Optimal Production Planning Models for Parallel Batch Reactors with Sequence-dependent Changeovers

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Abstract

In this paper we address the production planning of parallel multi-product batch reactors with sequence-dependent changeovers, a challenging problem that has been motivated by a real world application of a specialty chemicals business. We propose two production planning models that anticipate the impact of the changeovers in this batch processing problem. The first model is based on underestimating the effects of the changeovers that leads to an MILP problem of moderate size. The second model incorporates sequencing constraints that yield very accurate predictions, but at the expense of a larger MILP problem. In order to solve large scale problems in terms of number of products, reactors or length of the time horizon, we propose a decomposition technique based on rolling horizon scheme and also a relaxation of the detailed planning model. Several examples are presented to illustrate the performance of the proposed models.

Introduction

Batch manufacturing units help companies respond to fluctuating customer demands by being able to shift production between many products. This flexibility however introduces complexity in the production planning process making it hard to assess the true production capacity of these units. Understanding the accurate representation of the capacity of the manufacturing facilities has a significant financial impact since it results in the increased ability to satisfy committed orders and also helps identifying new market opportunities.

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The aim in production planning is to determine the production capacity in terms of high level decisions such as production levels and product inventories for given marketing forecasts, and demands over a long time horizon ranging from several months up to a year. Typically, planning models are linear and simplified representations that are used to predict production targets and material flows. Generally the production targets obtained at this level are overly optimistic since the effect of changeovers is neglected. Changeovers occur when production on one line is changed from one product to another. These changeovers may be associated with changing the operating conditions (temperature, pressure) or with the cleaning of the equipment. If the changeovers are sequence-dependent, then the utilization of the capacity will depend on the sequence in which products are produced on the units. Depending on the magnitude of the changeovers, they can significantly reduce the capacity available for production. Therefore, failing to take into account these change-over times can result in over estimation of the available production capacity and overly optimistic production targets, which may not be realized at the scheduling level. Hence, there is an incentive to develop models and approaches that can accurately represent the available production capacities of assets by accounting for the sequence-dependent changeovers.

Several tactical production models have been proposed that address the problem of determining the available production capacity. As one example McDonald and Karimi (1997) present a multiperiod midterm planning model for semi-continuous processes where the main goal is optimal allocation of assets to production tasks in order to satisfy the fluctuating demands over an extended horizon. Actual timing and sequencing of production campaigns are not determined. However, minimum run lengths are imposed to alleviate the effect of sequence-dependent changeovers. As another example, Bok et al (2000) present a multiperiod planning model for continuous process networks over a short time horizon ranging from 1 week to 1 month. The proposed model incorporates inventory profile, intermittent supplies and production shortfalls. The effect of changeovers is reflected through costs. In order to take into account sequence-dependent change-over costs without increasing the size of the model, the authors adopt one day time periods and enforce the condition that

each process should be operated with exactly one production scheme during each one-day periods.

An alternative approach for addressing the production capacity determining problem could be to formulate a simultaneous planning and scheduling model that spans the entire planning horizon of interest. However, the limitation with this approach is that when typical planning horizons are considered, the size of the detailed scheduling model becomes intractable due to the potential exponential increase in computation. The traditional approach of addressing this issue has been to follow a hierarchical strategy (Bitran and Hax, 1977) in which the planning problem is solved first to define the production targets. The scheduling problem, which is reduced to a sequencing subproblem, is solved next so as to meet the targets set by the planning. The problem with this approach is that a solution determined at the planning level does not necessarily lead to feasible schedules and most of the work that has been reported applies heuristic techniques to overcome the feasibilities that occur in the scheduling problem and does not guarantee global optimal solutions.

Bassett et al (1996) proposed a decomposition scheme for multipurpose batch plants where an aggregate planning problem is solved in the upper level, and detailed scheduling problems are independently solved for each planning period in the lower level. The authors apply heuristic techniques that make use of shifting of operations to overcome the inconsistencies between planning and scheduling. Subrahmanyam et al (1996) proposed a hierarchical decomposition scheme for batch plants, where the planning problem is updated at each iteration by disaggregating the aggregate constraints for all infeasible scheduling subproblems within the planning problem. Stefansson et al (2006) proposed a planning and scheduling approach based on a hierarchically structured moving horizon framework for multipurpose batch plants. On each level of the hierarchically structured framework, they propose optimization models to provide support for relevant decisions where each level differs regarding the scope and availability of the information. A second method for dealing with the computational difficulties is to use aggregation of constraints. Wilkinson et al (1996) used such an approach to obtain approximate solutions to the large scale production and distribution planning problems for multi-site production sites that are represented with Resource Task Network (Pantelides, 1994). In the proposed approach the authors split the planning horizon into smaller portions denoted as the aggregated time periods (ATP). They describe each ATP by aggregated variables each of which is equivalent to a weighted sum of the corresponding detailed variables over the time intervals. The aggregate formulation is then generated by replacing groups of related variables from the detailed formulation with corresponding aggregated variables in order to reduce the size of the problem. Birewar and Grossmann (1990) proposed a multiperiod linear programming (LP) formulation for the simultaneous planning and scheduling of multiproduct batch plants with flowshop structure. In this formulation, the batches that belong to the same products are aggregated and sequencing considerations are accounted for at the planning level by approximating the makespan with the cycle time. Another approach for addressing the simultaneous planning and scheduling problem is the bi-level decomposition. Erdirik-Dogan and Grossmann (2006) have proposed a bi-level decomposition algorithm where they decompose the original detailed model into an upper level planning and a lower level planning and scheduling problem. Since the former yields an upper bound and the latter a lower bound, convergence is achieved when the bounds lie within a given tolerance. Finally, a recent approach by Sung and Maravelias (2007) consists in using the production attainable region (PAR) framework for production planning problems. These authors propose replacing the scheduling models (e.g. STN model) with an approximation of the feasible region in which the scheduling model is projected onto relevant planning variables such as production flows using a numerical procedure for finding convex hulls.

This paper has been motivated by a real-world application in the Dow Chemical Company. The specific goal is to propose multiperiod MILP models for planning of parallel multiproduct batch reactors that anticipate the impact of sequence-dependent changeovers as accurately as possible, while determining production levels, inventory levels and allocation of products to available equipment. We also investigate solution strategies such as rolling horizon approach and relaxation of the detailed planning model for reducing the computational expense of large problems. The paper is organized as follows. In the following section the problem definition is presented. We then introduce the relaxed planning model where the effects of the changeovers are underestimated. In section 3, we describe the detailed planning model that incorporates sequencing constraints. The rolling horizon decomposition algorithm and the relaxed detailed planning model are presented in section 4. Finally, the application of the proposed models is illustrated with several examples.

1. Problem Statement

The problem we will address in this paper is as follows (see Figure 1). Given is a plant that contains batch reactors that operate in parallel. The batch reactors are to be used to manufacture intermediates and final products. A subset of the final products is produced in a single reaction stage, while the remaining final products require intermediates, thus involving two reaction stages. Each final product is fed to a dedicated storage tank. In order to formulate this problem we assume that we are given the products each reactor can produce, as well as the batch times and batch sizes for each product and the corresponding reactor. While the batch times and batch sizes are fixed, the number of batches of each product is a variable that is to be determined. Sequence-dependent changeover times and the total time each reactor is available in each month are given. Given are also raw material costs and availability, and storage tanks with associated capacities. Given is also a production horizon composed of a certain number of time periods given by due dates in which demands are specified as lower bounds. The problem is to determine the optimal production plan in terms of monthly production quantities and inventory levels so as to maximize the profit.



Figure 1. Representation of the problem

2. Relaxed Planning Model (RP)

We first propose an aggregate planning model that is based on a network that involves two type of nodes: one for tasks i and one for products j. The nodes are connected with streams that represent the flow of material. Each task i is characterized by a main product j. However, each product j can be consumed by other tasks i.

This model is based on the idea of ignoring detailed timing constraints and sequencing constraints, while accounting for some lower bounds for the changeovers for each assigned product. The goal of the planning model is to determine the optimal production quantities for each unit over a long range horizon (6-12 months), while taking into account the unit capacities, raw material availabilities, raw material costs, product prices and storage capacities. The decisions that we are concerned with are (i) the assignment of task i to unit m at each time period t, $YP_{i,m,t}$, (ii) number of each batches of each task i in each unit m at each period t, NB_{imt} , (iii) corresponding amount of material processed by each task i, FP_{imt} , and (iv) inventory levels of each product j at each time period t, INV_{ji} . The objective is to select these decisions in order to maximize profit in terms of sales minus inventory, operating and changeover costs.

The MILP model (RP) for the production planning problem is as follows:

a) Material handled and capacity requirements:

$$FP_{imt} \le Bound_{imt} \cdot YP_{imt} \quad \forall i \in I_m, m, t \tag{1}$$

The amount of material that will be carried out by task i in unit m at time period t is limited by the maximum batch capacity times the largest number that the task can be repeated (H_t/BT_{im}) , which leads to $Bound_{imt} = H_t \cdot Q_{im}/BT_{im}$. Note that constraint (1) forces the batch size to be zero if task i is not assigned to unit m at time t. The batch size of each task in each equipment is fixed to Q_{im} . Therefore, the amount of material consumed or produced by task i to unit m during time t, has to be at least the capacity of the unit m when processing task i.

$$FP_{int} \ge Q_{int} \cdot YP_{int} \quad \forall i \in I_{m}, m, t$$
⁽²⁾

b) Number of batches of each product:

$$NB_{i,m,t} = FP_{i,m,t} / Q_{i,m} \quad \forall i \in I_m, m, t$$
(3)

Constraint (3) determines the total number of batches of each task performed by the corresponding task in each unit at each time period. It should be noted that in the above inequality it is important to treat $NB_{i,m,t}$ as an integer variable in order to predict tighter bounds of the objective function in (11).

c) Mass Balances on the state nodes

We define set PS(j) to be the index set of tasks i that produce product j, and CS(j) as the index set of tasks i that consume product j. Then the mass balance is given by constraint (4), where for each product j the total amount of purchases plus the amounts produced within the network must be equal to the sum of sales, and the total consumption within the network plus the change in the inventory level.

$$P_{jt} + \sum_{i \in PS_j} \rho_{ji} \sum_{m \in M_i} FP_{imt} = S_{jt} + \sum_{i \in CS_j} \overline{\rho}_{ji} \sum_{m \in M_i} FP_{imt} + INV_{jt} - INV_{jt-1} \quad \forall j, t$$
(4)

We should note that since the detailed timing of production is neglected, the mass balances are handled in an aggregate manner. For products that are produced in two stages, the model makes sure that the mass balance holds within each time period. However, the model does not guarantee the assignment of the intermediate product required for the production of the end product before the assignment of the end product.

d) Demands

$$S_{j,t} \ge D_{j,t} \quad \forall j,t \tag{5}$$

Constraint (5) is added to ensure that demands that vary throughout the planning horizon are met and that the production may be exceeded.

e) Changeover times and costs

In this model, detailed timing constraints and sequencing constraints are ignored, and therefore exact changeover times and costs are not computed. However, the idea here is to account for lower bounds for changeovers by selecting a minimum changeover time for each assigned product so that the knowledge of the exact sequence is not required. This model yields tighter production estimates than a simpler model that totally ignores the changeovers.

We define the parameter $TR_{i,m} = \underset{i,i' \in IM(m), i' \neq i}{Min} \{\tau_{i,i',m}\}$ as the minimum changeover time for each product i, which is added to the processing time for each assigned product for each unit, for each time period. As an example, consider Figure 2 in which products A, B and C are



Figure 2. Assignments of products and minimum changeover times

$$\sum_{i \in I_m} NB_{i,m,t} \cdot BT_{i,m} + \sum_{i \in I_m} TR_{i,m} \cdot YP_{i,m,t} \le H_t \qquad \forall m,t$$
(6)

Constraint (6) defines the time balance such that the summation of the batch times of the assigned products plus the summation of the minimum changeover times for the assigned products must be less than or equal to the available time for reactor m at time period t. Note, however, that since we do not know the exact sequence of production at each time period, we cannot predict whether the production on the line at the end of each time period has been changed to another product or not. For cases where the last product of time period t and first

product of the subsequent period t+1 corresponds to the same product, constraint (6) results in an overestimation of the changeover times (See Figure 3).



Figure 3. Overestimation of changeover times

In order to avoid this overestimation, we neglect the changeover times across adjacent weeks. In this way, the total number of changeovers assigned will be equal to the total number of products minus one. Therefore, the maximum of the minimum changeover times should be subtracted from constraint (6), as is shown in constraints (7) and (8).

$$U_{m,t} \ge TR_{i,m} \cdot YP_{i,m,t} \quad \forall i \in I_m, m, t \tag{7}$$

$$U_{m,t} \le \max_{i \in I_m} \left\{ TR_{i,m} \right\} \quad \forall m,t$$
(8)

$$\sum_{i \in I_m} NB_{i,m,t} \cdot BT_{i,m} + \sum_{i \in I_m} TR_i \cdot YP_{i,m,t} - U_{m,t} \le H_t \qquad \forall m,t$$
(9)

In this way, according to constraint (9), the summation of the batch times of the assigned products plus the summation of the minimum changeover times for each assigned product minus the maximum of the minimum changeover times should be less than or equal to the total available time.

$$U_{m,t} \leq \sum_{i \in I_m} TR_i \cdot YP_{i,m,t} \quad \forall m,t$$
(9a)

Note that constraint (9) can lead to weak relaxations for widely different values of the minimum changeover times of the assigned products. In order to tighten the formulation we introduce constraint (9a). Constraint (9a) makes sure that maximum of the minimum change over times is less than the summation of the minimum changeover times of the assigned products.

Constraints (10a) and (10b) are introduced to account for the changeover costs and they are developed in analogy to constraints (7), (8) and (9). We define $TRC_{i,m} = \underset{i,i' \in M(m), i' \neq i}{Min} \left\{ C_{trans_{i,i'm}} \right\}$ to

be the minimum changeover cost for each task assigned to unit m during time t.

$$UT_{m,t} \ge TRC_{i,m} \cdot YP_{i,m,t} \quad \forall i \in I_m, m, t$$
(10a)

$$UT_{m,t} \le \max_{i \in I_m} \left\{ TRC_{i,m} \right\} \quad \forall m,t$$
(10b)

The term $\sum_{t} \sum_{m} (\sum_{i \in I_m} (TRC_{i,m} \cdot YP_{i,m,t}) - UT_{m,t})$, which is an underestimation of the changeover

costs, is then subtracted from the objective function.

$$UT_{m,t} \le \sum_{i \in I_m} (TRC_{i,m} \cdot YP_{i,m,t}) \quad \forall m,t$$
(11)

Finally, we introduce constraint (11) to tighten the formulation. Constraint (11) ensures that the maximum of the minimum changeover costs is less than the summation of the minimum changeover costs of the products that are assigned to unit m during time period t.

f) Objective function

The profit is given by the sum of sales revenues, the inventory costs, the operating costs, the changeover costs within each time period.

$$Max \qquad Z^{RP} = \sum_{j} \sum_{t} cp_{jt} \cdot S_{jt} - \sum_{j} \sum_{t} c^{inv}_{jt} \cdot INV_{jt} - \sum_{i \in I_m} \sum_{m} \sum_{t} c^{oper}_{it} \cdot FP_{imt} - (\sum_{t} \sum_{m} (\sum_{i \in I_m} TRC_{i,m} \cdot YP_{i,m,t}) - UT_{m,t})$$
(12)

Remarks:

- 1. The relaxed planning model described by constraints (1)-(12) assumes sequence independent changeovers resulting in underestimation of changeover times and costs.
- 2. Due to the underestimation of the effect of the changeovers, (RP) can result in overestimation of the available production capacities. However, being a low dimensional model (compared to the detailed planning model), it has the advantage of requiring lower computational efforts.

3. Detailed Planning Model (DP)

Although the relaxed planning model (RP) accounts for the lower bounds of the changeover times, for scenarios with high demand rates where the capacity utilization becomes

significant, or for the scenarios where the difference of the changeover times is high, (RP) might lead to a significant overestimation of the available production capacity. Therefore, we propose the detailed planning model (DP), which is in essence similar to the (RP) model. However, instead of accounting for only lower bounds of the changeovers as in constraint (9), we account for sequence-dependent changeovers by introducing sequencing constraints without determining the detailed timings of the tasks. Hence, the assignment constraints and the mass balances are the same as the (RP) model, but in order to handle the sequence-dependent changeovers, we introduce new sequencing variables and constraints that yield more accurate estimations for changeovers in the time balance constraint and the objective function will be modified.

The MILP model (DP) is as follows:

a) Material handled and capacity requirements:

$$FP_{imt} \le Bound_{imt} \cdot YP_{imt} \qquad \forall i \in I_m, m, t \tag{1}$$

$$FP_{imt} \ge Q_{im} \cdot YP_{imt} \qquad \forall i \in I_m, m, t$$
⁽²⁾

b) Number of batches of each product:

$$NB_{i,m,t} = FP_{i,m,t} / Q_{i,m} \qquad \forall i \in I_m, m, t$$
(3)

c) Mass Balances on the state nodes

$$P_{jt} + \sum_{i \in PS_j} \rho_{ji} \sum_{m \in M_i} FP_{imt} = S_{jt} + \sum_{i \in CS_j} \overline{\rho}_{ji} \sum_{m \in M_i} FP_{imt} + INV_{jt} - INV_{jt-1} \quad \forall j, t \quad (4)$$

d) Demands

$$S_{j,t} \ge D_{j,t} \quad \forall j,t \tag{5}$$

e) Changeover times and costs:

In order to account for the sequence-dependent changeover times and costs, we propose to find the minimum changeover time sequence within the assigned products within each time period, while maximizing the profit and satisfying the demands at the due dates. In this way, the determination and allocation of number of batches of each task and their sequencing are determined simultaneously. The idea for the sequencing is to generate a cyclic schedule within each time period that minimizes changeover times amongst the assigned products, and then to determine the optimal sequence by breaking one of the links in the cycle as described in Birewar and Grossmann (1990). As will be seen, the proposed sequencing constraints can be regarded as a relaxation of the traveling salesman problem (Nemhauser and Wolsey, 1988).

To generate a cyclic schedule, the decisions to be made concern the sequence of production that is represented by the binary variable $ZP_{ii'mt}$, which becomes 1 if product i precedes product i' in unit m at time period t, and zero otherwise. To obtain a specific sequence, the location of the link to be broken is determined with, $ZZP_{ii'mt}$, which becomes 1 if the link between products i and i' is to be broken, otherwise it is zero (see example in Figure 4).



Figure 4. Cylic schedule and the location of the link to be broken.

The following logic constraints are proposed for generating a cyclic schedule within each time period:

$$YP_{imt} \Leftrightarrow \bigvee_{i'} ZP_{ii'mt} \qquad \forall i \in I_m, m, t$$
(13)

$$YP_{i'mt} \Leftrightarrow \bigvee ZP_{ii'mt} \qquad \forall i' \in I_m, m, t \tag{14}$$

According to logic proposition (13), product i is assigned to unit m during period t if and only if there is exactly one transition from product i to product i' in unit m at time period t. Similarly, according to proposition (14), product i' is assigned to unit m at period t if and only if there is exactly one transition from any product i to product i' in unit m at time period t. These constraints can be mathematically written as follows (see also Sahinidis and Grossmann, 1990):

$$YP_{imt} = \sum_{i'} ZP_{ii'mt} \qquad \forall i \in I_m, m, t$$
(15)

$$YP_{i'mt} = \sum_{i} ZP_{ii'mt} \qquad \forall i' \in I_m, m, t$$
(16)

Constraints (15) and (16) will generate a cyclic schedule within each time period provided no subcycles are obtained. The total number of links (changeovers), *NL*, within each cycle will be equal to the total number of products assigned to that time period. According to the location of the link that is to be broken, a total of *NL* different schedules can be generated from each cycle. In order to determine the optimal sequence amongst the *NL* possible sequences, the cycle will be broken at the link with the highest changeover time. We introduce the binary variable ZZP_{iimit} to represent location of the link to be broken to obtain the specific sequence (see example in Figure 5).



Figure 5. Derivation of the schedule.

Equation (17) states that exactly one of the links in the optimal cycle can be broken.

$$\sum_{i \in I_m} \sum_{i' \in I_m} ZZP_{ii'mt} = 1 \qquad \forall m, t$$
(17)

Also, according to inequality (18), a link cannot be broken if the corresponding pair is not selected in the cycle.

$$ZZP_{ii'mt} \le ZP_{ii'mt} \qquad \forall i, i' \in I_m, m, t \tag{18}$$

We should note that if the cyclic schedule implied by (13)-(14) has no subcycles then constraints (15)-(18) will lead to a sequence in which the changeovers are exactly taken into account. In the case when there are subcycles, these constraints will lead to subsequences as seen in Figure 6. While these will not correspond to a complete feasible sequence, they do correspond to a valid lower bounding representation for the changeover times, which in turn leads to a valid upper bound to the profit. Since in the planning model we are not concerned with detailed scheduling, this does not pose any difficulty.





Figure 6. Subcycles leading to a valid upper bound

We should also note that in constraints (15) and (16), products i and i' may correspond to the same product. Forcing i and i' to be different would lead to infeasible schedules for the cases where only a single product is assigned to unit m in time period. On the other hand, allowing the constraints to hold true for i = i', would yield schedules consisting of self loops (see example in Figure 7) as this leads to zero change-over times, and consequently to a more optimistic bound for the profit.



Figure 7. Subcycles for multiple products

In order to overcome the above difficulty, we introduce the following expression where we allow a self changeover (a product followed by the same product) if and only if that product is the only product assigned to that unit during that time period. That is,

$$YP_{imt} \wedge \left[\bigwedge_{i \neq i} \neg YP_{i'mt}\right] \quad \Longleftrightarrow \quad ZP_{iimt} \quad \forall i \in I_m, m, t$$
(19)

According to expression (19), if product i is assigned in unit m at time period t, and none of the products i' different than i are assigned in the same unit at the same time period, then product i can be followed by product i. Also, if product i is followed by product i in unit m at period t, then only product i is assigned in unit m for period t and none of the products i' other than i are assigned to the same unit at the same time period. The expression in (19) can be written mathematically as follows:

$$YP_{imt} \ge ZP_{i,i,m,t} \qquad \forall i \in I_m, m, t$$
(20)

$$ZP_{i,i,m,t} + YP_{i',m,t} \le 1 \qquad \forall i, i' \in I_m, i' \neq i, m, t$$

$$\tag{21}$$

$$ZP_{i,i,m,t} \ge YP_{i,m,t} - \sum_{\substack{i' \neq i \\ i' \in I_m}} YP_{i',m,t} \qquad \forall i \in I_m, m, t$$
(22)

The total changeover time within each period, $TRNP_{m,t}$, is then given by the summation of the changeover times corresponding to each existing pair $(ZP_{i,i',m,t})$ minus the changeover time corresponding to the link that is broken from the sequence $(ZZP_{i,i',m,t})$.

$$TRNP_{m,t} = \sum_{i \in I_m} \sum_{i' \in I_m} \tau_{i,i'} \cdot ZP_{i,i',m,t} - \sum_{i \in I_m} \sum_{i' \in I_m} \tau_{i,i'} \cdot ZZP_{i,i',m,t} \qquad \forall m,t$$
(23)

Note that changeover costs are assumed to be directly proportional to changeover times. Furthermore, the variable $ZZP_{i,i',m,t}$ has a negative coefficient in the time balance and a positive coefficient in the objective function. Therefore, the model will choose the link corresponding to the pair with the highest changeover time as the link to break the optimal cycle. Therefore, the optimal sequence obtained at each time period will correspond to the sequence with the minimum changeover times.

In order to be able to account for the changeover times and costs across adjacent weeks, we need to determine the first and last element of each sequence obtained at each time period. These elements correspond to the pair where the cycle is broken to form the sequence. According to their relative position in the cycle, the head of the cycle will correspond to the first element and the tail will correspond to the last element (see example in Figure 8).



Figure 8. First and last elements of the sequence

Defining the binary variables $XF_{i,m,t}$ and $XL_{i,m,t}$ for the first and last tasks in the sequence, the implication in (24) states that if at least one of the links that point from any product i to product i' is broken, then product i' becomes the first product in the optimal sequence obtained for unit m during time period t. Similarly, according to the implication in (25) if at least one of the links pointing from product i to any product i' is broken, then product i becomes the last product in the optimal sequence obtained for unit m during time period t. Note that with constraint (17), we guarantee that in each unit during each time period, exactly one link in the cycle can be broken.

$$\bigvee_{i \in I_m} ZZP_{i,i',m,t} \Longrightarrow XF_{i',m,t} \qquad \forall i' \in I_m, m, t$$
(24)

$$\bigvee_{i'\in I_m} ZZP_{i,i',m,t} \Longrightarrow XL_{i,m,t} \qquad \forall i \in I_m, m, t$$
(25)

The implications in (24) and (25) can be expressed mathematically as follows:

$$XF_{i',m,t} \ge \sum_{i \in I_m} ZZP_{i,i',m,t} \qquad \forall i' \in I_m, m, t$$
(26)

$$XL_{i,m,t} \ge \sum_{i' \in I_m} ZZP_{i,i',m,t} \qquad \forall i \in I_m, m, t$$
(27)

Furthermore, exactly one product must be the first to be processed, and exactly one product must be the last to be processed. This is represented with constraints (28) and (29).

$$\sum_{i \in I_m} XF_{imt} = 1 \qquad \forall m, t \tag{28}$$

$$\sum_{i \in I_m} XL_{imt} = 1 \qquad \forall m, t \tag{29}$$

Note that if only one type of product is assigned, then that product gets to be both the first and the last product.

The changeover time across adjacent time periods depends on the last product of the current time period, XL_{imt} , and the first product of the next time period, $XF_{i'mt+1}$ (see example in Figure 9).



Figure 9. Changeovers across adjacent time periods

Constraint (30) defines the sequence-dependent changeover variable $ZZZ_{i,i',m,t}$ which becomes 1 if product i at time t is followed by product i' at time t+1 in unit m. Since the changeover

costs are minimized in the objective function, the variable $ZZZ_{i,i',m,t}$ can be treated as continuous, $0 \le ZZZ_{i,i',m,t} \le 1$.

$$ZZZ_{i,i',m,t} \ge XL_{i,m,t} + XF_{i',m,t+1} - 1 \quad \forall i,i' \in I_m, m,t \in T - \{\overline{t}\}$$

$$(30)$$

Another way of enforcing the same condition is to use the following set of constraints (Sahinidis and Grossmann, 1990):

$$\sum_{i'\in I_m} ZZZ_{i,i',m,t} = XL_{i,m,t} \quad \forall i \in I_m, m, t$$

$$\sum_{i\in I_m} ZZZ_{i,i',m,t} = XF_{i',m,t+1} \quad \forall i' \in I_m, m, t \in T - \{\overline{t}\}$$
(30a)
(30b)

According to (30a), exactly one changeover occurs from product i at the end of time period t in unit m, if and only if i is the last produced last at time period t. Similarly, according to (30b), exactly one changeover to product i' occurs at the beginning of time period t+1 in unit m if and only if product i' is produced the first at time period t+1 in unit m. Constraints (30a) and (30b) yield a tighter formulation than constraint (30), and require fewer constraints.

Finally, the following constraint corresponds to the time balance. It states that the total allocation of production times plus the total changeover time within that time period (constraint 23) plus the changeover time to the adjacent period (constraints 30a and 30b) cannot exceed the available time for each unit.

$$\sum_{i \in I_m} NB_{i,m,t} \cdot BT_{i,m} + TRNP_{m,t} + \sum_{i \in I_m} \sum_{i' \in I_m} ZZZ_{i,i',m,t} \cdot \tau_{ii'} \le H_t \qquad \forall m,t$$
(31)

f) Objective function

$$Max \quad Z^{p} = \sum_{j} \sum_{t} cp_{jt} \cdot S_{jt} - \sum_{j} \sum_{t} c_{jt}^{inv} \cdot INV_{jt} - \sum_{i \in I_{m}} \sum_{m} \sum_{t} c_{it}^{oper} \cdot FP_{imt}$$
$$- \sum_{i \in I_{m}} \sum_{i' \in I_{m}} \sum_{m} \sum_{t} c_{i,i'}^{trans} \cdot (ZP_{i,i',m,t} - ZZP_{i,i',m,t} + ZZZ_{i,i',m,t})$$
(32)

The last term of the objective function stands for the changeover costs: the first term in the summation accounts for the changeover costs within each cycle, the second term stands for

the changeover cost of the link that was broken, and the last term stands for the changeover costs of the changeovers that occur across adjacent weeks.

Remarks:

1. For the cases where all the products are produced in a single stage and there are no subcycles, the detailed planning model yields the exact scheduling solution since the information of the timing of the individual batches is not required for this case.

2. As was pointed out before, the formulation of the DP model given by equations (1)-(4), (12)-(31), might exhibit subcycles. In this case although no complete sequences are obtained, constraints (15)-(18) represent a relaxation and hence a valid bounding representation. The upper bound on the profit, however, will be higher compared to the case where there are no subcycles since the corresponding solution will result in an underestimation of the actual changeover times. Subcycles could be eliminated by the introduction of subtour elimination constraints as described in Birewar and Grossmann (1990).

3. Each cycle is broken at the link corresponding to the highest changeover time within that cycle. This is ensured by the fact that changeover times are directly proportional to changeover costs and also the variable responsible from breaking the cycle ($ZZP_{i,i',m,t}$) has a positive coefficient in the objective function.

4. The proposed detailed planning model (DP) is significantly larger in size than the relaxed planning model (RP) (see the examples in section 5), but predicts tighter upper bounds on the profit.

6. Minimum number of batches can be imposed by the following constraint:

$$NB_{i,m,t} \ge MRL_i \cdot YP_{i,m,t} \quad \forall i \in I_m, m, t$$
(33)

where *MRL* is the parameter denoting the minimum number of batches.

4. Solution Strategies

The MILP models presented in the previous sections can be solved directly with branch and bound enumeration procedures. For large problems and long time horizons, however, the computational expense for solving the detailed planning (DP) model can be high. Therefore, we consider as alternative a rolling horizon algorithm and also a relaxed version of the detailed planning model.

4.1. Rolling Horizon Approach

In this section, we describe a forward rolling horizon algorithm, which is a heuristic approach used to reduce the computational expense for solving the detailed planning model. Instead of solving the entire planning horizon with the detailed planning model, we decompose the problem into a sequence of sub-problems that are solved recursively (Dimitriadis et al, 1997). In each sub-problem only the initial part of the horizon is modeled with the detailed planning model (DP) and the rest of the horizon is modeled with the relaxed planning model (RP). The solution of the detailed part is then fixed giving rise to the next sub-problem.

As shown in Figure 10, with each sub-problem the time periods covered by the detailed model grows successively whereas the time periods covered by the relaxed model shrinks. The computational cost of the problem is kept low despite the growing DP blocks by fixing the binary variables for the assignment and sequencing to their optimal values obtained in previous sub-problems. This recursive scheme continues until the entire planning horizon is solved with DP.



Figure 10. Rolling horizon algorithm

Although it is possible to fix all the continuous and the binary variables to their optimal values obtained in previous sub-problems, we fix only the binary variables responsible from the assignment, YP_{int} , and the sequencing, $ZP_{ii'nt}$ in order to reduce infeasibilities.

Another decision concerns the length of the planning horizon that will be solved by the detailed planning model in each sub-problem. Depending on the computational effort required to solve the detailed planning models, a two period (week) rolling horizon or a three period (week) rolling horizon approach might be adopted instead of one in order to increase the accuracy of the solution (see Figure 11).



Figure 11. Rolling horizon with (a) two periods, (b) three periods

We should note that the sequence-dependent changeovers across adjacent periods are accounted for within each detailed time block. However, they are neglected at the boundary between the detailed time block and the aggregated time block.

4.2. Relaxed Detailed Planning Model

The relaxed planning model (DP*) is in essence the same with the detailed planning model which was described with constraints (1)-(5), (15)-(18), (20)-(23), (26)-(29), (30a)-(30b), (31-33) with the exception that in (DP*) we declare the variable number of batches ($NB_{i,m,t}$) to be continuous variables as opposed to integer variables. Since we are maximizing the profit, (DP*) will yield a valid upper bound on the profit. And as will be seen by the results, declaring the variable $NB_{i,m,t}$ as continuous variables can significantly reduce the computational expense.

5. Examples

The application of the proposed models RP, RP*, DP, DP* and the rolling horizon algorithm (RH) will be illustrated with examples. Model RP is described by constraints (1)-(9), (9a), (10a)-(11b), (11), (12) and (33) where as in model RP* we eliminate constraints (9a) and (11). Models DP and DP* on the other hand involve constraints (1)-(5), (15)-(18), (20)-(23), (26)-(29), (30a)-(30b), (31)-(33). For the representation of the rolling horizon algorithm (RH), (DP) is used for representing the detailed blocks whereas (RP*) is used to denote the aggregate blocks.

In this section we present four different examples, with the last example corresponding to an industrial-sized problem. It should be noted that all the models presented in this paper have been implemented in GAMS 22.3 and solved with CPLEX 10.1 on an 2X Intel Xeon 5150 at 2.66 GHz machine. The data for Example 1 is given in Appendix A and the data for all the other examples are available upon request. It is also interesting to note that no subcycles were obtained in any of the examples.

Example 1

This example consists of five different products, A-E to be processed on two reactors. Each reactor can process only a subset of products (see Figure 12). Namely reactor R1 can process products A, B and E, whereas reactor R2 can process products C and D. All the products except product B are produced in a single stage, whereas product B requires product a as an intermediate.



Figure 12. Schematic representation of Example 1

Example 1a.

The model and solution statistics for a planning horizon of 6 weeks for detailed planning model (DP), detailed planning model with continuous number of batches (DP*), relaxed planning (RP) and rolling horizon (RH) is given in Table 1. The first three columns indicate the problem sizes in terms of number of binary variables, number of continuous variables and number of equations. The fourth column shows the CPU s and the last column shows the profit that was obtained. All of the solutions presented in Table 1 are obtained for a 0% optimality tolerance. The detailed planning model (DP) yields a profit of \$4,599,724 in 9 CPUs whereas the relaxed planning model overestimates the profit by 53.4% to \$7,057,649 due to underestimating the changeover times and costs. Relaxing the integer number of batches condition (DP*) resulted in 6.82% overestimation in profit yielding a profit of \$4,913,459. For the application of the rolling horizon algorithm, the length of the detailed time block is selected as 2 weeks and thus the problem is solved in 3 iterations. As can be seen from Table 1, the rolling horizon resulted in the exact solution as the detailed planning model (DP). Note that the size reported for the rolling horizon algorithm corresponds to the size of the third iteration, in other words to the last iteration. Since at each iteration we do not fix all variables, but only the binary variables representing the assignments and the sequence within each week, the total number of constraints in the last iteration is the same as the detailed model. However, there is a slight decrease in the number of variables.

	number of	number of	number of	time	solution
method	binary variables	continuous variables	equations	(CPU s)	(\$)
detailed planning (DP)	276	452	567	9	4,599,724
detailed planning (DP*)	246	452	567	7.5	4,913,459
relaxed planning (RP)	60	175	289	0.64	7,057,649
rolling horizon (RH)	204	444	567	1.5	4,599,724

Table 1. Model and Solution Statistics of Example 1 for 6 Weeks of Planning Horizon

*continuous number of batches

Table 2. Objective Function Cost Items for Example 1 for 6 Weeks

	detailed	detailed	relaxed	rolling
(\$)	planning	planning *	planning	horizon
sales	10,187,300	10,771,300	11,809,100	10,187,300
operating costs	3,806,240	3,974,750	4,368,080	3,806,240
inventory costs	31,336	33,091	23,371	31,336
transition costs	1,750,000	1,750,000	360,000	1,750,000



Figure 13. Objective function terms for Example 1 for 6 Weeks

In Table 2, the objective function cost items in (\$) are shown for the proposed models and the rolling horizon algorithm (see also Figure 13). As can be seen from Table 2, the relaxed planning model overestimates the sales by 16%, and underestimates the changeover costs by 80% compared to the detailed model. If we are to analyze the results obtained by (DP*), we can see that (DP*) overestimates the sales by 6% due to non-integer number of batches whereas it yields the exact changeover costs as the detailed planning model (DP).



Figure 14. Optimal schedule generated by (DP) for Example 1a

Figure 14 shows the number of batches of each product and the optimal sequence predicted for each time period in each unit. The solution did not exhibit any subcycles. Note, however, that despite the fact that product B required product A as an intermediate and that the initial inventory level for product A was zero, product B was assigned before product A. This is due to the fact that the mass balances are handled in an aggregate manner and the model tends to minimize the total changeover times and costs. Although the model ensures that the mass balances hold within each time period, it does not guarantee the assignment of the intermediate before the end product. Therefore, the schedule obtained by the detailed model does not correspond to a feasible schedule.

Example 1b.

This example is essentially the same as Example 1b except for the extension of the planning horizon to 12 weeks. Table 3 shows the model and solution statistics for this example, whereas Table 4 shows the objective function items in terms of sales, operating costs, inventory costs and changeover costs. Once again the solutions reported for Example 1b were obtained for a 0% optimality tolerance. The detailed planning model yielded a solution of \$9,501,060 in 153 CPUs, which is 51% more accurate than the result obtained from the relaxed planning model, but with the expense of increasing the solution time 10 times and increasing the number of variables 3 times. While (DP*) overestimates the total profit by 7% compared to (DP), its computational requirements were reasonable. The rolling horizon algorithm on the other hand overestimated the total profit by only 2%, while reducing the CPU time by a factor of 7.

method	number of binary variables	number of continuous variables	number of equations	time (CPU s)	solution (\$)
detailed planning (DP)	552	908	1143	153	9,501,060
detailed planning (DP*)	492	908	1143	29.89	10,120,472
relaxed planning (RP)	120	349	577	14.76	14,351,686
rolling horizon (RH)	372	900	1143	22.8	9,343,221

 Table 3. Model and Solution Statistics of Example 1 for 12 Weeks of Planning Horizon

Figure 15 shows the cost items in (\$) for (DP), (DP*), (RP) and (RH). Note that, underestimating the effects of the changeovers in the relaxed planning model resulted in 11% overestimation in the total sales value and 83% underestimation in the changeover costs compared to the detailed planning model.



Figure 15. Objective function terms for Example 1 for 12 Weeks

Example 1c.

Table 5 shows the results for the same 5 products, 2 reactors example for a time horizon of 24 weeks. For 0% optimality gap the detailed planning model yielded a profit of \$17,939,396 in 22,000 CPUs; when the optimality gap is set to 5% it yields a profit of \$17,570,013 in 279 CPUs.

In the last row of Table 5, we show the results of the relaxed planning model (RP*) when none of the tightening constraints (9a), (9b) and (11) are added to the model.

	number of	number of	number of	time	solution
method	binary variables	continuous variables	equations	(CPU s)	(\$)
detailed planning (DP)	1104	1820	2295	22000	17,939,396
detailed planning (DP*)	984	1820	2295	164	19,102,539
relaxed planning (RP)	240	697	1153	15904	27,413,277
relaxed planning (RP*)	240	697	1009	160	30,477,546

Table 5.Model and Solution Statistics for Example 1 for 24 Weeks

In Table 6, the objective cost items for (RP) and (RP*) are compared. Note that due to the absence of the tightening constraints, (RP*) underestimates the changeover costs by 173%. Also note that (RP) predicts the profit more accurately (11%) compared to (RP*) but at the expense of increasing the CPU time by a factor of 99. As can be seen from Table 6, (RP*) results in negative changeover costs. The reason for this is the variable $UT_{m,t}$ has a positive cost coefficient in the objective function and in the absence of constraint (11) the model tends to set $UT_{m,t}$ to the maximum available value since we are maximizing the profit.

	relaxed	relaxed
(\$)	planning*	planning
sales	47,152,800	46,209,744
operating costs	17,595,240	17,243,335
inventory costs	140,014	113,132
transition costs	-1,060,000	1,440,000

 Table 6. Objective function items for RP* and RP for Example 1c

Table 7 shows the effect of optimality tolerance on the rolling horizon algorithm. As the results suggest, decreasing the tolerance results in more accurate values of the objective function but at the expense of increased solution times.

	time	solution
method	(CPU s)	(\$)
rolling horizon (RH) (0%)	1283	17,446,011
rolling horizon (RH) (1%)	1180	17,286,999
rolling horizon (RH) (5%)	38.51	15,874,108

Example 2.

In this example, there are 3 reactors (R1-R3) and 8 products (A-H) where all the products are produced in a single production stage. Each reactor can process a subset of the products (see Figure 16).



Figure 16. Schematic representation of Example 2

Table 8 shows the problem sizes and the solution times for 6 weeks. The results presented are obtained for 0% optimality gap. Although, even for this small instance the detailed planning model requires more than 900 times the computational effort of the relaxed planning model, it results in 14% more accurate estimation of the profit compared to the relaxed planning problem. In fact, since in this example all the products are produced in a single production stage, and there are no subcycles in the solution (see figure 17a), the schedule obtained by the detailed planning model corresponds to the actual schedule.

	number of	number of	number of	time	solution
method	binary variables	continuous variables	equations	(CPU s)	(\$)
detailed planning (DP)	864	1327	1483	1667	11,819
detailed planning (DP*)	792	1327	1483	96	12,211
relaxed planning (RP)	144	349	553	1.75	13,460
rolling horizon (RH)	624	1,291	1,483	322	11,377

 Table 8. Model and Solution Statistics for Example 2 for 6 Weeks

Figure 17, compares the number of batches of products and the sequences generated by DP and DP* where the number of batches are regarded as continuous variables. Note that, DP* not only results in non-integer number of batches but also different sequences for each unit and each time period compared to DP.

Figure 18a presents the variation of the profit for DP*, RP and RH for 5% optimality gap for planning horizons of 6, 12, 18 and 24 weeks. Figure 18b displays the corresponding CPU times on a logarithmic scale.



Figure 17. Comparison of DP and DP* for Example 2 for 6 Weeks



Figure 18. Results for Example 2 for 6 – 24 Week

Example 3.

This example is much larger in size compared to Example 1, specifically there are 10 products (A-K) and 4 reactors (R1-R4). Products B and G are produced in two stages and require intermediates A and F respectively. As can be seen from Figure 19, reactor R1 can process products A, B and E, reactor R2 can process products C and D, R3 can process F, G and K, and finally R4 can process products H and J.



Figure 19. Example 3 with 10 Products and 4 Reactors

Example 3a.

In Example 3a, we present the results for a planning horizon of 6 weeks. Table 9 shows the model size and statistics for this example. The first row stands for the results obtained by the detailed planning model (DP) whereas the second row presents the results for (DP*) detailed planning model with continuous number of batches. The third row and the fourth row show the results for relaxed planning model (RP) and the rolling horizon approach (RH), respectively. The results shown in this table are obtained for a 0% optimality gap. The relaxed planning model overestimates the profit by 40% whereas (DP*) overestimates the

total profit by 7%. The rolling horizon approach resulted in the exact same solution as the detailed model.

Table 10 presents the objective function items for the models corresponding to Table 9. It shows that the relaxed planning model overestimates the total sales by 12% and underestimates changeover costs by 60% with respect to the detailed planning model. (DP*) on the other hand, overestimates the total sales by only 5% while resulting in the same total changeover costs with the detailed planning model (DP).

Table 9. Model and Solution Statistics for Example 3a for 0% optimality tolerance

	number of	number of	number of	time	solution
method	binary variables	continuous variables	equations	(CPU s)	(\$)
detailed planning (DP)	552	903	1133	56.421	9,199,448
detailed planning (DP*)	492	903	1133	18	9,826,918
relaxed planning (RP)	120	349	469	12.56	12,901,329
rolling horizon (RH)	408	887	1133	7.17	9,199,448

 Table 10.Objective Function Items for Example 3a for 0% Optimality Tolerance

	detailed	detailed	relaxed	rolling
(\$)	planning	planning*	planning	horizon
sales	20,374,600	21,342,600	22,778,000	20,374,600
operating costs	7,612,480	7,949,500	8,489,600	7,612,480
inventory costs	62,671	66,182	47,071	62,671
transition costs	3,500,000	3,500,000	1,340,000	3,500,000

Table 11 compares the number of batches obtained by the detailed planning model and the relaxation of the detailed planning model where the number of batches was declared as continuous variables.

Example 3b.

In part b of Example 3, we extend the planning horizon to 12 weeks. Table 12 presents the results obtained for (DP), (DP*), (RP) and (RH) for 0% optimality tolerance. The detailed planning model yields a profit of \$ 18,951,172 in 27,000 CPUs on the other hand if the optimality gap is set to 5%, then a profit of \$ 16,681,769 is obtained in 3,500 CPUs. As Table 12 suggests, (DP*) overestimates the profit by 7% with respect to (DP), whereas (RP) overestimates the profit by 44% with respect to (DP).

Number of batches obtained from (DP)						
	T1	T2	T3	T4	T5	T6
A in R1	2	6	0	0	4	10
B in R1	2	4	2	0	3	0
E in R1	6	0	7	11	3	0
C in R2	4	0	4	6	2	0
D in R2	2	8	2	0	5	8
F in R3	2	6	0	0	4	10
G in R3	2	4	2	0	3	0
K in R3	6	0	7	11	3	0
H in R4	4	0	4	6	2	0
J in R4	2	8	2	0	5	8
	Nu	mber of bate	ches obtai	ined from (I	OP*)	
	T1	T2	T3	T4	T5	T6
A in R1	2	6.437	0	0	3.203	10.5
B in R1	2	4	2	0	3	0
E in R1	6	0	7.2	11.2	4.051	0
C in R2	3	0	2	7	2	0
D in R2	3.9	8.4	4.5	0	5.15	8.4
F in R3	2	6.437	0	0	3.203	10.5
G in R3	2	4	2	0	3	0
K in R3	6	0	7.2	11.2	4.051	0
H in R4	3	0	2	6.717	2	0
J in R4	3.9	8.4	4.5	0	5.15	8.4

Table 11. Comparison of Number of Batches obtained by (DP) and (DP*) for Example 3a

Table 12. Objective Function Items for Example 3b for 0% Optimality Tolerance

method	number of binary variables	number of continuous variables	number of equations	time (CPU s)	solution (\$)
detailed planning (DP)	1104	1815	2285	27000	18,951,172
1 0 0					
detailed planning (DP*)		1815	2285	308	20,205,487
relaxed planning (RP)	240	697	1033	435	27,310,348
rolling horizon (RH)	744	1799	2285	1192	17,246,014

Example 3c.

We extend the planning horizon to 24 weeks in this example. The detailed planning model becomes computationally very expensive to solve this example. Therefore, we present the results for (DP*), (RP) and (RH).

Tables 13 and 14, display the sizes and results for 5% and 3% optimality tolerances, respectively. The last three rows of both tables correspond to the rolling horizon algorithm by using 2, 3 and 4 detailed time periods per iteration. As the results suggest, the accuracy increases as the number of detailed time periods increase but at the expense of increased solution times.

Table 13. Problem Sizes for Example 3c

	number of	number of	number of
method	binary variables	continuous variables	equations
detailed planning (DP*)	1968	3639	4589
relaxed planning (RP)	480	1393	1873
rolling horizon (RH) (2B)	1416	3623	4589
rolling horizon (RH) (3B)	1452	3623	4589
rolling horizon (RH) (4B)	1488	3623	4589

 Table 14. Results for Example 3c for 3% and 5% optimality tolerance

	3%		5%	/0
	time	solution	time	solution
method	(CPU s)	(\$)	(CPU s)	(\$)
detailed planning (DP*)	17977	44,927,589	890	44,782,747
relaxed planning (RP)	428	54,793,780	30	54,122,362
rolling horizon (RH) (2B)	1199	37,570,228	158	38,605,704
rolling horizon (RH) (3B)	2464	40,303,229	165	39,047,238
rolling horizon (RH) (4B)	2932	40,967,510	1196	39,625,581

Example 4

In this final example we present an industrial-sized case study that consists of 15 Products and 6 reactors. Figure 20 shows which products can be processed by each of the units. Table 15 presents the results for a planning horizon of 48 weeks for 6% optimality tolerance. Since this problem is much larger compared to the previous examples, both in terms of size and the length of the planning horizon considered, the detailed planning model became very expensive to solve, and hence we present only the results for the relaxed planning (RP) model and rolling horizon (RH). As we have mentioned before, in the rolling horizon algorithm, we only fix the binary variables denoting the assignments and sequencing within each time period. In the last row of Table 15, we show the results for the rolling horizon algorithm where all the binary variables are fixed through the iterations. Fixing all the binary variables reduce the computational time by a factor of 5 however, at the cost of decreasing the accuracy by 2%.

 Table 15. Results for Example 3c for 3 % optimality tolerance

	number of	number of			
	binary	continuous	number of	time	solution
method	variables	variables	equations	(CPU s)	(\$)
relaxed planning (RP)	2,592	5,905	9,361	362	224,731,683
rolling horizon (RH)	10,092	25,798	28,171	11,656	184,765,965
rolling horizon (RH**)	1,950	25,798	28,171	4,554	182,169,267

** All binary variables fixed



Figure 20. Batch processing plant of Example 4

Figure 21 shows the variation of profit and CPU time for Example 4 with respect to 6, 12, 24 and 48 weeks of planning horizons.



Figure 21. Variation of Profit (\$) and CPU time with respect to periods for Example 4

6. Conclusions

This paper has addressed the production planning of parallel multi-product batch reactors with sequence-dependent changeovers. We have proposed two alternative MILP models for handling sequence-dependent change-over times and costs. Both models determine the allocation of products to available equipment, number of batches of each product for each unit, each time period as well as production and inventory levels. The difference between the two models lies in the handling of the sequence-dependent change-over times. The first model (RP) is based on underestimating the effects of changeovers, and therefore results in an overestimation of sales and the profit. The second model (DP), on the other hand, explicitly accounts for scheduling via sequencing variables and constraints. Due to its ability to incorporate scheduling at the planning model, it results in more accurate production plans compared to (RP). In fact, in the absence of sub-cycles in the solution and for the case of a single stage, (DP) produces the exact production schedule as a corresponding detailed scheduling model would. However, as has been shown with numerical results, there is a trade-off between the extent of scheduling decisions incorporated and the size of the resulting problem. The detailed planning model (DP) yields more realistic production plans compared to (RP) but at the expense of increasing the number of binary variables, continuous variables and the number of constraints.

The results have shown that the detailed planning model has good computational performance for modest sized problems, but it becomes computationally expensive for large scale problems. In order to tackle large problems without giving up significantly the solution quality, we have presented a rolling horizon algorithm (RH) and a relaxation of the detailed planning model (DP) in which the number of batches is treated as a continuous variable. The rolling horizon provides a lower bound on the profit, and for small problems it tends to yield the same solution as the detailed planning model, whereas for larger problems it underestimates the profit typically by up to 10%. Relaxing the detailed planning model by declaring the number of batches as continuous variables (DP*) over estimates the profit by up to 8% but greatly decreases the computational effort.

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Appendix A

Data for Example 1:

	Batch Siz	e (lb)				
	R1					
Α	80,000	80,000				
B	96,000	96,000				
С	120,000	120,000				
D	100,000	100,000				
Ε	150,000	150,000				
	Batch Tir	Batch Time (hrs)				
	R1	R2				
Α	16	16				
B	10	10				
С	25	25				
D	20	20				
Е	15	15				

 Table A1. Batch Sizes and Batch Times for Example 1

 Table A2. Changeover Times and Changeover Costs for Example 1

	Product				
Product	Α	В	С	D	Ε
		Т	'ransition ti	mes (hrs)	
Α	0	25	30	20	35
В	22	0	42	8	40
С	25	5	0	15	32
D	22	12	28	0	17
Ε	29	4	45	21	0
			Transition o	costs (\$)	
Α	0	250	300	200	350
B	220	0	420	90	400
С	250	50	0	150	320
D	220	120	280	0	170
E	290	40	450	210	0

		selling	inventory
	operating	price	costs
Product	costs (\$/lb)	(\$/lb)	(\$/(lb w))
Α	0.35	0.95	0.01496
В	0.34	0.99	0.01339
С	0.36	0.9	0.01418
D	0.37	1	0.01539
E	0.3	0.85	0.01618

Table A3. Selling Price and Cost Data for Example 1

Table A4. Minimum Number of Batches for Example 1a, 1b, and 1c

Min Run Lengths (hrs)						
	6 Weeks	12 Weeks	24 Weeks			
Α	2	2	2			
В	2	2	3			
С	2	2	2			
D	2	2	3			
Е	2	2	2			

Table A5. Lower Bounds for Demands for Example 1a

	time period					
Product	1	2	3	4	5	6
Α	80,000	80,000	80,000	160,000	320,000	80,000
В	192,000	384,000	96,000	96,000	192,000	96,000
С	240,000	120,000	120,000	120,000	240,000	120,000
D	200,000	100,000	100,000	200,000	300,000	200,000
Е	150,000	300,000	150,000	100,000	150,000	300,000

Demand (lb/w)

Table A6. Lower Bounds for Demands for Example 1b

	Demand (lb/w)					
	time period	time period	time period	time period	time period	time period
Product	1	2	3	4	5	6
Α	80,000	80,000	80,000	160,000	320,000	80,000
В	192,000	384,000	96,000	96,000	192,000	96,000
С	240,000	120,000	120,000	120,000	240,000	120,000
D	200,000	100,000	100,000	200,000	300,000	200,000
E	150,000	300,000	150,000	100,000	150,000	300,000
	time period	time period	time period	time period	time period	time period
Product	7	8	9	10	11	12
Α	160,000	80,000	80,000	160,000	80,000	160,000
В	192,000	192,000	96,000	96,000	192,000	192,000
С	240,000	480,000	120,000	120,000	240,000	120,000
D	100,000	300,000	200,000	200,000	300,000	100,000
Ε	300,000	150,000	300,000	150,000	150,000	300,000

	Demand (lb/w)						
	time period	time period	time period	time period	time period	time period	
Product	1	2	3	4	5	6	
Α	80,000	80,000	80,000	160,000	320,000	80,000	
В	192,000	384,000	96,000	96,000	192,000	96,000	
С	240,000	120,000	120,000	120,000	240,000	120,000	
D	200,000	100,000	100,000	200,000	300,000	200,000	
E	150,000	300,000	150,000	100,000	150,000	300,000	
	time period	time period	time period	time period	time period	time period	
Product	7	8	9	10	11	12	
Α	160,000	80,000	80,000	160,000	80,000	160,000	
В	192,000	192,000	96,000	96,000	192,000	192,000	
С	240,000	480,000	120,000	120,000	240,000	120,000	
D	100,000	300,000	200,000	200,000	300,000	100,000	
Е	300,000	150,000	300,000	150,000	150,000	300,000	
	time period	time period	time period	time period	time period	time period	
Product	13	14	15	16	17	18	
Α	160,000	80,000	320,000	160,000	320,000	80,000	
В	192,000	384,000	96,000	192,000	384,000	96,000	
С	240,000	120,000	120,000	240,000	0	120,000	
D	400,000	300,000	100,000	100,000	100,000	200,000	
E	300,000	0	300,000	150,000	300,000	300,000	
	time period	time period	time period	time period	time period	time period	
Product	19	20	21	22	23	24	
Α	80,000	320,000	80,000	80,000	160,000	160,000	
В	192,000	384,000	768,000	384,000	192,000	384,000	
С	120,000	480,000	120,000	120,000	240,000	480,000	
D	100,000	200,000	400,000	200,000	100,000	400,000	
Е	300,000	150,000	150,000	0	300,000	150,000	

Table A7. Lower Bounds for Demands for Example 1c

REFERENCES

- 1. Wilkinson, S. J.; Shah, N.; Pantelides, C.C. Aggregate Modeling of Multipurpose Plant Operation. *Comput. Chem. Eng.* **1996**, *19*, Supplement 1,11 583,588.
- Dimitriadis, A.D.; Shah, N.; Pantelides, C. C. RTN-based Rolling Horizon Algorithms for MediumTerm Scheduling of Multipurpose Plants. *Comput. Chem. Eng.* 1997, 21, 1061-1066.

- Bassett, M. H.; Pekny, J. F.; Reklaitis, G. V. Decomposition Techniques for the Solution of Large-Scale Scheduling Problems. *AIChE J.* 1996, *42*, 3373-3384.
- Subrahmanyam, S.;Pekny, J. F.; Reklaitis, G. V. Decomposition Approaches to Batch Plant Design and Planning. *Ind. Eng. Chem. Res.* 1996, 35, 1866-1876.
- 5. Birewar, D. B.; Grossmann I. E. Simultaneous Production Planning and Scheduling in Multiproduct Batch Plants. *Ind. Eng. Chem. Res.* **1990**, *29*, 570-580.\
- Birewar, D. B.; Grossmann I. E. Efficient Optimization Algorithms for Zero-Wait Scheduling of Multiproduct Batch Plants. *Ind. Eng. Chem. Res.* 1989, 28, 1333-1345.
- Bok, J.-K., I. E. Grossmann, and S. Park, "Supply chain optimization in continuous flexible process networks," Ind. Eng. Chem.Res., 39, 1279–1290 (2000).
- McDonald, C.; Karimi, I.A. "Planning and Scheduling of Parallel Semicontinuous Processes 1. Production Planning," Ind. Eng. Chem. Res., 36, 2691 (1997).
- Pantelides, C. C. "Unified Frameworks for the Optimal Process Planning and Scheduling," in Proceedings on the Second Conference on Foundations of Computer Aided Operations, 253-274 (1994).
- 10. Stefansson, H., Shah, N., and Jensson, P., "Multiscale planning and scheduling in the secondary pharmaceutical industry," AIChE Journal, 52,12, 4133-4149, (2006)
- Dogan, M.E.; Grossmann I.E., "A Decomposition Method for the Simultaneous Planning and Scheduling of Single-Stage Continuous Multiproduct Plants," Ind. Eng.Chem. Res., 45, 299-315, (2006).
- 12. Bitran, G.R.; Hax, A.C., "On the design of hierarchical production planning systems", Decision Science, 8, 28-55, (1977).

- Nemhauser, G.; Wolsey, L. Integer and Combinatorial Optimization; John Wiley & Sons: NewYork, 1988.
- 14. Sahinidis, N.V.; Grossmann, I.E. MINLP model for cyclic multiproduct scheduling on continuous parallel lines. *Comput. Chem. Eng.* 15,2,85, (1991a)
- 15. Sung, C.; Maravelias, C. T. An Attainable Region Approach for Effective Production. Planning of Multi-product Processes. To appear in *AIChE J*. 2007

Nomenclature:

Indices

<i>i</i> , <i>i</i> '	tasks
j	products
т	units
t	time periods
\overline{t}	last time period
Sets	
Ι	set of tasks
I_{m}	set of tasks that can be processed in unit m
PS_{j}	set of tasks that produce product j
CS_{j}	set of tasks that consume product j
М	set of units
$M_{_i}$	set of units that can process task i
Parame	ters

*Bound*_{imt} maximum amount of material that can be processed by task i in unit m during time period t

$BT_{i,m}$ batch processing time of task i in uni	t m
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- $Q_{i,m}$ batch size of task i in unit m
- ρ_{ii} mass balance coefficient for the production of product j by task i

 $\overline{\rho}_{ii}$ mass balance coefficient for the consumption of product j by task i

- D_{it} demand for product j at the end of time period t
- $TR_{i.m}$ minimum changeover time for task i in unit m
- $\tau_{i,i',m}$ changeover time required to change the operation from task i to task i' in unit
- m
- H_t duration of the tth time period
- *TRC*_{*i.m*} minimum changeover cost for task i in unit m
- c_{it}^{oper} operating cost of task I in unit m
- c_{jt}^{inv} inventory cost of product j at the end of time period t
- cp_{it} selling price of product j at the end of time period t
- $c_{i,i',m}^{trans}$ changeover costs of changing the production from task i to i' in unit m

Variables

 $YP_{i,m,t}$ binary variable denoting the assignment of task i to unit m at each period t

 NB_{imt} integer variable denoting number of each batches of each task i in each unit m at each period t

FP_{int} amount of material processed by each task i

 INV_{it} inventory levels of each product j at each time period t

 P_{it} the total amount of purchases of product j during time period t

 S_{ii} sales of product j at the end of time period t

 $U_{m,t}$ maximum of the minimum changeover times of products assigned to unit m during time t

 $UT_{m,t}$ maximum of the minimum changeover costs of products assigned to unit m during time t

 $ZP_{ii'mt}$ binary variable becomes 1 if product i precedes product i' in unit m at time period t, 0 otherwise

 $ZZP_{ii'mt}$ binary variable which becomes 1 if the link between products i and i' is to be broken, otherwise it is zero

 $TRNP_{m,t}$ total changeover time for unit m within each period

 $XF_{i,m,t}$ binary variable denoting the first task in the sequence

*XL*_{*i.m.t*} binary variable denoting the last task in the sequence

 $ZZZ_{i,i',m,t}$ changeover variable denoting the changeovers across adjacent periods