SCHEDULING WITH EQUIPMENT REDESIGN IN MULTIPURPOSE BATCH PLANTS

Samuel Moniz[1,3], Ana Paula Barbosa-Póvoa[1*], Jorge Pinho de Sousa[2,3]
[1]Centro de Estudos de Gestão, Instituto Superior Técnico,
Universidade Técnica de Lisboa, 1049-001 Lisboa, Portugal
[2]INESC Porto
[3]Faculdade de Engenharia da Universidade do Porto

Abstract

The objective of this paper is to present a new formulation for the optimal scheduling of multipurpose batch plants where equipment redesign is considered simultaneously with the scheduling decisions. The equipment redesign is characterized by the implementation of modifications in the existent processing units so as to change their suitability to perform certain tasks, while regarding tasks' characteristics inside a given scheduling horizon. This approach may be advantageous in cases where no schedule solutions are found with the existent equipments and where, with minor technology modifications on the processing units, feasible schedules can be obtained. Each of these changes has a cost and requires a certain time to be implemented. In order to model such problem a simple Mixed Integer Linear Programing formulation (MILP) is proposed having as basis the unified Resource-Task Network (RTN) representation presented by Pantelides (1994). An example motivated by a chemical-pharmaceutical industry is used to demonstrate the applicability of the proposed formulation.

Keywords

Multipurpose batch plants, simultaneous scheduling and design, equipment redesign

Introduction

The chemical-pharmaceutical industry has been facing an increasing demand for the production of a high variety of low volume products at a minimum cost. Such pressure leads to the need of production systems that run efficiently both in terms of cost and time. Consequently, production flexibility is required so as to accommodate the customers' orders within acceptable response times and costs – usually imposed by the market. To compete in such environment, the chemical industry has been using multipurpose batch plants that are characterized by having a set of resources (processing units, raw materials, utilities, manpower, etc.) that can be shared, so as to produce several products. These plants are especially attractive in situations where product demands and formulations change rapidly, since they can be easily adapted to the production specificities of each product. Moreover, changes in a plant such as the addition of new processing units or connections and the removal of old inefficient units are decisions that can also be considered. In this context, planning and scheduling become important functions of the production system enabling a flexibility increase of the multipurpose batch plants while minimizing costs. This problem has been addressed in the literature as the design and retrofit of multipurpose batch plants. For the most recent review on these issues see Barbosa-Póvoa (2007). The design of batch plants from scratch is referred as a grassroot problem while the redesign of an existing plant is denoted as a retrofit problem. Two additional concepts have been used

---

[*] To whom all correspondence should be addressed, apovoa@ist.utl.pt

to categorize these research problems: "*basic design*" and "*extended design*". As stated by Barbosa-Póvoa (2007) the former refers to the simple choice of equipments and associated scheduling, while the latter goes further and addresses scheduling and detailed design where not only the choice of the equipment is considered but also topology and operational aspects are explored. A number of papers have been published on these topics and the proposed models cover a large number of problem features such as: the selection of the processing units and their sizes; addition of storage vessels; storage policies; design of equipment units' connections; operating mode – cyclic and non-cyclic; campaign structure; and 2D and 3D layout design.

Furthermore, when looking into the batch scheduling problem as a standalone problem, the aim is to operate a set of resources so as to produce a set of products within a defined scheduling period. For a detailed review on this topic the work of Mendez et al. (2006) should be analyzed. Batch scheduling problems need to deal with a great variety of aspects that are intrinsically linked to the problem structure. Some of the most important of these aspects are: multiproduct and multipurpose batch topologies; equipment connectivity; inventory storage policies; material transfer; batch size and batch processing time; and changeovers. When modeling such problems one of the most important issues is the time representation, which can be discrete or continuous. Discrete formulations have been shown to be a good approach for those scheduling problems that can be represented with a reasonable, not too large, number of time intervals (Castro et al., 2003). Continuous formulations explicitly represent the timing decisions as a set of continuous variables, as a way to define the exact time at which the events occur. Typically, this results in the reduction of the number of variables of the model. Despite the added flexibility, continuous formulations tend to increase the models complexity by means of the use of big-M constraints.

As mentioned before most of the work performed on the scheduling problem of multipurpose batch plants mainly addresses the optimal utilization of a set of existent resources so as to produce what the customers need. On the other hand, the design and retrofit of multipurpose batch plants looks into the need of designing a plant from scratch or redesigning the existing plant, by adding new units or connections. Nevertheless, an intermediate problem, somewhere between the design and the scheduling problem, is often faced by multipurpose process companies when trying to produce a new set of products, see Figure 1. This problem is related to the need of performing changes in the existing processing units – equipment redesign – so as to improve the existent equipment suitability, thus providing more flexibility to the plant. The timing of the equipment redesign decisions is similar to the scheduling decisions since their scope is also of short-term. Furthermore, the retrofit and grassroots design take time to be implemented in the shop-floor and may require large investments, hence these decisions must be considered in the long-term planning. The equipment redesign assumes more relevance in industries that perform process development, since the production recipes evolve with it and for that reason it may be necessary to modify the processing units.

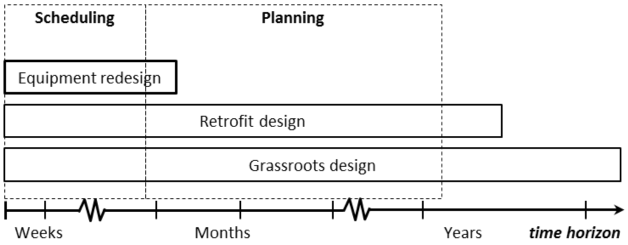

Figure 1. Impact of scheduling, planning and design decisions over the time horizon.

As an example, we have the addition or removal of cleaning-in-place (CIP) systems as well as the addition or removal of temperature or sampling systems. Such operations allow for changes in the equipment's suitability so as to perform new process recipe tasks. Doing this, new design and scheduling alternatives are then generated at lower cost and with smaller time consumption.

This problem is addressed in the current paper and has emerged from a real problem that is been addressed by the authors in a chemical-pharmaceutical industry. Unlike the previous research on this topic, that has been addressing the plant design as grassroot or retrofit problems at the global plant level, we consider that performing specific changes in the processing units can be an alternative to tackle scheduling and design problems simultaneously. A Mixed Integer Linear Programming (MILP) model is proposed based on the Resource-Task Network (RTN) representation presented by Pantelides (1994).

The remaining of the paper is structured as follows. We first present the problem definition as well as the modeling framework that is being used. Two ways of modeling the equipment redesign problem are then characterized. One uses the original RTN formulation and the other is an extended RTN formulation. We present the computational results of a scheduling problem motivated by the chemical-pharmaceutical industry under study, where equipment "redesign" is a regular approach when performing the production schedule. We finish the paper with the conclusions and some future work is also suggested.

Problem Definition

As referred above the generic scheduling problem assumes that, when performing scheduling, there must be a perfect match between the tasks requirements and the existent processing units' characteristics. Clearly, this is not easy to do due to the large number of processing units existing in the plant and due to the various recipes requirements. Finding a schedule solution without relaxing any of these inputs is often difficult to accomplish, mainly when the plant operates close to the maximum capacity and when new products are frequently being introduced. In these cases to get feasible schedules usually requires re-negotiating new order due dates with the customers. Nevertheless, new alternatives for the schedules can also be generated with some equipment modifications involving little costs and time.

The use of multipurpose reactors is indeed advantageous in these situations since such units are very flexible and can often perform several tasks. Additionally, their operating range can be increased by doing small equipment modifications. The same reasoning can be applied to all processing units whose suitability to execute tasks can be changed quickly. The redesign problem takes into account the setup-time to perform the equipment modifications and, at the same time, the resources that are needed to do the modification. This approach transforms the processing units into more generic units capable of executing more tasks. From the point of view of the operations this adds flexibility, since more scheduling alternatives can be explored. Such scheduling with equipment redesign is modeled in the present work, and can be described as follows:

Given:

- the RTN representation of the process (tasks and resources);
- the number of processing units available, and their maximum and minimum capacity;
- the scheduling granularity and time horizon;
- the production requirements during the time horizon;
- the auxiliary equipments that can change the suitability of the processing units;
- the cost and setup-time to add and remove auxiliary equipments;

Determine:

- a process schedule such that the processing units suitability change during the time horizon;
- an equipment modification plan to respond to the above schedule, taking into account the setup times for adding and removing the auxiliary equipments and their limited availability;

Minimize:

- the processing units modification costs plus the operational costs, while respecting the delivery due dates.

Problem Modeling

The problem considered here is modeled with a discrete time formulation based on the Resource-Task Network representation proposed by Pantelides (1994). The scheduling of a set of products is performed in a set of existing equipments allowing for modifications in some resources. The set of modifications is identified simultaneously with the definition of the production schedule, within a pre-defined time horizon.

Resource Task Network discrete formulation

The Resource-Task Network representation proposed by Pantelides (1994) involves two types of entities, *tasks* and *resources*. A *task* is an abstract operation that consumes and/or produces a specific set of resources (material, equipment items, utilities, etc.). For the purposes of the discrete time formulation presented in this paper, the time discretisation is made fine enough so that all tasks can be considered to start and end at a time interval boundary. Each task has a fixed duration τ_k and the execution of task k starting at time t is characterised by its "extent" - a pair of variables (N_{kt},ξ_{kt}). N_{kt} is the number of instances (either 0 or 1) of task k starting at time t while, ξ_{kt} is the total amount of material that is processed by all these instances. Resources are produced and consumed at discrete times, during the execution of the task. The amount of resource r produced or consumed by a task k at different times over its duration τ_k can be obtained from the values of the "extent" variables. Changes to the resource utilisation can occur only at interval boundaries. The amount of unused ("excess") resource r, held over time interval t, is denoted by R_{rt}.

As presented by Pantelides (1994) the RTN discrete scheduling problem can be described by the following three types of constraints:

$$R_{rt} = R_{r,t-1} + \sum_{k\in K_r}\sum_{\theta=0}^{\tau_k}\left(\mu_{kr\theta}N_{k,t-\theta} + \upsilon_{kr\theta}\xi_{k,t-\theta}\right) + \Pi_{rt} \qquad \forall r\in R, t\in H \tag{1}$$

$$0 \le R_{rt} \le R_{rt}^{\max} \qquad \forall r\in R, t\in H \tag{2}$$

$$V_{kr}^{\min}N_{kt} \le \xi_{kt} \le V_{kr}^{\max}N_{kt} \qquad \forall r\in E, k\in K_r, t\in H \tag{3}$$

Constraints (1) express resource balancing through the variables R_{rt}, that state the availability of resource r at time t. The amount of resource r consumed and produced at each time is expressed by the integer and continuous part of constraints ($\mu_{kr\Theta}N_{k,t-\Theta}+v_{kr\Theta}\xi_{k,t-\Theta}$). $N_{k,t-\Theta}$ is a binary variable that takes the value 1 if task k starts at time t, and $\xi_{k,t-\Theta}$ indicates the amount of material being produced at each time period, *i.e.*, the batch size. The parameters $\mu_{kr\Theta}$ and $v_{kr\Theta}$ represent the fixed and variable resource consumption/production respectively. Constraints (2) limit the availability the resources to the maximum value $R_{rt}^{\max}$ during the time horizon. And constraints (3) set the batch sizes within the limits of the resource capacity $V_{kr}^{\min}$ and $V_{kr}^{\max}$, where E is the subset of R for the processing units, and K_r is the set of tasks that use resource r.

Equipment redesign problem using the RTN

Applying the existing formulation to the equipment redesign problem requires the explicit representation of all possible modification alternatives. Hence, we need to create new tasks to explicitly take into account all steps required to modify the processing units, *i.e.* to model the addition and removal of auxiliary equipments. This approach will make the network of processing tasks very complex and more difficult to tackle.

Figure 2 shows how the RTN formulation can deal with the equipment redesign problem. To consider the setup time for adding and removing the auxiliary equipment CIP on Reactor1, we need to create two additional tasks (Add_CIP and Remove_CIP), and one extra resource (Reactor1_CIP). This allows us to model the availability of Reactor1 after the modification, *i.e.*, having Reactor1 with a CIP system installed.

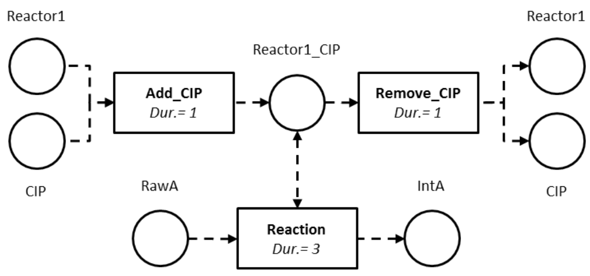

Figure 2. RTN of the equipment redesign problem (reversible modification)

If the modification is irreversible there is no removing task; if the modification is reversible it is necessary to create two tasks: one to add the auxiliary equipment to the processing unit, representing the equipment modification, and another task to remove the previously installed auxiliary equipment, providing the processing unit with its initial suitability. The network of processing tasks requires the explicit representation of all possible combinations of auxiliary equipments (e.g. CIP, sampling devices and temperature systems) and processing units (e.g. reactors, filters, dryers). In the case of the reversible modifications, two additional tasks and one extra resource will be added to the model for each equipment modification needed. For these reasons, the model complexity for representing the problem using the RTN formulation rises. The same obviously happens with the computational time needed to obtain a solution.

Equipment redesign problem using an extended RTN formulation

An alternative approach to tackle this problem is to create two additional sets of binary variables to control when the processing unit needs to be modified in order to be suitable for the task execution, see constraints (4).

$$
\begin{aligned}
R_{rt} = {} & R_{r,t-1} + \sum_{k\in K_r}\sum_{\theta=0}^{\tau_k}\left(\mu_{kr\theta}N_{k,t-\theta} + \upsilon_{kr\theta}\xi_{k,t-\theta}\right) \\
& + \sum_{k'\in K'_r}\sum_{u=0}^{s_{k'}}\left(\lambda_{k'ru}M_{k',t-u} + \gamma_{k'ru}\overline{M}_{k',t-u}\right) \\
& + \Pi_{rt} \qquad \forall r\in R, t\in H
\end{aligned}
\tag{4}
$$

To express the redesign of the processing units, we will use the binary variables M_{kt} and $\overline{M}_{kt}$ that will be equal to 1 if a modification (addition or removal respectively) occurs by means of the task k at the time interval t. The parameter λ_{kru} denotes the resources r that will be consumed (*e.g.*, CIP and Reactor1) by an equipment modification required by a task k during the interval u, once the modification has started. The parameter γ_{kru} denotes the reverse operation. It consumes the modified resource (*e.g.*, Reactor1) and releases back the resources (*e.g.*, CIP and Reactor1). The setup-time required for each modification is given by the parameter s_k. Constraints (1) are modified and a third term is added to reflect this behavior. The $\left(\lambda_{kru}M_{k,t-u}\right)$ expression enforces the modifications to be done by each task k, while the $\left(\gamma_{kru}\overline{M}_{k,t-u}\right)$ part denotes the removal of the auxiliary equipment from the processing units.

The entire formulation also guarantees that the auxiliary equipment cannot be removed during the task execution and that the setup-times s_k for modifying the processing units are respected. K'_r is a subset of K_r that denotes the tasks that require redesign through the resources r. More specifically, for the example given in Figure 2, we get the $\lambda_{Reaction,Reactor1,0} = \lambda_{Reaction,CIP,0} = -1$ and $\lambda_{Reaction,Reactor1,1} = 1$ and $\gamma_{Reaction,Reactor1,0} = -1$ and $\gamma_{Reaction,Reactor1,1} = \gamma_{Reaction,CIP,1} = 1$, see Figure 3.

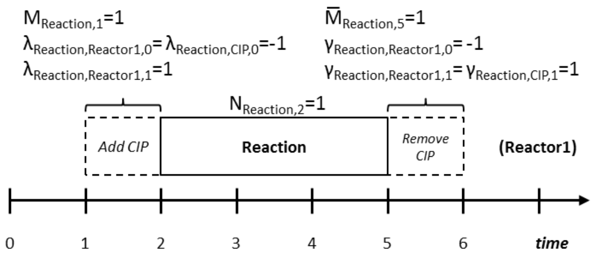

Figure 3. Equipment redesign modeling with the alternative formulation

An additional constraint type is also needed for the correct assignment of the M_{kt} and $\overline{M}_{kt}$ binary variables. Since the equipment modification needs to be done before the task starts, constraints (5) guarantee that the auxiliary equipment has been previously installed. A is the subset of R which has auxiliary equipments needed to modify the processing units, and K_{kr} is the set of tasks that share the auxiliary equipment r.

$$N_{k,t} <= \sum_{\theta=0}^{t} \sum_{k' \in K_{kr}} \left(M_{k',\theta} - \overline{M}_{k',\theta} \right) \quad \forall r \in A, k \in K_r, t \in H \tag{5}$$

When the binary variables N_{kt} are equal to 1, the right hand side of the constraints needs also to be 1, therefore having at that time instant a sum (involving the M_{kt} and $\overline{M}_{kt}$ variables) equal to 1. In practice, this means that the auxiliary equipment needs to be previously consumed by that task, or by other task that was executed in the past and that required the same auxiliary equipment in the same processing unit.

With this formulation, there is no need to explicitly write the modification tasks. Instead two sets of additional binary variables are added to the model to express the addition and removal of auxiliary equipments to the processing units. The resources are still treated uniformly as they are in the original RTN formulation.

Finally, for both formulations the objective function considered in this work is the minimization of the processing units modification costs C_k and, $\overline{C}_k$ as well as the operational costs O_k , see equation (6).

$$\min \sum_{k} \sum_{t} \left(O_k N_{k,t} \right) + \\ \sum_{k \in K'} \sum_{t} \left(C_k M_{k,r,t} + \overline{C}_k \overline{M}_{k,r,t} \right) \tag{6}$$

Case Study

A real world problem from a chemical-pharmaceutical industry is solved using both presented formulations. The company performs the development and production of complex and fine chemicals to the pharmaceutical industry and biotechs. Its core business is the development and manufacture of new active pharmaceutical ingredients (APIs). In this business, the chemical industry is continuously challenged to respond within short time windows. On the one hand, the company needs to manage small batches of under development products and, on the other hand, needs to produce large batches of products in commercialization. Thus, operations flexibility is required to respond to this heterogeneous demand. This adds extra complexity to operations management especially to the planning and scheduling functions.

The product object of our analysis goes through a sequence of tasks such as reaction, precipitation, crystallization, filtration, suspension, drying, quality control and packaging, which can be performed by the following resources: four reactors, one vessel, one filter, one dryer and a packaging room. The typical production time is around ten days. For illustration purposes, we will focus here on the multipurpose reactors since these are the most difficult resources to schedule, thus imposing the schedule of the remaining resources. Devices such as CIP and temperature systems (TS) are considered auxiliary equipments that can be used for the reactors redesign. The reaction, precipitation, crystallization and suspension tasks can either be executed in reactors that do not require modifications but have small capacity, or can be executed in reactors with higher capacity but need to be modified at a certain cost. The product must be delivered at a date and quantity agreed with the customer. The objective is to get the optimal schedule for this product, minimizing the global operation and modification costs, while respecting the product delivery date.

Case Study Results

The scheduling problem was solved for a time horizon of ten days. The time was discretized to one shift of eight hours, which resulted in a scheduling horizon of 30 time intervals (three shifts per day). We have considered an operational cost for each task depending on the processing unit that is used. Tasks that take place in low capacity reactors (capacity of 4,000 liters) have an operational cost of 70 mu (monetary units) and tasks that are performed in high capacity reactors (capacity of 10,000 liters) have a cost of 100 mu. In the course of the recipe production the tasks' characteristics may change requiring the processing units redesign. For instance, precise temperature control is needed on Mixing and Precipitation tasks at Reactor1 and Reactor2, and a CIP system must be available in Reactor2 and Reactor3 when performing Reaction and Stirring tasks, respectively. The costs to modify a reactor with a CIP and TS are, respectively, 3 mu and 5mu. The setup-time to modify the reactors with a CIP is 8 hours, while for a TS is 16 hours. The time required to remove those systems from the reactors in order to restore their original suitability is equal to 8 hours for both auxiliary equipments. One final product delivery of 2 tons is scheduled for the entire schedule horizon. The optimal schedule obtained for our example is depicted in Figure 4. This optimal solution has a value of 2074 mu. Although this test instance is relatively simple, it allows us to understand the tradeoffs existing in the equipment redesign problem, between equipment's suitability and the setup-time and costs to perform the equipments modifications. As can be seen in Figure 4, to respect the delivery date, equipment redesign tasks must take place. To perform the Reaction task in Reactor2 it is necessary to add a CIP, and to do the Precipitation task in this same reactor it is necessary to add a TS. These tasks can be seen at the time interval 0 and 5 of the schedule, respectively. The same reasoning applies to the Mixing task at Reactor1 and to the Stirring task at Reactor3. But note that no auxiliary equipments were defined for the Crystallization task at Reactor2 and for the Cooling task at Reactor3, that nevertheless were modified previously. In the end of this schedule Reactor2 had a TS installed, while Reactor3 had a CIP mounted. The MILP model using Pantelides formulation resulted in 1178 binary variables, 2202 continuous variables and 5085 constraints. Optimality could be proved in 3.15 seconds. The extended formulation has 775 binary variables, 1396 continuous variables, 2853 constraints and reached the optimal solution in 1.78 seconds.

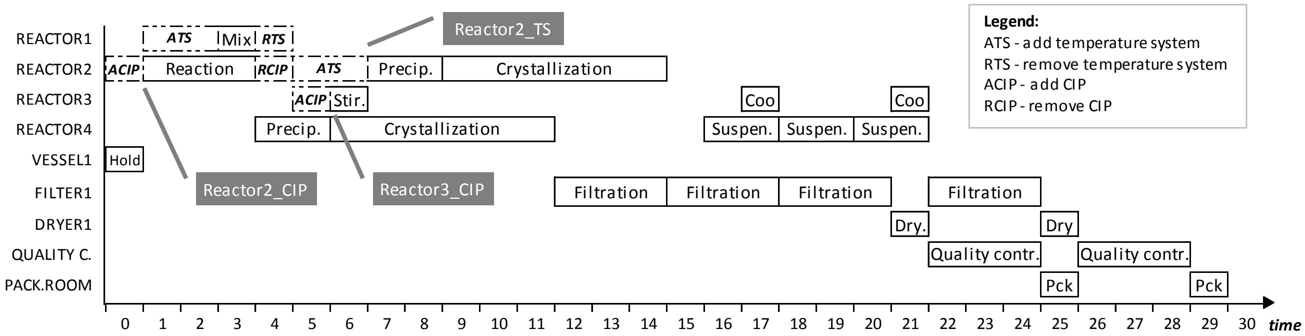

Figure 4. Optimal production schedule with the equipment redesign plan

The model was implemented using ILOG/CPLEX version 12.2 on an Intel Core i7 at 2.67GHz with 4 GB of RAM. The extended formulation has less binary and continuous variables and a smaller number of constraints.

When analyzing these results some disadvantages can be pointed to the original RTN formulation when using it in the redesign problem. It requires the representation of all modification tasks, which results in a complex network of processing tasks. One needs to create additional resources to manage the modified equipments, such as for instance: Reactor2_CIP and Reactor2_TS; these are two additional resources that define Reactor2 modified with a CIP and a TS, respectively. At the same time, since we are assuming the redesign process increases the processing units' suitability such that more tasks can be performed, we must represent all new production alternatives. For instance, the Crystallization task does not require any change on Reactor2, nevertheless if this reactor is modified with a CIP or TS, becoming Reactor2_CIP, Reactor2_TS or Reactor2_CIPTS, we need to create several additional tasks to allow for the possibility of the task being executed in one of these resources. This kind of tasks needs to be created for all resources that can be modified, thus increasing the model size. These drawbacks are overcome in the proposed formulation by replacing the redesign tasks by M_{kt} and $\overline{M}_{kt}$ binary variables. The resulting model is smaller and it is easier to write since it does not require the representation of additional tasks. The redesign tasks are simply modeled by the M_{kt} and $\overline{M}_{kt}$ variables. For that reason, the resulting MILP has less binary and continuous variables. Nevertheless, the use of the M_{kt} and $\overline{M}_{kt}$ variables limits the equipment modification to one auxiliary equipment per task. The possibility of doing more than one modification per task would clearly be an interesting extension of our model.

Conclusions

This paper has addressed a new type of problem that is being faced by the chemical-pharmaceutical industry using multipurpose batch plants, and performing simultaneous design and scheduling within a short period of time. The equipment redesign problem concerns the need to perform changes in the processing units such that their suitability is increased and therefore the units are capable to perform additional tasks. The redesign tasks can be seen as an additional way to increase flexibility of these plants. The redesign problem was formulated using the RTN formulation introduced by Pantelides and an extension to this formulation was also proposed in this work. While the RTN formulation requires the explicit representation of all production alternatives, taking into account the different states of the modified resources, the extension here developed deals with the equipment redesign decisions through two extra groups of binary variables. Preliminary computational results show that the proposed formulation has better performance. The formulation applicability was tested in an industrial example and the achieved results are promising but improvements should be further explored. Namely, it would be interesting to extend the formulation to deal with multiple modifications per task. Also more comprehensive tests need to be performed to further compare the two analyzed formulations.

Acknowledgement

The authors would like to thank Pedro Duarte from Hovione FarmaCiencia SA for his continuous help and gratefully acknowledge the financial support of Hovione and Fundação para a Ciência e Tecnologia under the grant No. SFRH/BD/33970/2009.

References

Barbosa-Póvoa, A. P. (2007). A critical review on the design and retrofit of batch plants. Computers & Chemical Engineering, 31, 833-855.

Castro, P. M., Barbosa-Póvoa, A. P., & Matos, H. A. (2003). Optimal periodic scheduling of batch plants using RTN-based discrete and continuous-time formulations: A case study approach. Industrial & engineering chemistry research, 42, 3346-3360.

Mendez, C. A., Cerda, J., Grossmann, I. E., Harjunkoski, I., & Fahl, M. (2006). State-of-the-art review of optimization methods for short-term scheduling of batch processes. Computers & Chemical Engineering, 30, 913-946.

Pantelides, C. C. (1994). Unified frameworks for optimal process planning and scheduling. In (pp. 253-274): Cache Publications New York.