200	31,100	0.60
8	75	150	300	600	900	9760	0.65
9	2	4	6	8	10	151,312	0.65
10	100	200	300	400	600	7255	0.65
11	50	100	150	200	300	31,100	0.60

References: 1: biomass fermentor, 2: alcohol fermentor 1, 3: alcohol fermentor 2, 4: centrifuge, 5: evaporator, 6: dryer, 7: distiller feed vessel, 8: distiller evaporator, 9: column, 10: condenser, 11: distillate tank.

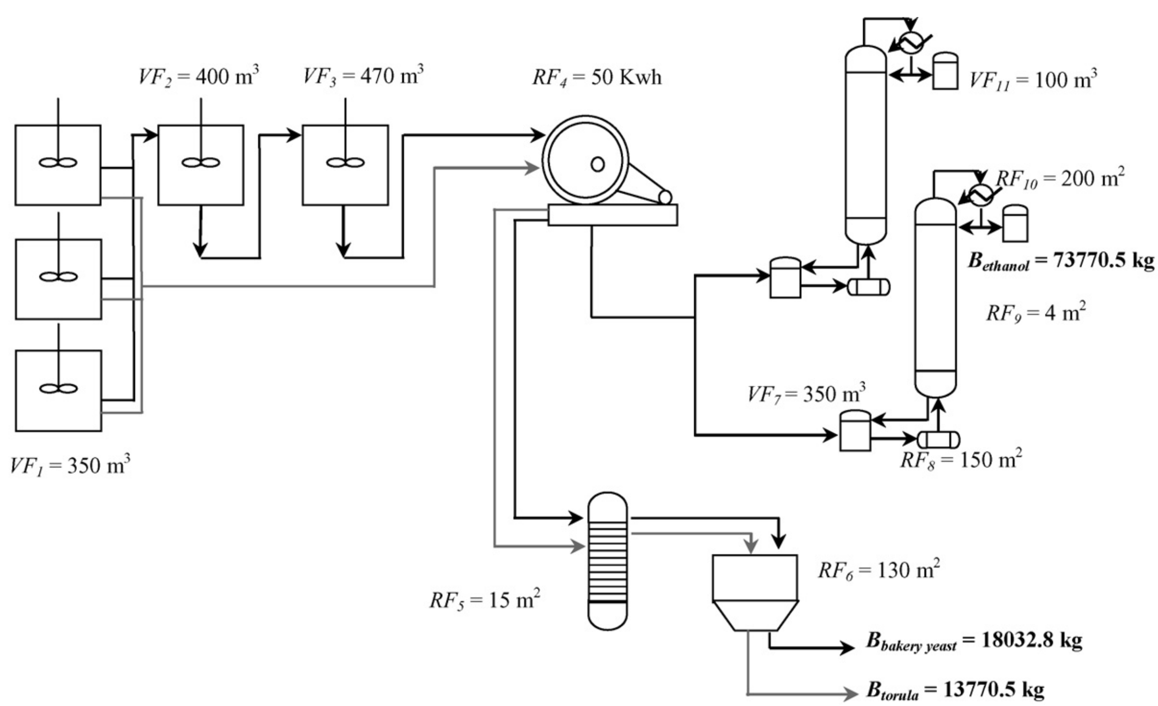

Fig. 6. Example 1: optimal plant design.

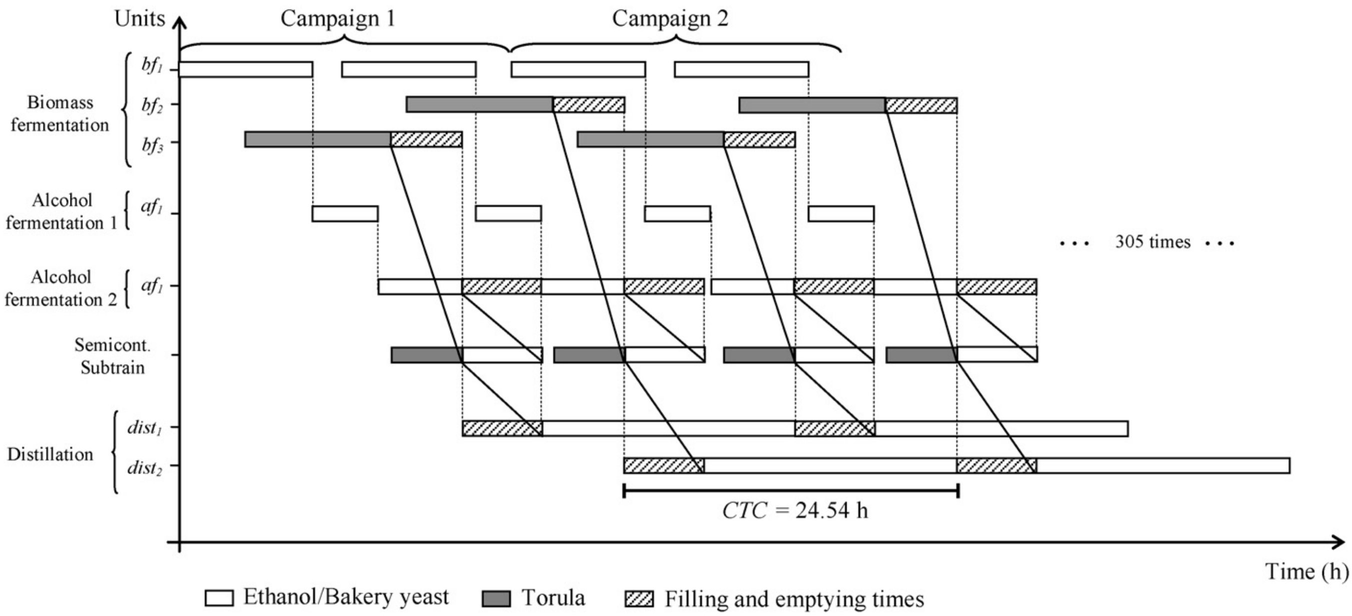

Fig. 7. Example 1: Gantt chart for ethanol plant.

campaign is not suitable since huge stocks are accumulated and, therefore, the products are decomposed.

The SPC formulation is performed for the same model parameters of the previous instance. This MILP model comprises 287 constraints, 165 binary variables and 395 continuous variables and it was solved in a CPU time of 0.076 s. The optimal solution increases the investment costs to $13,549,638. The plant design consists of the duplication of biomass fermentation and distillation stages as is shown in Fig. 8. The figure also shows unit sizes and batch sizes for each product. Ethanol is produced along 381 batches and its cycle time is equal to 12.27 h, since torula cycle time is equal to 7.98 h and its production is repeated 352 times as is shown in Fig. 9.

Apart from the disadvantages previously cited, the use of SPC for sequential multipurpose plants presents longer idle times in some unit. Besides, for products that do not use all the plant stages, some units are inactive during its production.

In this example, the plant configuration selects two biomass fermentors in order to reduce the torula cycle time, but the second biomass fermentor is not used for ethanol production, and therefore it is inactive during nearly 4700 h. On the other hand, torula production does not use alcohol fermentation and distillation stages. Then, these stages are idle during practically 2800 h. Hence, when SPC is applied, equipment is sub-occupied.

The number of batches of each product through the time horizon is decreased due to the idle times increase. Therefore larger batch

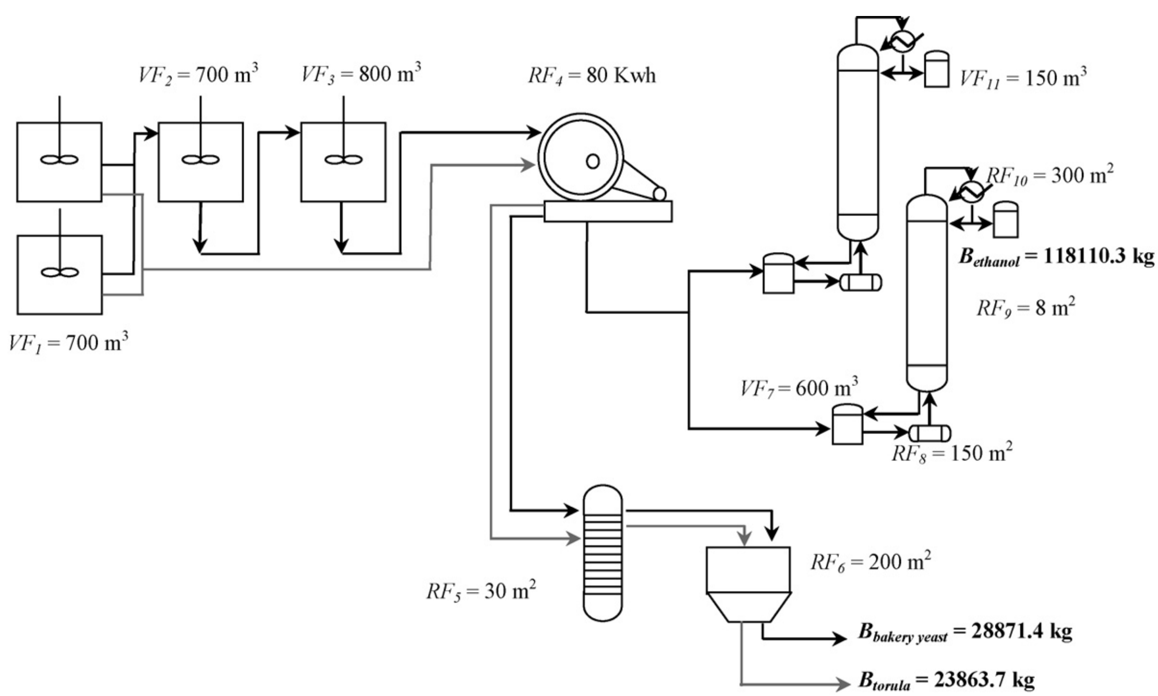

Fig. 8. Example 2: optimal plant design for SPC model.

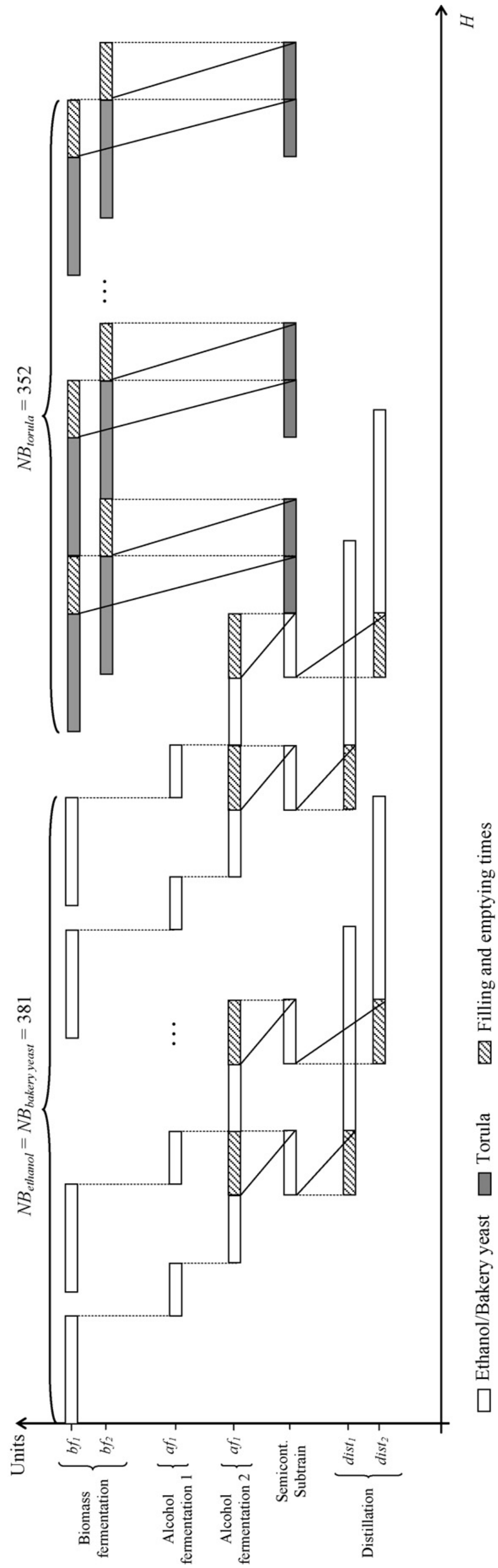

Fig. 9. Example 2: Gantt chart for SPC model.

Table 4
Computational performance for Example 1 with different values of NBC_i^{UP}.

NBC_{torula}^{UP}	$NBC_{ethanol}^{UP}$	No. of constraints		No. of binary variables		No. of continuous variables		CPU time (s)	
		Using Eq. (30)	Without Eq. (30)	Using Eq. (30)	Without Eq. (30)	Using Eq. (30)	Without Eq. (30)	Using Eq. (30)	Without Eq. (30)
3	4	3623	5496	593	695	1068	1252	33.02	95.61
4	4	4358	6662	660	780	1201	1369	37.38	96.74
5	5	7200	11,727	883	1069	1526	1775	160.57	310.62
6	6	11,911	19,042	1157	1402	1911	2225	685.3	1137.48
7	7	17,210	29,033	1428	1779	2281	2719	1661.24	3840.88

Table 5
Product demands for each case of Example 3.

	Demand: Q_i (kg)		
	Torula yeast	Ethanol	Bakery yeast
Case 1	6, 500, 000	40,000,000	10,000,000
Case 2	9, 000, 000	46,000,000	11,500,000

Table 6
Optimal variables for Example 3, Cases 1 and 2.

	Case 1	Case 2
CTC (h)	24.54	31.87
NC	296	311
Campaign composition	1 Torula batches–2 ethanol batches	2 Torula batches–2 ethanol batches
Torula batch size (kg)	21,959.5	14,469.5
Ethanol batch size (kg)	67,567.6	73,955
Bakery yeast batch size (kg)	16,892	18,488.8
Time to fulfill required demands (h)	7264	9911.57

sizes are needed to fulfill the product demands. Then, unit sizes are increased and hence the investment cost is 17.6% higher that the MPC optimal solution.

It is worth mentioning that a characteristic of torula yeast and bakery yeast productions is its fast degradation, since they have to be consumed in 72 h. Therefore, the SPC forces to consume the product that cannot be stored while the production is carried out. Besides, when it is not produced, demand cannot be satisfied. In other words, since they are perishable, they can be only seasonally supplied.

In short, the drawbacks of SPC are: longer idle times, bigger unit sizes, inactive units for long times, huge stocks, and inappropriate scheduling policy for perishable products.

4.3. Example 3

A usual industrial practice consists of planning the production for a fixed time horizon in a given plant. The objective of this example is to apply the proposed approach as a planning tool, where the plant configuration and unit sizes are known. In this case, the analysis is focused on the number and size of production batches that compose the campaign, and on different scheduling decisions as assignment and sequencing of batches in each unit.

Suppose that a facility, with the configuration and sizing as it is shown in Fig. 10, is given. Different scenarios can be posed depending on the operation manager requirements. In this example, two cases were defined by changing the required demands for a time horizon of 7500 h (Table 5). The proposed MILP model was adapted to perform the planning for each case, fixing the plant design to the configuration and unit sizes showed in Fig. 10. The problem objective function is the minimization of the campaign cycle time since the plant is already installed. In both cases, the maximum number

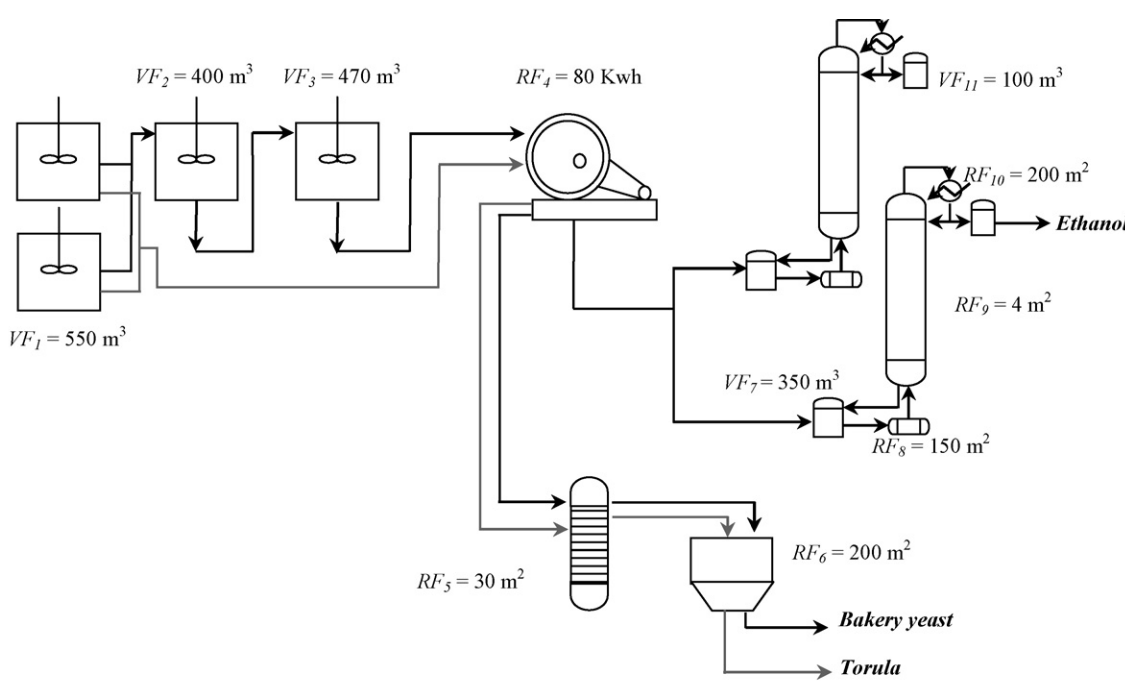

Fig. 10. Example 3: plant design for planning approach.

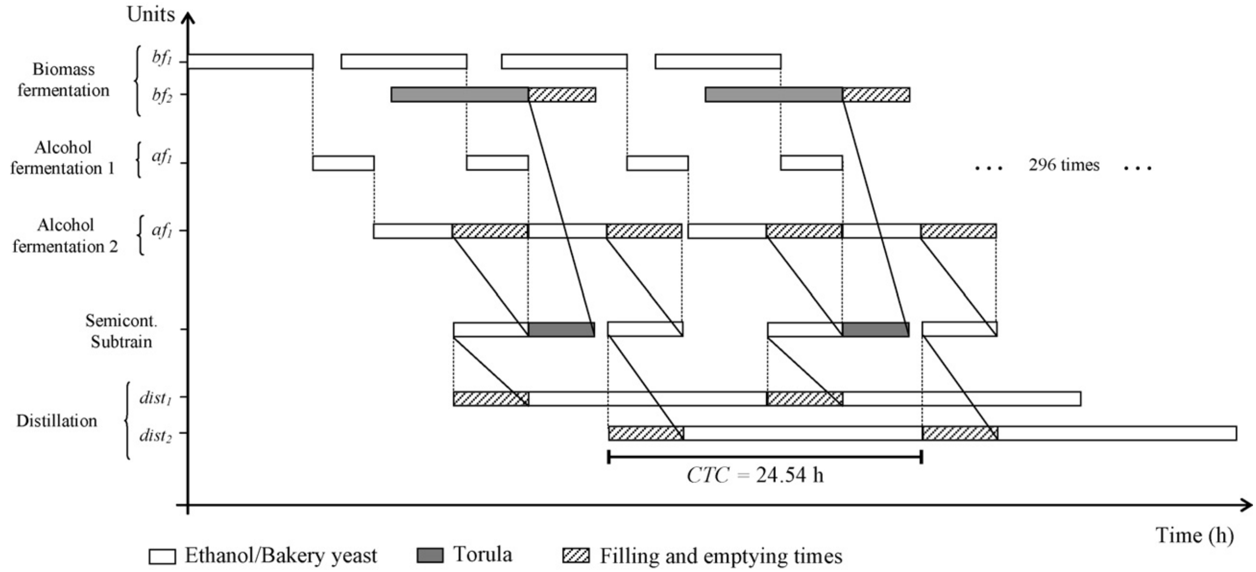

Fig. 11. Example 3: Case 1 – optimal production planning.

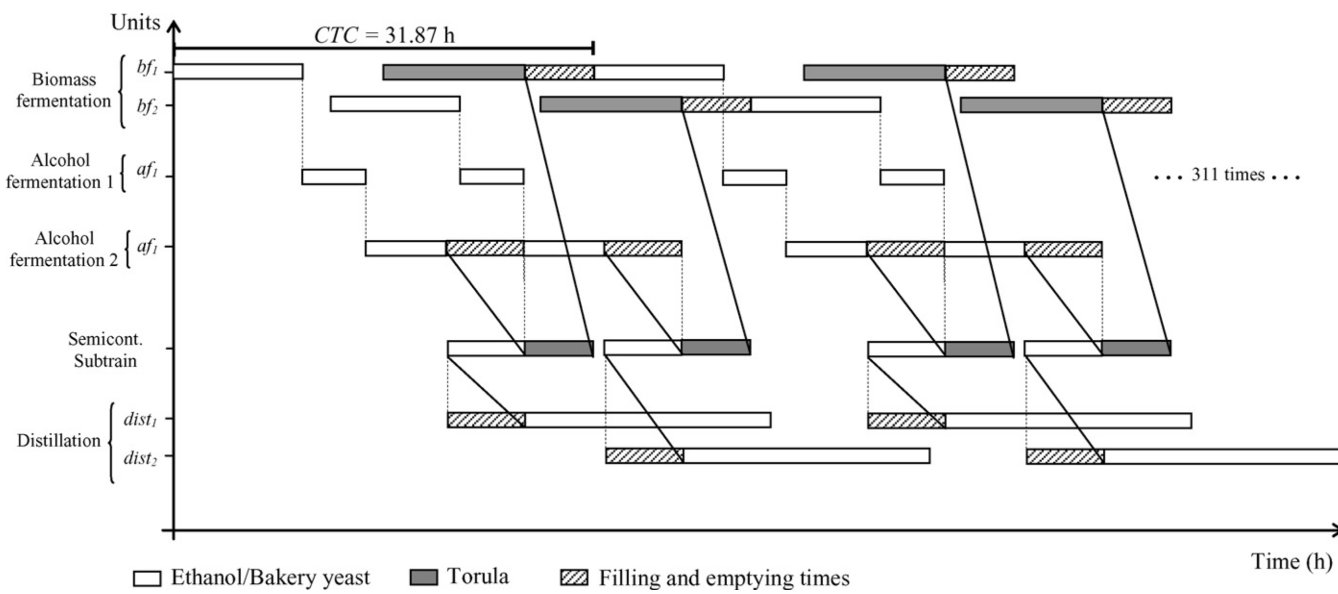

Fig. 12. Example 3: Case 2 – optimal production planning.

of batches of each product in the campaign was stated equal to four for all products.

4.3.1. Case 1

The MILP formulation for this case study comprises 3240 constraints, 472 binary variables and 1073 continuous variables and it was solved in a CPU time of 0.179 s. The Gantt chart of Fig. 11 illustrates the optimal production sequence on each unit for different stages and first column of Table 6 shows the most relevant optimal variables.

Similarly to Example 1, the limiting time stage is distillation, and there are not idle times in units of this stage. Batch sequencing does not follow the same order in all the units. It can be observed in Fig. 11 how a torula batch is inserted between two ethanol batches in order to reduce the cycle time at semicontinuous stages.

The model allows determining if the available time horizon is sufficient to satisfy the required demands. If this is so, the model selects the best campaign configuration with minimum cycle time. In this case, the necessary time to fulfill market requirements is approximately 7264 h, relatively less than 7500 h. Then, the model can be used by the planner as a tool to assess the convenient operation mode for the remaining time, for example, if the campaign is repeated for storage or new campaigns are processed for future demands.

4.3.2. Case 2

In this case, the model is solved according to product demands showed in Table 5. The number of constraints is 3240, the number of binary and continuous variables is 472 and 1073 respectively, and the CPU time is 87.99 s.

The model solution is infeasible and, therefore, the demands cannot be fulfilled over the time horizon of 7500 h. Consequently, the model is used by the operation manager as a tool for determining the required minimum time horizon and the appropriate production campaign to assure the product demands. Therefore, Eqs. (24) and (25) are modified, including a longer time horizon.

After solving the new model, the optimal campaign involves two batches of torula and two batches of ethanol/bakery yeast, and the production sequence in each unit is showed in Fig. 12. The optimal variables are depicted in Table 6. It is worth noting that ethanol and bakery yeast batch sizes are bigger than those obtained in Case 1, but even though torula demand is greater, its batch size is smaller since the number of batches involved in the campaign is duplicated.

According to this solution, the operation manager has to decide if the plant continues the production plan along near 2500 h more to complete the new demands or if production is shut down without satisfying the demands.

In this last example a new scenario has been solved. Unlike the previous examples, in this case the plant is given. Only planning (number of batches and product batch sizes) and scheduling (batch assignment and sequencing) decisions have to be considered. However this scenario is usual because operating, production and market conditions can change. Then production planning has to be adjusted to satisfy these new requirements. This example shows how the proposed model can be used as a tool for planning the production of a given plant and for analyzing different production schemes. The cycle time minimization as objective function allows attaining the shortest production time in the time horizon. Therefore, the equipment is better occupied. If the horizon time is partially used, the campaign can be repeated more times for storage or new campaigns can be processed for future demands. Thus the plant can be appropriately operated and controlled. On the other hand, if the demands cannot be fulfilled in the time horizon, the operation manager can modify the production requirements or extend the available time.

5. Conclusions

In this work a MILP model is proposed for simultaneous design and scheduling of sequential multipurpose plants with batch and semicontinuous units. The model was applied for an ethanol plant where yeast production is also considered as a sustainable alternative. Due to yeast degradation and with the objective of providing a stable product supply, the most appropriate scheduling policy is MPC. Besides, the use of MPCs allows taking advantage of the structure of sequential multipurpose plants, because long idle times and significant overdesign of the plant are avoided. Therefore, a set of novel scheduling constraints was formulated in order to obtain the batch assignment and sequencing simultaneously with the plant design. When design and scheduling decisions are jointly approached, the campaign cycle time has to be determined, since the production campaign is cyclically repeated through the time horizon. The cycle time calculation involves considering initial and final times for each unit and therefore the problem size is increased. In this work a novel expression for postulating the number of slots for each unit was presented, and thus, the problem size was significantly reduced.

The model was formulated for sequential multipurpose plants but it is also valid for multiproduct plants. Another contribution of this work is the consideration of batch and semicontinuous units, and the corresponding scheduling constraints for this kind of mixed plants.

The production of renewable energy is an interesting problem that had paid much attention in the industrial and scientific communities. The ethanol plant model proposed in this work allows producing sustainable and renewable fuels. Besides, a stable context can be assumed, where demands can be appropriately forecast. Thus the joint resolution of design and scheduling can be effectively addressed over long time horizons.

In order to show the advantages of the proposed formulation, several scenarios were treated in the ethanol and derivatives industry. A first case was solved using MPC and SPC approaches in order to assess the differences between them. Better solutions were obtained for the proposed model with MPC. Additionally, the trade-offs among design and scheduling decisions can be effectively assessed. Besides, in order to show the possible applications of this formulation, it was used for the optimal production planning of this kind of plants.

Nomenclature

Sets

BI_i	batches proposed of product i in a campaign
EB_i	batch processing stages utilized for the manufacturing of product i
ES_i	semicontinuous processing stages utilized for the manufacturing of product i
I_j	products that stage j can process
SR_j	available discrete sizes for semicontinuous units of stage j
SV_j	available discrete sizes for batch units of stage j

Indices

i	product
j	stage
k	unit
l	slot
m	discrete size for semicontinuous unit
M_j	number of available standard sizes for semicontinuous stage j
n	number of batches of a product
p	discrete size for batch unit
P_j	number of available standard sizes for batch stage j

Parameters

CCF	capital charge factor
CTC^{UP}	upper bound for variable CTC
D_{ij}	duty factor of product i in semicontinuous stage j
H	time horizon
K_j	maximum number of available identical parallel units at batch stage j
L_{kj}	number of slots postulated for unit k of stage j
NBC_i^{UP}	maximum number of batches of product i in the composition of a campaign
Q_i	demand of product i over the time horizon H
RF_{jm}	discrete size m for semicontinuous units of stage j
SF_{ij}	size factor of product i in batch stage j
t_{ij}	processing times for product i in stage j
T_{ij}	time that a unit of stage j will be occupied to process a batch of product i
VF_{jp}	discrete size p for batch units in stage j
α_j	cost coefficient for units of stage j
β_j	cost exponent for units of stage j
λ	weighting factor for variable CTC in the objective function

Binary variables

r_{jm}	denotes if units of semicontinuous stage j have size m
u_{ijmn}	represents the bilinear term $r_{jm}\, x_{in}$
v_{jp}	denotes if units of batch stage j have size p
w_{ijpn}	represents the bilinear term $v_{jp}\, x_{in}$
x_{in}	denotes if n batches of product i are processed in the campaign
X_{jkl}	indicates if slot l of unit k in stage j is employed
Y_{bjkl}	specify if batch b is assigned to slot l and processed in unit k of stage j
z_{jk}	specify if unit k of stage j is employed

Continuous variables

B_i	batch size of product i
CTC	cycle time of the campaign
e_{jkp}	product of binary variables $z_{jk}\, v_{jp}$
ee_{jkm}	product of binary variables $z_{jk}\, r_{jm}$
IC	annual investment cost of the batch plant
NBC_i	number of batches of product i included in the campaign
NB_i	total number of batches of product i in the time horizon
NC	number of times that the campaign is cyclically repeated over the time horizon
R_j	processing rate for semicontinuous stage j
TF_{jkl}	final processing time of slot l in unit k of stage j
TI_{jkl}	initial processing time of slot l in unit k of stage j
uu_{ijmn}	cross product $u_{ijmn}CTC$
V_j	size of a batch unit in stage j
ww_{ijpn}	cross product $w_{ijpn}CTC$

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