Short-Term Scheduling of Batch Plants with Parallel Reactors Forming Mobile Work Groups

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Abstract

We address the problem of short-term scheduling of parallel batch reactors followed by continuously operating finishing trains to form work groups which is motivated by a real world problem at the Dow Chemical Company. The proposed MILP formulation is based on the recent planning model of Erdirik-Dogan and Grossmann (2007), and features additional constraints for handling complex arrangements arising from the workgroups. Several examples are presented to illustrate the proposed model.

Keywords: *batch reactors, scheduling, sequence-dependent changeovers, mobile work groups, MILP*

1. Introduction

This work has been inspired by a real world application originating from the specialty chemicals business at the Dow Chemical Company which is characterized by the manufacture of a large product portfolio (see Erdirik-Dogan et al., 2007, 2008). The specialty chemicals business is subject to constant change with respect to the products in the portfolio. The relative demand for individual products can fluctuate widely over time as conditions change in the many markets that are served. The price and profitability among products varies greatly and can shift over time. New product introductions and

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experimental product runs occur several times a year and must be worked into the production schedule. Many high margin products are subject to spot orders that are hard to forecast. All of these conditions create a challenging production scheduling environment.

We address the short-term scheduling of a multi-product batch plant which consists of parallel batch reactors that are connected to continuously operating finishing trains to form work groups. Finishing operations in the specialty chemicals business are required to convert the outputs from the reactors to trade products for a diverse set of markets and customers. Depending on the business, finishing trains can simply purify the crude reactor grade product or they may include blending operations for additives.

A complication that arises in this type of plant is that each time a product switch occurs, not only the reactors but also the finishing trains need to be cleaned up and made ready for the next product. Since these clean up operations involve sequence-dependent changeovers, determining the optimal sequence of production is of great importance for improving equipment utilization and reducing the costs. The main challenge of modeling this scheduling problem arises from the structure of the plant, where the work groups are not fixed, but are flexible in the sense that subsets of work groups can be selected by manipulating valves that interconnect the reactors with the finishing trains. Therefore, in addition to the challenge of determining the optimal production sequence given the sequence-dependent changeovers with high variance, there is also the challenge of regrouping the units periodically when the demand varies from one period to the next one, or when new products are introduced while maximizing profit. This problem is somewhat unique as it does not fit conventional batch scheduling problems that have been considered before in the literature (for a review see Shah, 1998; Kallrath, 2002; Mendez et al, 2006).

In order to address the aforementioned issues, we propose in this paper an MILP optimization model which is the extension of the recent work of Erdirik-Dogan and Grossmann (2007) for long-term planning of two-stage parallel batch reactors to the case of short-term scheduling of single stage, parallel batch reactors connected to continuously operating finishing trains. The paper is organized as follows. In the next section, we present the problem statement. This is followed by the proposed MILP formulation. In section 4, we present several examples to show the application and effectiveness of the model, and finally, section 5 summarizes some conclusions and recommendations for future work.

2. Problem Statement

Given is a plant consisting of several identical batch reactors operating in parallel, and which are connected via valves to intermediate storage tanks dedicated to each finishing train, which in turn are connected to continuously operating finishing trains to from work groups. Each finishing train is connected to any of the dedicated storage tanks where products are stored. As seen in Figure 1, reactors R1 and R3 can be connected to finishing train A to form work group 1; Reactors R1, R2 and R5 can be connected to finishing train B to work group 2 and so on.

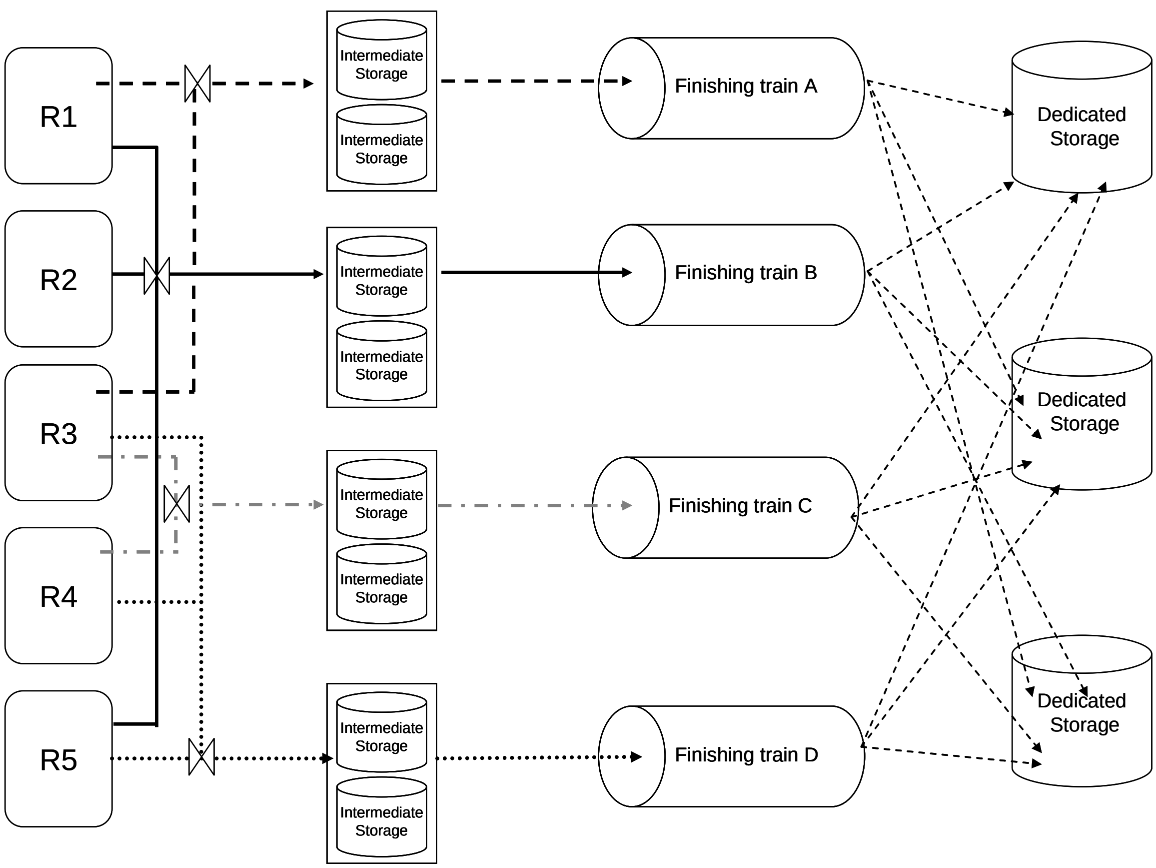

Figure 1. Schematic representation of the problem

A combination of two intermediate storage tanks is dedicated to each finishing train to act as a buffer between batch reactors and continuously operating finishing trains as shown in Figure 1. Reactors and the associated intermediate storage tank are connected through a single valve. Hence the material transfer from the parallel reactors to this tank occurs simultaneously. When a product switch occurs, one of the intermediate tanks is run dry, cleaned and made ready for the next product while the other tank is feeding the first product to the finishing train. After the processing of the first product is completed, both the finishing train and the tank feeding it are cleaned and made ready for the next product as well. Since the intermediate storage tanks do not represent a bottleneck in terms of capacity and since we are not concerned with the detailed timing of operations in this work, we have simplified the problem as shown in Figure 2 where the intermediate storage tanks are removed from the system.

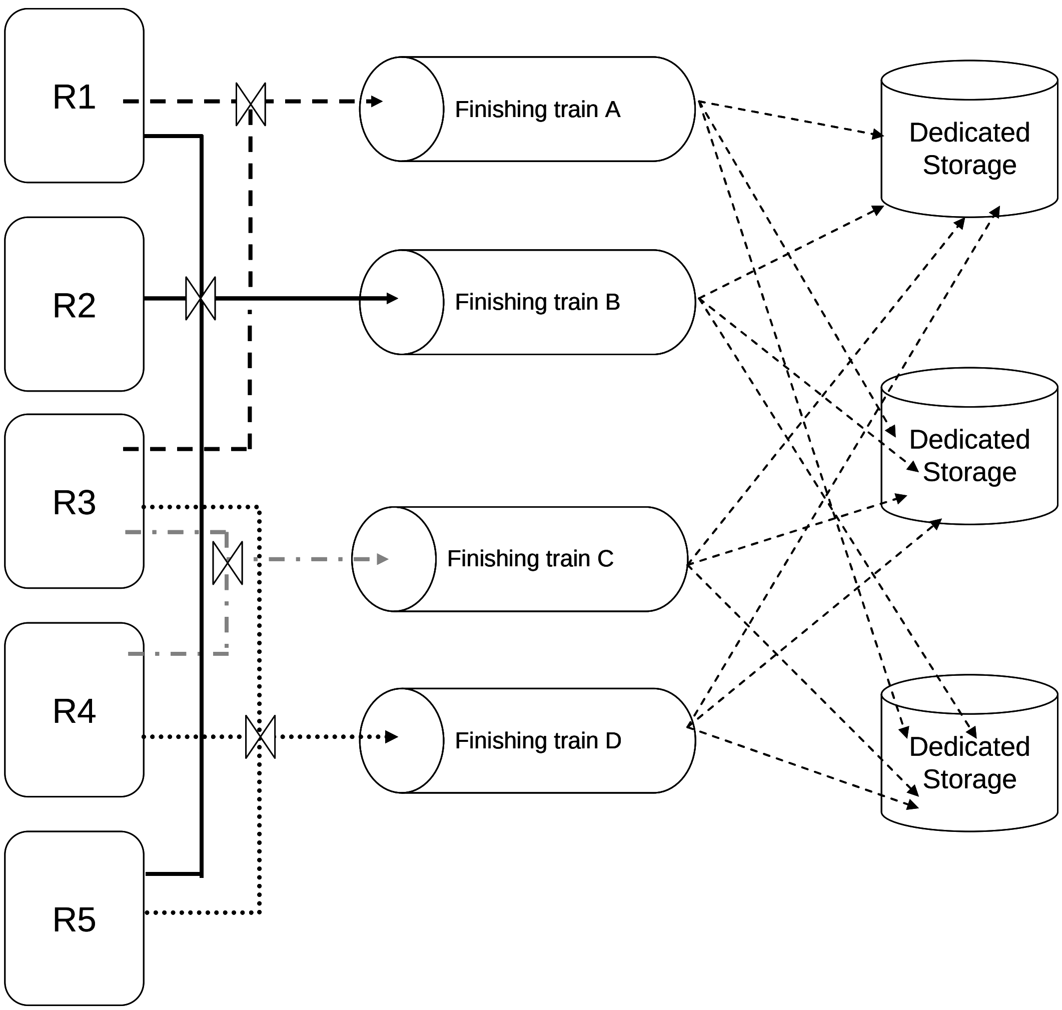

Figure 2. System of reactors, finishing trains and dedicated storage tanks

Each reactor can have potential connections with more than one finishing train. Hence each reactor can be involved with more than one work group. Moreover, the connection between a specific reactor and potential finishing trains is flexible in the sense that one reactor can be connected to one finishing train during one period, but can be connected to another finishing train in the subsequent time period. In other words, assignment of a reactor to a work group is not fixed throughout the horizon, but can change from one time period to another. As an example consider Figure 2 where reactor R1 can be connected to finishing train A during time period t but can be connected to finishing train B during the subsequent time period, $t+1$.

For this scheduling problem, we assume that the following information is given:
(a) Potential connections between a reactor and a work group; (b) subset of products that each reactor can process; (c) batch times and batch sizes of each product for the corresponding units; (d) sequence-dependent changeover times and costs; (e) operating costs, inventory costs, selling price associated with each product; (f) due dates and demands to be satisfied; (g) time horizon under consideration.

The problem is then to determine optimum values of the following items so as to maximize the profit while satisfying production demands at the specified due dates: (i) allocation of units to potential workgroups during each time period (connection of each reactor to each finishing train during each time period); (ii) production sequence on each unit during each time interval; (iii) number of batches of each product in each unit during each time interval; (iv) production and inventory levels; (v) amounts of products sold at the end of each time period. The objective is to select these items in order to maximize the profit.

3. Mathematical Model

The mathematical model proposed for the problem described in this paper is based on the recent work by Erdirik-Dogan and Grossmann (2007) where a method for simultaneously determining the number of batches of each product together with their allocation and sequencing on the available units has been proposed. The proposed model explicitly accounts for sequence-dependent changeover times and costs by immediate precedence sequencing variables and sequencing constraints which correspond to a relaxation of the traveling salesman problem (Nemhauser and Wolsey, 1988). We should note that the proposed model does not involve detailed timing variables as would be the case of a slot-based model (e.g. see Sundaramoorthy, A. & Karimi, I.A., 2005; Erdirik and Grossmann, 2008). Main reason behind this simplification is that the planning model by Erdirik and Grossmann (2007), which is used as a basis for this work, provides an exact schedule for single stage plants when there are no subcycles.

In this paper that work is extended to accommodate the case of parallel batch reactors connected to continuously operating finishing trains to form work groups. The extension involves the introduction of a new binary variable and several constraints which will be explained in detail in the problem constraints sub-section. Moreover, the model of Erdirik-Dogan and Grossmann (2007) has the potential drawback of generating solutions featuring subcycles. For the cases when subcycles are encountered, the model will not be able to generate a feasible schedule. In order to guard against such a case, we add subtour elimination constraints iteratively until feasible schedules are found.

The following assumptions hold for this scheduling model:

1. The model parameters are deterministic.
2. Single stage production is assumed.
3. Transfer time of material from the reactors to the finishing trains is negligible.
4. The production process is non-preemptive.
5. Each reactor can process a subset of products. However, the units are identical in terms of the batch times, batch sizes and production costs.
6. Transition times and costs are sequence-dependent, but independent of the units.
7. Connections between reactors and finishing trains can only change between time periods.

Since the proposed formulation uses as a basic building block the work of Erdirik-Dogan and Grossmann (2007), for the sake of completeness, we first briefly outline that model. Next, we introduce the additional constraints and variables to be able to accommodate the extension to the connection with continuously operating finishing trains. And finally, we address the aforementioned subtour elimination constraints.

3.1. Outline of the Erdirik-Dogan and Grossmann (2007) model

Material handled and capacity requirements:

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

Number of batches of each product:

$$NB_{i,m,t} = FP_{i,m,t} / Q_{i,m} \quad \forall i \in I_m, m, t \tag{2}$$

Mass Balances on the state nodes

$$P_{j,t} + \sum_{i \in PS_j} \rho_{j,i} \sum_{m \in M_i} FP_{i,m,t} = S_{j,t} + \sum_{i \in CS_j} \bar{\rho}_{j,i} \sum_{m \in M_i} FP_{i,m,t} + INV_{j,t} - INV_{j,t-1} \quad \forall j, t \tag{3}$$

Demands

$$S_{j,t} \geq D_{j,t} \quad \forall j, t \tag{4}$$

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

Demands can be defined as hard upper bounds, soft lower bounds or both where it is given by a range of values. The lower bounds represent fixed orders, whereas the upper bounds represent maximum projected demands that can be sold in the market during each time period.

Changeover times and costs

We account for the sequence-dependent changeover times and costs through sequencing constraints similar to the ones from the traveling salesman problem and through time balances. The basic idea is to find the minimum transition time sequence within the assigned products within each period while maximizing the profit and satisfying the demands at the due dates. In order to do that, a cyclic schedule is first generated within each period that minimizes transition times amongst the assigned products. Next, one of the links in the cycle is broken to determine the optimal sequence (see also Birewar and Grossmann, 1990).

The following constraints are proposed for generating cyclic schedules in each unit, each time period.

$$YP_{imt} = \sum_{i'} ZP_{ii'mt} \quad \forall i \in I_m, m, t \tag{6}$$

$$YP_{i'mt} = \sum_{i} ZP_{ii'mt} \quad \forall i' \in I_m, m, t \tag{7}$$

Constraints (8) and (9) determine the location of the cycle to be broken.

$$\sum_{i \in I_m} \sum_{i' \in I_m} ZZP_{ii'mt} = 1 \quad \forall m, t \tag{8}$$

$$ZZP_{ii'mt} \leq ZP_{ii'mt} \quad \forall i, i' \in I_m, m, t \tag{9}$$

Constraint (10) defines the total transition time within each time period ($TRNP_{m,t}$), which is given by the summation of the transition times ($\tau_{i,i'}$) corresponding to each existing pair ($ZP_{ii'mt}$) minus the transition time corresponding to the link that is broken ($ZZP_{ii'mt}$).

$$TRNP_{m,t} = \sum_{i \in I_m} \sum_{i' \in I_m} \tau_{i,i'} \cdot ZP_{i,i',m,t} - \sum_{i \in I_m} \sum_{i' \in I_m} \tau_{i,i'} \cdot ZZP_{i,i',m,t} \qquad \forall m,t \tag{10}$$

The following constraints (11)-(16) are introduced to be able to account for the transitions across adjacent time periods. The elements that correspond to the pair where the cycle is broken to form the sequence, represent the head, $XF_{i,m,t}$, and the tail, $XL_{i,m,t}$, of the sequence.

$$XF_{i',m,t} \geq \sum_{i \in I_m} ZZP_{i,i',m,t} \qquad \forall i' \in I_m, m, t \tag{11}$$

$$XL_{i,m,t} \geq \sum_{i' \in I_m} ZZP_{i,i',m,t} \qquad \forall i \in I_m, m, t \tag{12}$$

$$\sum_{i \in I_m} XF_{i,m,t} = 1 \qquad \forall m,t \tag{13}$$

$$\sum_{i \in I_m} XL_{i,m,t} = 1 \qquad \forall m,t \tag{14}$$

$$\sum_{i' \in I_m} ZZZ_{i,i',m,t} = XL_{i,m,t} \quad \forall i \in I_m, m, t \tag{15}$$

$$\sum_{i \in I_m} ZZZ_{i,i',m,t} = XF_{i',m,t+1} \quad \forall i' \in I_m, m, t \in T - \{\overline{t}\} \tag{16}$$

Finally, through the time balances given by constraint (17), the total allocation of production times plus the total transition times is enforced not to exceed the available time for each unit.

$$\sum_{i \in I_m} NB_{i,m,t} \cdot BT_{i,m} + TRNP_{m,t} + \sum_{i \in I_m} \sum_{i' \in I_m} ZZZ_{i,i',m,t} \cdot \tau_{i,i'} \leq H_t \qquad \forall m,t \tag{17}$$

Objective function

The objective is to maximize the profit in terms of sales revenues, inventory costs, operating costs and changeover costs.

$$\begin{aligned} Max \quad Z^p = & \sum_j \sum_t cp_{j,t} \cdot S_{j,t} - \sum_j \sum_t c^{inv}_{j,t} \cdot INV_{j,t} - \sum_{i \in I_m} \sum_m \sum_t c^{oper}_{i,t} \cdot FP_{i,m,t} \\ & - \sum_{i \in I_m} \sum_{i' \in I_m} \sum_m \sum_t c^{trans}_{i,i'} \cdot (ZP_{i,i',m,t} - ZZP_{i,i',m,t} + ZZZ_{i,i',m,t}) \end{aligned} \tag{18}$$

3.2. Constraints for the connection of parallel batch reactors to continuously operating finishing trains

In order to model these constraints we will define the boolean variables $YP_{i,m,t}$ and $VY_{m,w,t}$ to represent assignment of product i to unit m during time period t and assignment of unit m to workgroup w during time period t, respectively. We also define the subset W_m to represent the workgroups that can potentially include unit m.

Assignment of any task i in unit m during period t, triggers the assignment of unit m to one of the potential workgroups $w \in W_m$ it can belong to.

According to the implication in constraint (19), if unit m is selected to operate during time period t, then one of the work groups which m can be a part of must also be selected. This implication can be mathematically written as shown in constraint (20),

$$YP_{i,m,t} \rightarrow \bigvee_{w \in W_m} VY_{m,w,t} \quad \forall i, m \in M_i, t \tag{19}$$

$$YP_{i,m,t} \leq \sum_{w \in W_m} VY_{m,w,t} \quad \forall i \in I_m, m, t \tag{20}$$

Assignment of unit m to workgroup $w \in W_m$ during time period t, activates the assignment of all the other units belonging to workgroup w during time period t.

Assignment of a unit to a work group w during time period t, implies that the work group w has been selected to operate during time t, which further implies that all the units associated with that work group must also be selected. This is represented in the implication (21) which is written mathematically as shown in constraint (22).

$$VY_{m,w,t} \rightarrow \bigwedge_{\substack{m' \in M_w \\ m' \neq m}} VY_{m',w,t} \quad \forall m, w \in W_m, t \tag{21}$$

$$VY_{m',w,t} \geq VY_{m,w,t} \quad \forall m \in M_w, m' \in M_w, m \neq m', w, t \tag{22}$$

During each time period, unit m can operate as a part of at most one potential work group $w \in W_m$.

Since the valves connecting units to finishing trains can be turned on or off only between time periods, each unit is dedicated to at most one work group during each time period. Therefore, if unit m is selected to operate during time period t, then it can operate as a part of at most one work group which is represented by constraint (23).

$$\sum_{w \in W_m} VY_{m,w,t} \leq 1 \quad \forall m, t \tag{23}$$

The units belonging to a specific workgroup at any time period must have the same assignments and sequence on all units within that time period.

In the previous paper, we did not consider the connections between reactors and finishing trains where any reactor could be directly connected to any of the storage tanks. Thus, the reactors were independent in the sense that the assignments of products and their sequences in each unit were allowed to be unique. However, taking into account the connection between reactors and finishing trains brings up a new issue. Specifically, since, materials are fed simultaneously from the reactors to the finishing trains, contamination in the finishing trains may occur. As an example consider the workgroup shown in Figure 3, where product A is produced in reactor R1 while product B is produced in reactor R2. At the end of the production, transferring A and B simultaneously to the finishing train will cause A and B to mixed and will result in an off-specification product. In order to avoid the aforementioned problem, the units operating as a workgroup must be synchronized during that time period.

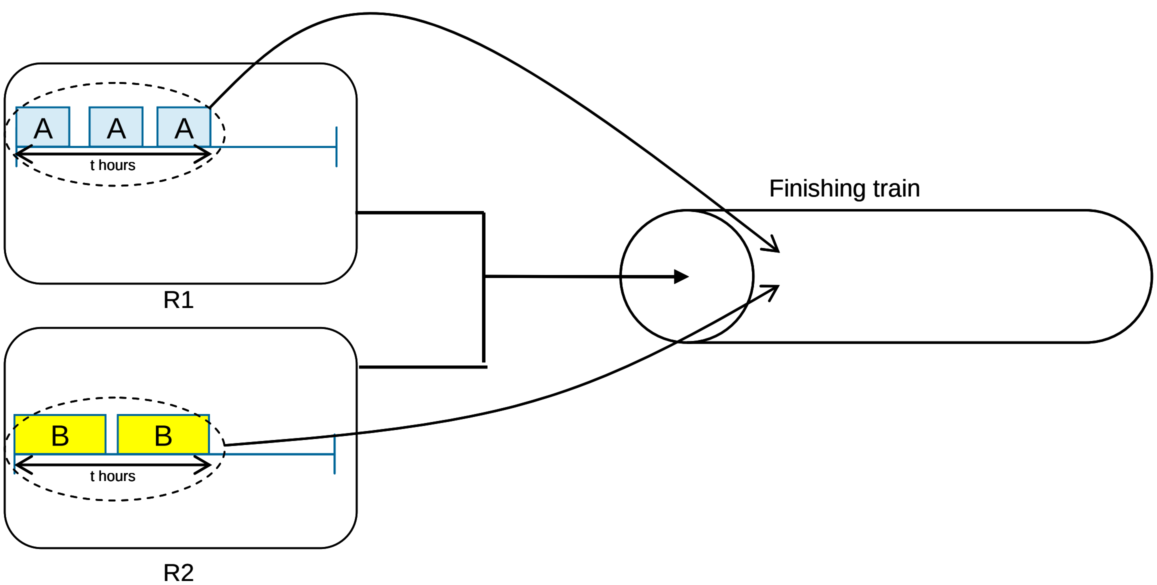

Figure 3. Contamination in the finishing trains due to a synchronized schedules

The following constraint is proposed to ensure that the units operating as a part of the same work group will have the same product assignments during that time period. The implication in constraint (24) states that if product i is assigned to unit m during time period t, and unit m operates as a part of work group w during time period t, and if any other unit m’ is also operating as a part of work group w within that time period, then product i will also be assigned for production on unit m’ during that time period. Constraint (24) is then transformed into an inequality with 0-1 variables to yield constraint (25).

$$\left(YP_{i,m,t} \wedge VY_{m,w,t} \wedge VY_{m',w,t}\right) \rightarrow YP_{i,m',t} \quad \forall i \in (I_m \cap I_{m'}), m \in M_w, m' \in M_w, m \neq m', w, t \tag{24}$$

$$YP_{i,m',t} \geq YP_{i,m,t} + VY_{m,w,t} + VY_{m',w,t} - 2 \quad \forall i \in (I_m \cap I_{m'}), m \in M_w, m' \in M_w, m \neq m', w, t \tag{25}$$

We should note that enforcing the same product assignments within all units associated with a work group is not sufficient to obtain the same sequences in all the units involved with that work group. This is due to the fact that the reactors operating in parallel in one time period could be coupled with other reactors, and could have different product assignments in the subsequent time period. Hence, for the sake of minimizing transitions across adjacent weeks, different sequences could be assigned to units belonging to the same work group unless that condition is explicitly enforced. This is illustrated in the example of Figure 4. Units R1 and R2 are connected via the same finishing train in the first week but the connection is severed in the second week and new connections between R1 and R3 and R2 and R4 are made. Since the product assignments change for both R1 and R2 from week 1 to week 2, the model yields different schedules in the first week for R1 and R2 in order to minimize the transitions across adjacent weeks.

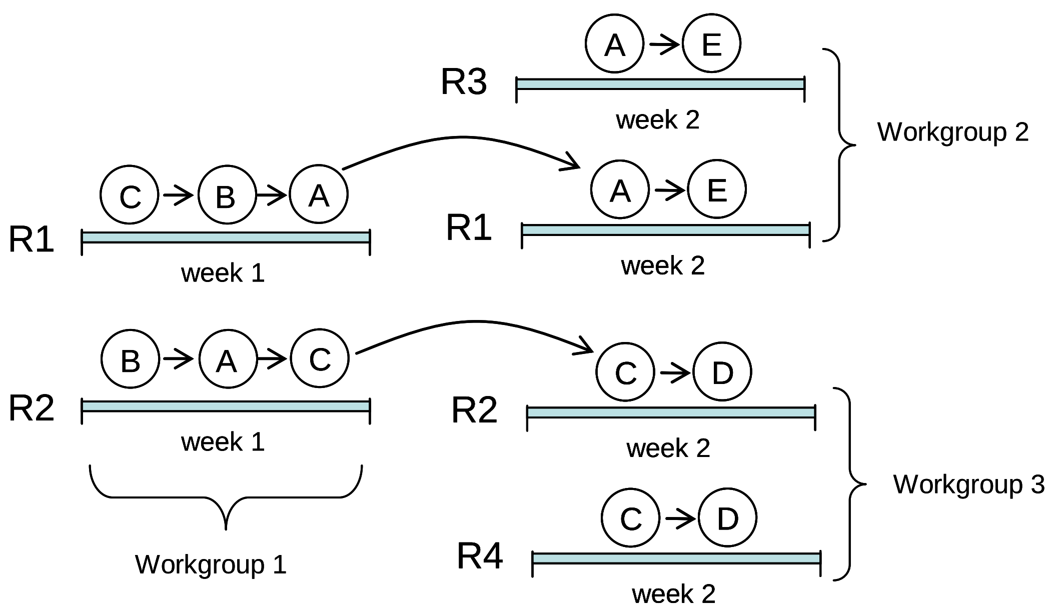

Figure 4. Transitions across adjacent periods for units belonging to different workgroups in adjacent periods

In order to ensure that the units operating as a work group have the same sequence within a given time period, we must enforce the condition that the cycles generated for the units under consideration are broken from the same location. This is because of the way we handle the sequence of production.

Specifically, the order of products in the generated cycles will be the same for all the units that have the same product assignments since the goal is to minimize the total transition time. However, according to the location of the link to be broken, different cycles can be obtained. As an example consider Figure 5 where the same cycle of three products can lead to three different sequences according to the location of the link to be broken.

Hence, by enforcing the cycle to be broken at the same location, or in other words, enforcing that the generated sequences have the same heads ($XF_{i,m,t}$) and tails ($XL_{i,m,t}$) through constraints (26) and (27), we ensure that units connected to the same finishing train at a given period will have the same sequences.

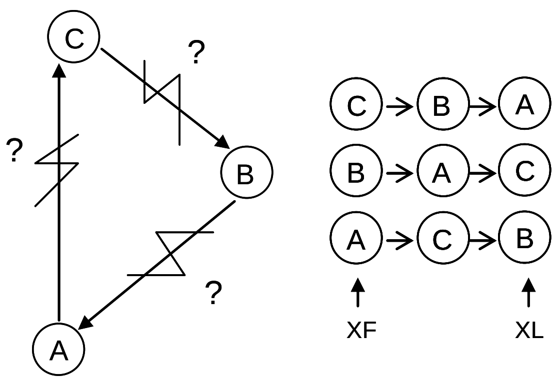

Figure 5. One cycle, three different sequences

Constraints (26) and (27) are derived in analogy to constraint (24), and can be written mathematically as shown in constraints (28) and (29), respectively.

$$\left(XF_{i,m,t} \wedge VY_{m,w,t} \wedge VY_{m',w,t}\right) \rightarrow XF_{i,m',t} \quad \forall i \in (I_m \cap I_{m'}), m \in M_w, m' \in M_w, m \neq m', w, t \tag{26}$$

$$\left(XL_{i,m,t} \wedge VY_{m,w,t} \wedge VY_{m',w,t}\right) \rightarrow XL_{i,m',t} \quad \forall i \in (I_m \cap I_{m'}), m \in M_w, m' \in M_w, m \neq m', w, t \tag{27}$$

$$XF_{i,m',t} \geq XF_{i,m,t} + VY_{m,w,t} + VY_{m',w,t} - 2 \quad \forall i \in (I_m \cap I_{m'}), m \in M_w, m' \in M_w, m \neq m', w, t \tag{28}$$

$$XL_{i,m',t} \geq XL_{i,m,t} + VY_{m,w,t} + VY_{m',w,t} - 2 \quad \forall i \in (I_m \cap I_{m'}), m \in M_w, m' \in M_w, m \neq m', w, t \tag{29}$$

3.3. Subcycle elimination constraints

The formulation given by constraints (1)-(17), (20), (22), (23), (25), (28), (29), and objective in (18), might exhibit subcycles. Although, for asymmetric sequence-dependent changeovers the likelihood of subcycles is small (Pekny and Miller, 1992), there is no guarantee that this will be the case. In this subsection, we will discuss the addition of constraints that will ensure obtaining sequences without any subcycles.

The first alternative is to introduce general subtour elimination constraints as shown in inequality (30) which are similar to the subtour elimination constraints used in the traveling salesman problem (see also Birewar and Grossmann, 1989).

$$\sum_{i \in Q_m} \sum_{i' \in Q_m'} ZP_{i,i',m,t} \geq 1 \qquad \forall m \in (M_i \cap M_{i'}), t$$
$$Q_m \subset I_m, Q_m \neq \emptyset, |Q_m| + |Q_m'| = N_m \tag{30}$$

where Q_m is a subset of products such that the cardinality of Q_m is strictly less than N_m and it is not an empty set. I_m is the set of all N_m products and Q'_m is the complement of Q_m. While including constraint (30) in the formulation will guarantee that the optimal solution is free of any subcycles, it increases the number of constraints by $(2^{N_m} - 2) \cdot |M| \cdot |T|$.

The second alternative is instead of adding subtour elimination constraints given in (30) for all possible subcycles, to introduce these constraints iteratively for only the set of products involved in the various subcycles until the solution is free of subcycles as shown in constraint (31).

$$\sum_{i \in Q_m} \sum_{i' \in Q_m'} ZP_{i,i',m,t} \geq 1 \qquad \forall m \in (M_i \cap M_{i'}), t$$
$$Q_m = S_1, S_2, \ldots\ldots, S_{N_s}, |Q_m| + |Q_m'| = N_m \tag{31}$$

where $S_1, \ldots.S_N$ are the sets of products that are involved in the corresponding subcyles, Q'_m is the complement of set Q_m, and N_m is the set of products that can be processed on unit m.

Constraint (31) forces the model to break one of the links in each subcycle Q_m and Q'_m and to form at least one connection between set Q_m and set Q'_m. After the addition of constraint (31), if the solution does not contain any subcycles the procedure is stopped. Otherwise, constraint (31) for the new subcycles is added iteratively until the model does not introduce new subcycles. We should also note that this procedure will not guarantee the global optimum solution since all we are aiming for is a feasible sequence.

4. Examples

In this section we present three different examples to illustrate the application of the proposed model. 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.

4.1. Example 1

The first example consists of six products, A-F, four reactors, R1-R4, and five finishing trains, FT1-FT5 whose structure is shown in Figure 6. Each reactor can process only a subset of products. Namely, Reactor R1 can process products A, B, C and F; R2 can process A, B, C, D, E; R3 can process A, B, and C; and finally R4 can process D, E and F. The potential connections between reactors and the finishing trains are as follows. Reactors R1 and R3 can be connected to FT 1 to form work group 1, R2 and R4 can be connected to FT 2 to form work group 2, R2 and R3 can be connected to W3 to form work group 3, R1, R2 and R3 can be connected to FT 4 to from work group 4, and finally, R1 and R4 can be connected to FT 5 to form work group 5. The data used for this example is presented in Appendix A. We should note that, the product demand is assumed to be flexible in the sense that it is bounded by a soft upper bound and a hard lower bound as shown in Table A4.

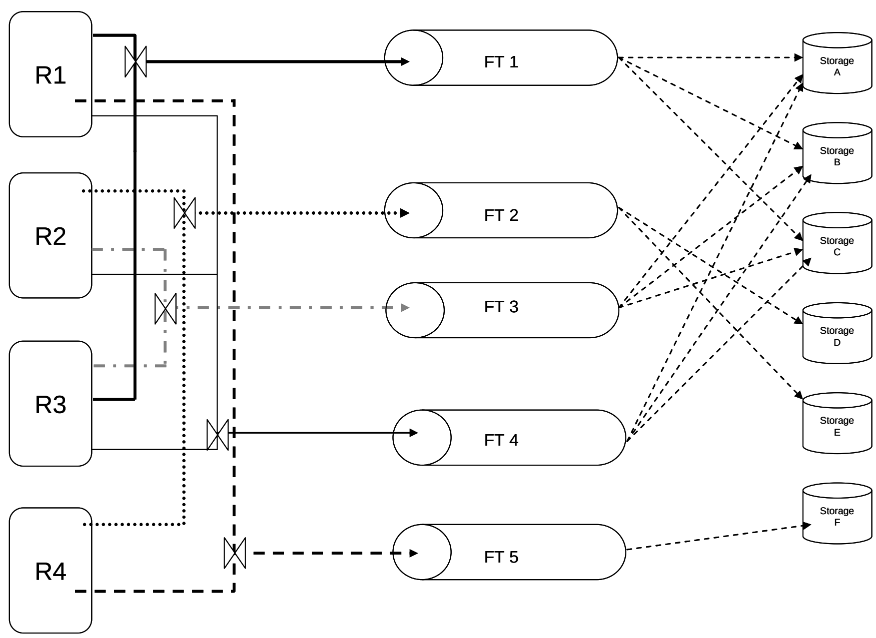

Figure 6. Schematic representation for Example 1

When the model is solved for a horizon of 3 weeks, it contains 1291 constraints, 858 continuous variables and 573 binary variables. The model yields the profit of $ 2,585,544 in 0.64 CPUs. Table 1 illustrates the computational performance of the model with respect to increasing time horizons. As can be seen, the time required to solve the problem increases dramatically with increasing time horizons. In fact, for the case of the 12 week horizon, the model failed to terminate in 10,000 CPUs yielding only a feasible solution of $ 10,791,100.

Table 1. Model and Solution Statistics for Example 1 for 3-12 Weeks

time horizon	number of binary variables	number of continuous variables	number of equations	time (CPU s)	solution ($)
3 weeks	573	858	1291	0.64	2,585,544
6 weeks	1164	1728	2611	29.82	5,478,987
12 weeks	2292	3468	5251	10,000*	10,791,100*

*Search terminated, best feasible solution posted

Figure 7 shows the optimal work groups for Example 1 which is for a horizon of 3 weeks. As can be seen, while for the first two weeks, reactors R1 and R3 connected to FT1 to form work group 1, and R2 and R4 connected to FT2 to form work group 2. In the third week these connections were severed and new connections were made between R2 and R3 to form work group 3 and R1 and R4 to form work group 5.

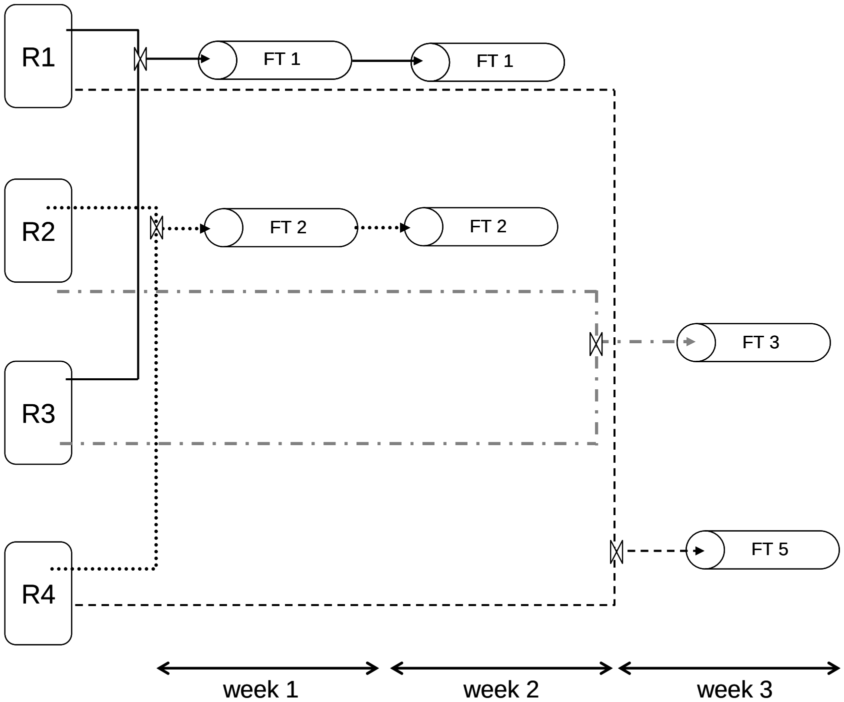

Figure 7. Optimal solution for work groups for Example 1

Figure 8 shows the optimal sequence obtained for each reactor as well as the finishing trains for each week. The numbers shown in parentheses represent the number of batches of each product. Since no subcycles were encountered in the solution, the schedule obtained corresponds to the actual schedule.

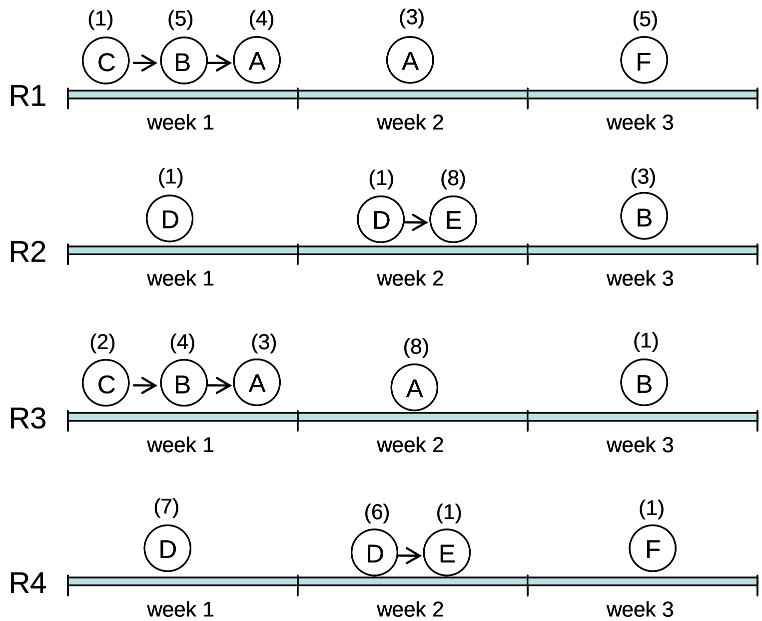

Figure 8. Optimal schedule obtained for Example 1 for 3 weeks

4.2. Example 2

In this example, we consider 10 products, A-K, 6 reactors, R1-R6 and a time horizon of 4 weeks. Each reactor can process only a subset of the products. Specifically, R1 can process A, B, C; R2 is capable of processing A, B, C, H, J, K; R3 can process C, H, J, K; R4 can process D, E, F, G, H, J, R5 can process D, E, F, G, K, and finally R6 is capable of processing D, E, F and G. The potential connections between the reactors and the finishing trains are shown in Figure 9.

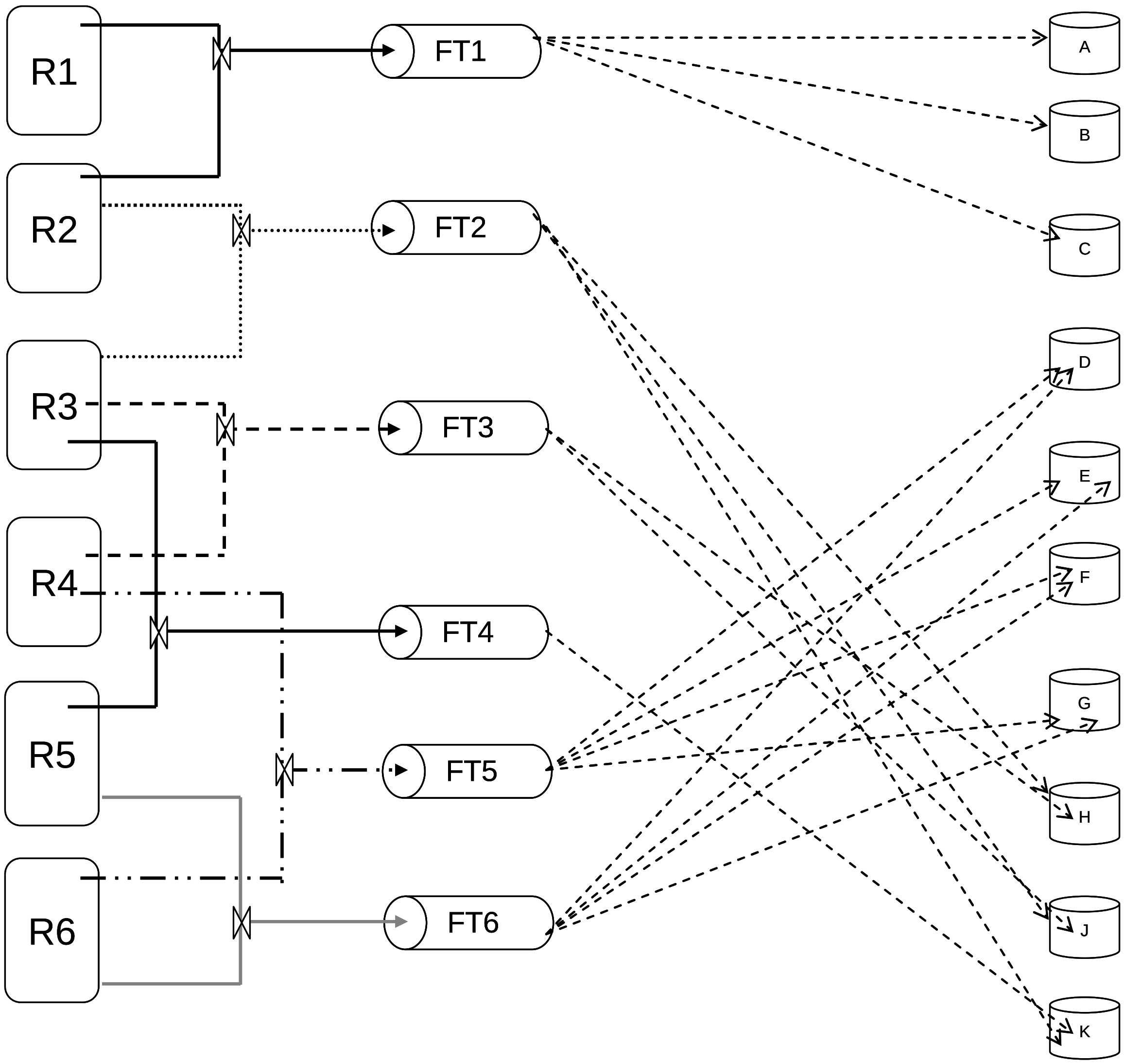

Figure 9. Schematic representation for Example 2

Table 2 shows the model and solution statistics for this example. The formulation consisted of 1992 binary variables, 2904 continuous variables and 6183 constraints. The optimal schedule with a profit of $7,986,674 was obtained in 644 CPUs.

Table 2. Model and Solution Statistics for Example 2

number of binary variables	number of continuous variables	number of equations	time (CPU s)	solution ($)
1992	2904	6183	644	7,986,674

Figure 10 shows the optimal connections between the reactors and the finishing trains for each time period. As can be seen, during weeks 1, 3 and 4 reactors R1 and R2; R3 and R4; and R5 and R6 operated as work groups, while in the second week only R1 and R2 continued to operate as a work group, and new connections were made between R3 and R5 to connect to FT4 and between R4 and R6 to connect to FT5.

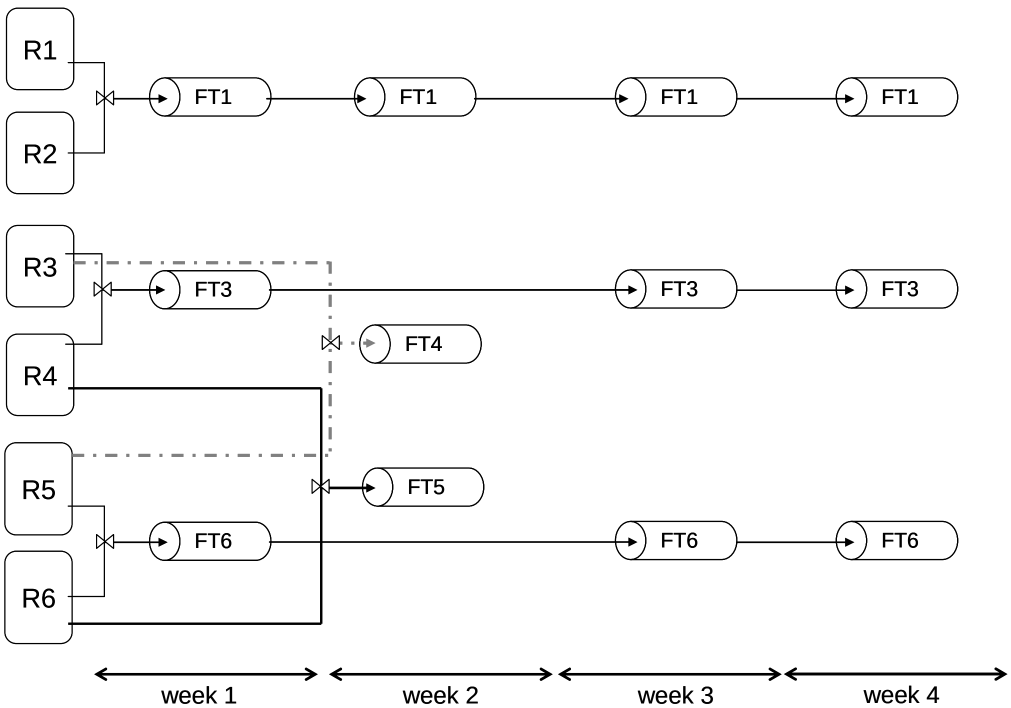

Figure 10. Optimal work group selection for Example 2

Figure 11 shows the optimal sequence and the number of batches of each product obtained for each reactor for each time period. We should note that the same sequences apply for the corresponding finishing trains. We should also note that no subcycles were encountered in the solution; hence the schedule obtained corresponds to the actual schedule.

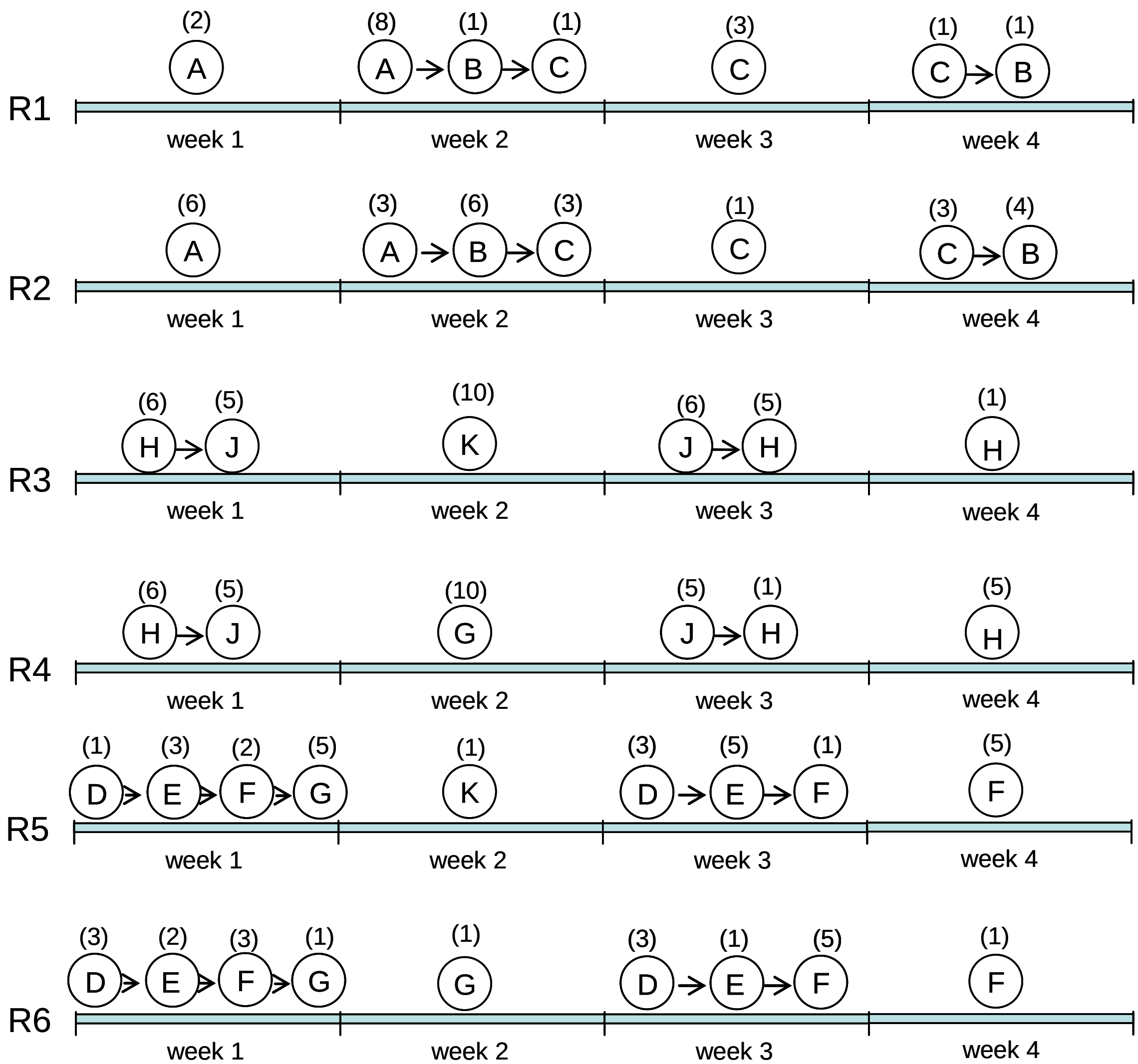

Figure 11. Optimal schedule obtained for Example 2 for 4 weeks

4.3. Example 3

The purpose of this example is to show the application of subcycle elimination constraints. The problem presented here is in essence the same as the one shown in Example 2 with the exception of the transition time and cost matrices. Since the likelihood of observing subcycles is higher in the presence of symmetric transition matrices, we have manipulated the transition time and cost values between products E and F and between products D and E as shown in Appendix A.

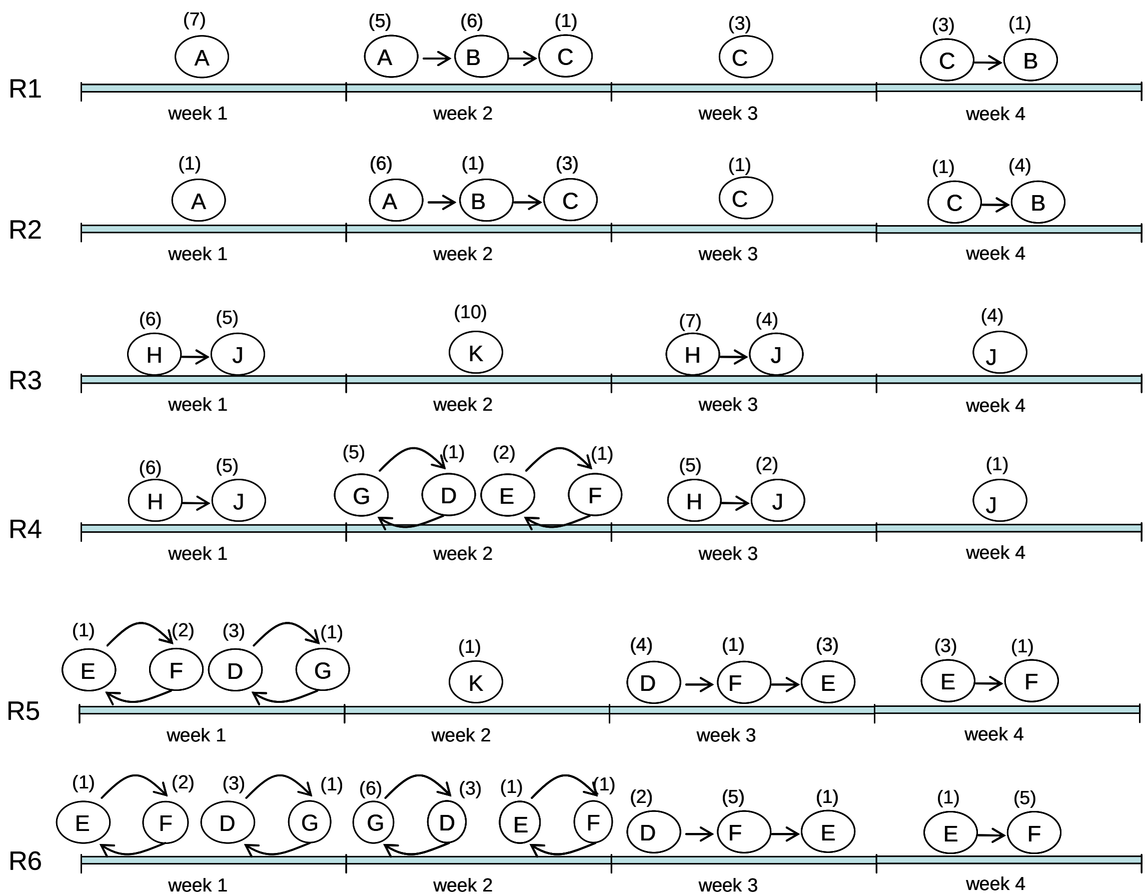

Figure 12. Optimal schedule obtained for Example 3

While there has been no change in the optimal work group selection, there have been some changes in the optimal production schedule. As can be seen from Figure 12, the solution exhibits subcycles, specifically, $S_1 = \{E, F\}$ and $S_2 = \{D, G\}$ for units R5 and R6 in the first week and for units R4 and R6 in the second week.

In order to eliminate these subcycles and to obtain a feasible production sequence, the formulation is resolved with the addition of the following four subcycle elimination constraints.

$$ZP_{D,E,R5,T1} + ZP_{D,F,R5,T1} + ZP_{G,E,R5,T1} + ZP_{G,F,R5,T1} \geq 1 \tag{32}$$

$$ZP_{D,E,R6,T1} + ZP_{D,F,R6,T1} + ZP_{G,E,R6,T1} + ZP_{G,F,R6,T1} \geq 1 \tag{33}$$

$$ZP_{D,E,R4,T2} + ZP_{D,F,R4,T2} + ZP_{G,E,R4,T2} + ZP_{G,F,R4,T2} \geq 1 \tag{34}$$

$$ZP_{D,E,R6,T2} + ZP_{D,F,R6,T2} + ZP_{G,E,R6,T2} + ZP_{G,F,R6,T2} \geq 1 \tag{35}$$

Figure 13 illustrates the optimal schedule obtained with the subcycle elimination constraints. Clearly, the solution is free of any subcycles.

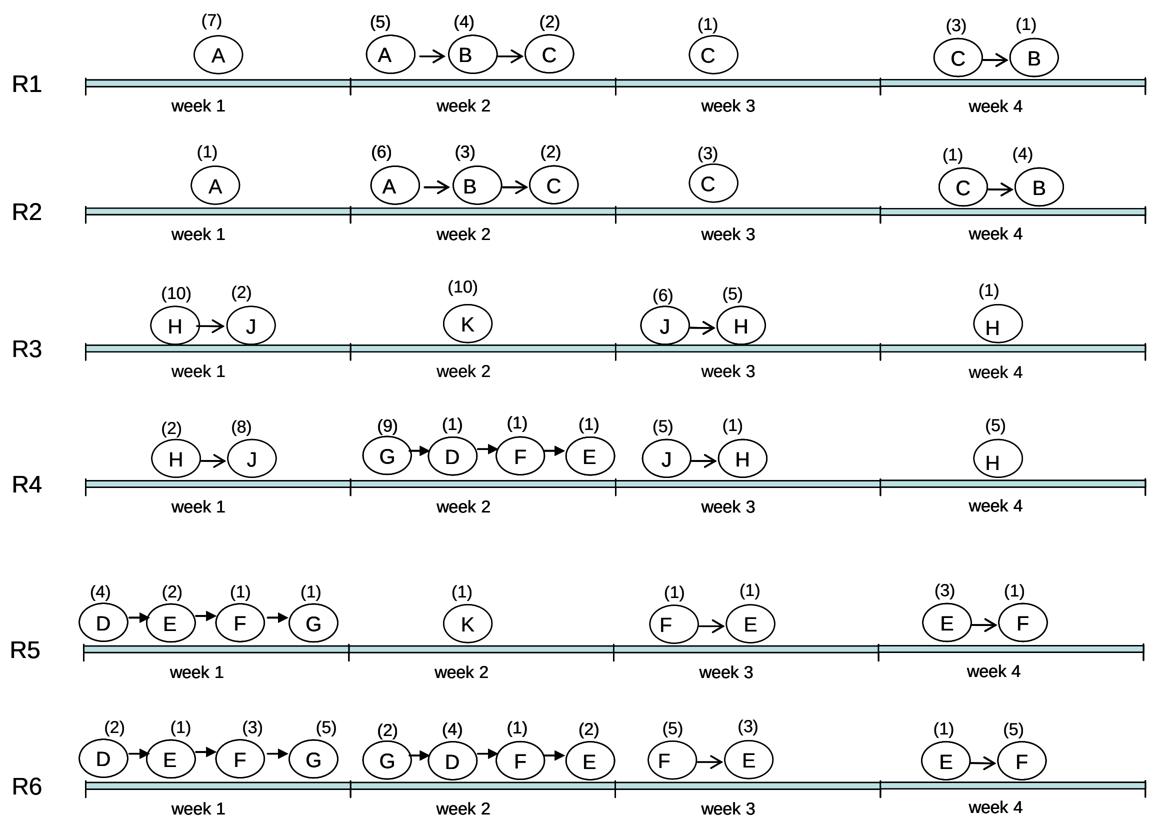

Figure 13. Optimal schedule obtained for Example 3 after introducing subcycle elimination constraints

Table 3. Model and Solution Statistics for Example 3

Model	number of binary variables	number of continuous variables	number of equations	time (CPU s)	solution ($)
original formulation	1992	2904	6183	299	8,462,343
formulation with subcycle elimination constraints	1992	2904	6187	91	8,284,540

Table 3 shows the model and solution statistics for this example. The first row represents the solution of constraints (1)-(18), (20), (22), (23), (25), (28), and (29), whereas in the second row constraints (32)-

(35) are also introduced. As can be seen the profit drops from $ 8,462,343 to $ 8,284,540 which means that in the worst case the schedule in Figure 13 has an optimality gap of 2 %.

5. Conclusions

This research note presented an MILP model for the short-term scheduling of parallel batch reactors followed by continuously operating finishing trains to form work groups. While, the recent work of Erdirik-Dogan and Grossmann (2007) has been used as a basis for the formulation given in this paper, several additional constraints and variables have been introduced to be able to accommodate this challenging problem. As has been shown with the numerical results, the computational requirements of the proposed formulation are reasonable. However, to extend this work to mid to long time horizons, a specialized solution strategy capable of dealing with the problem size would be required. Another possible extension of the application in future work is to deal with the detailed timing of production which would result in several additional challenges such as ensuring sufficient inventory levels in the intermediate storage tanks to avoid undue delays.

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Appendix A

Data for Example 1:

Table A1. Batch Sizes and Times for Example 1

	Batch Size (lb)			
	R1	R2	R3	R4
A	80,000	80,000	80,000	0
B	96,000	96,000	96,000	0
C	120,000	120,000	120,000	0
D	0	100,000	0	100,000
E	0	150,000	0	150,000
F	80,000	0	0	80,000
	Batch Time (hrs)			
	R1	R2	R3	R4
A	16	16	16	0
B	10	10	10	0
C	25	25	25	0
D	0	20	0	20
E	0	15	0	15
F	16	0	0	16

Table A2. Selling Price and Cost Data for Example 1

Product	operating costs ($/lb)	selling price ($/lb)	inventory costs ($/lb w)
A	0.35	0.95	0.01496
B	0.34	0.99	0.01339
C	0.36	0.9	0.01418
D	0.37	1.1	0.01539
E	0.3	0.85	0.01618
F	0.35	0.95	0.01496

Table A3. Changeover Times and Changeover Costs for Example 1

Product	A	B	C	D	E	F
Transition times (hrs)						
A	0	25	30	20	35	15
B	22	0	42	8	40	10
C	25	5	0	15	32	16
D	22	12	28	0	17	8
E	29	4	45	21	0	6
F	6	25	30	20	35	0
Transition costs ($/1000)						
A	0	250	300	200	350	150
B	220	0	420	90	400	100
C	250	50	0	150	320	160
D	220	120	280	0	170	80
E	290	40	450	210	0	60
F	60	250	300	200	350	150

Table A4. Upper and Lower Bounds for Demands for Example 1

Demand (lb/w)			
Upper Bounds			
Product	time period 1	time period 2	time period 3
A	640,000	720,000	160,000
B	480,000	480,000	384,000
C	600,000	480,000	480,000
D	500,000	500,000	500,000
E	450,000	750,000	600,000
F	640,000	480,000	480,000
Lower Bounds			
Product	time period 1	time period 2	time period 3
A	160,000	0	80,000
B	196,000	0	0
C	240,000	0	0
D	0	200,000	0
E	0	300,000	0
F	0	0	80,000

Data for Example 2:

Table A5. Batch Sizes and Times for Example 2

	Batch Size (lb)					
	R1	R2	R3	R4	R5	R6
A	80,000	80,000	0	0	0	0
B	96,000	96,000	0	0	0	0
C	120,000	120,000	120,000	0	120,000	0
D	0	0	0	100,000	100,000	100,000
E	0	0	0	150,000	150,000	150,000
F	0	0	0	80,000	80,000	80,000
G	0	0	0	90,000	90,000	90,000
H	0	90,000	90,000	90,000	0	0
J	0	125,000	125,000	125,000	0	0
K	0	120,000	120,000	0	120,000	0
	Batch Time (hrs)					
	R1	R2	R3	R4	R5	R6
A	16	16	0	0	0	0
B	10	10	0	0	0	0
C	15	15	15	0	15	0
D	0	0	0	20	20	20
E	0	0	0	15	15	15
F	0	0	0	16	16	16
G	0	0	0	9	9	9
H	0	12	12	12	0	0
J	0	15	15	15	0	0
K	0	10	10	0	10	0

Table A6. Selling Price and Cost Data for Example 2

Product	operating costs ($/lb)	selling price ($/lb)	inventory costs ($/lb w)
A	0.35	0.95	0.01496
B	0.34	0.99	0.01339
C	0.36	0.9	0.01418
D	0.37	1	0.01539
E	0.3	0.85	0.01618
F	0.35	0.95	0.01496
G	0.37	1.2	0.01339
H	0.37	1	0.01339
J	0.36	0.99	0.01839
K	0.36	1	0.02339

Table A7. Changeover Times and Changeover Costs for Example 2

Product	A	B	C	D	E	F	G	H	J	K
	Transition times (hrs)									
A	0	5	13	20	35	15	12	10	9	25
B	22	0	4	8	40	10	13	20	10	10
C	25	5	0	15	32	16	10	15	15	5
D	22	12	18	0	7	8	12	16	22	17
E	29	4	25	21	0	6	10	20	12	15
F	0	25	10	20	35	0	6	17	25	23
G	12	6	5	14	20	33	0	13	5	6
H	6	10	23	12	20	10	4	0	11	19
J	15	4	19	18	28	18	6	7	0	3
K	12	17	6	10	8	3	5	6	12	0
	Transition costs ($/1000)									
A	0	50	130	200	350	150	120	100	90	250
B	220	0	40	80	400	100	130	200	100	100
C	250	50	0	150	320	160	100	150	150	50
D	220	120	180	0	70	80	120	160	220	170
E	290	40	250	210	0	60	100	200	120	150
F	0	250	100	200	350	0	60	170	250	230
G	120	60	50	140	200	330	0	130	50	60
H	60	100	230	120	200	100	40	0	110	190
J	150	40	190	180	280	180	60	70	0	30
K	120	170	60	100	80	30	50	60	120	0

Table A8. Upper and Lower Bounds for Demands for Example 2

Demand (lb/w)				
Upper Bounds				
Product	time period 1	time period 2	time period 3	time period 4
A	560,000	560,000	320,000	480,000
B	480,000	480,000	288,000	480,000
C	240,000	480,000	480,000	480,000
D	500,000	400,000	400,000	500,000
E	450,000	450,000	600,000	600,000
F	320,000	160,000	480,000	480,000
G	540,000	270,000	180,000	540,000
H	540,000	630,000	540,000	540,000
J	625,000	625,000	750,000	625,000
K	600,000	600,000	480,000	480,000
Lower Bounds				
Product	time period 1	time period 2	time period 3	time period 4
A	0	0	0	0
B	0	0	0	0
C	0	0	0	0
D	0	0	0	0
E	0	0	0	0
F	0	0	0	0
G	0	0	0	0
H	0	0	90,000	0
J	0	0	125,000	0
K	0	0	0	0

Data for Example 3:

Table A9. Changeover Times and Changeover Costs for Example 3

Product	A	B	C	D	E	F	G	H	J	K
	Transition times (hrs)									
A	0	5	13	20	35	15	12	10	9	25
B	22	0	4	8	40	10	13	20	10	10
C	25	5	0	15	32	16	10	15	15	5
D	22	12	18	0	10	8	12	16	22	17
E	29	4	25	21	0	1	10	20	12	15
F	0	25	10	20	1	0	6	17	25	23
G	12	6	5	14	20	33	0	13	5	6
H	6	10	23	12	20	10	4	0	11	19
J	15	4	19	18	28	18	6	7	0	3
K	12	17	6	10	8	3	5	6	12	0
	Transition costs ($/1000)									
A	0	50	130	200	350	150	120	100	90	250
B	220	0	40	80	400	100	130	200	100	100
C	250	50	0	150	320	160	100	150	150	50
D	220	120	180	0	100	80	120	160	220	170
E	290	40	250	210	0	10	100	200	120	150
F	0	250	100	200	10	0	60	170	250	230
G	120	60	50	140	200	330	0	130	50	60
H	60	100	230	120	200	100	40	0	110	190
J	150	40	190	180	280	180	60	70	0	30
K	120	170	60	100	80	30	50	60	120	0

Nomenclature

Indices

i, i'	tasks
j	products
m	units
t	time periods
$\bar{t}$	last time period
w	work groups

Sets

I	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
M	set of units
M_i	set of units that can process task i
W	set of work groups
W_m	set of work groups that can involve unit m

Parameters

$Bound_{imt}$ 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 unit m

$Q_{i,m}$ batch size of task i in unit m

ρ_{ji} mass balance coefficient for the production of product j by task i

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

$D_{j,t}$ 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_{jt} 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

$VY_{m,w,t}$ binary variable denoting the assignment of unit m to work group w at period t

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

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

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

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

$S_{j,t}$ 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

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