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# Production Scheduling of a Multi-Grade PET Resin Plant

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**Abstract**

We present a discrete-time, Mixed Integer Linear Programming (MILP) model for the production scheduling of a continuous-process multi-grade PET resin plant. The objective is to minimize the cost associated with grade changeovers in order to avoid undesirable variations in base resin properties and process conditions that occur during such changes. The constraints of the model include requirements related to sequence-dependent changeovers, sequential processing with production and space capacity, mixed and flexible finite intermediate storage, and intermediate demand due-dates. We present a case study that illustrates the application of the model on a real problem scenario and provides insight into its behavior. The numerical experience demonstrates that the computational requirements of the model are quite reasonable for problem sizes that typically arise in practical applications.

**Key words:** Polymer industry, PET resin, continuous multi-grade process, production scheduling, mixed integer linear programming.

## 1. Introduction

Chemicals and plastics production is based on the processing of oil, natural gas and coal. It starts from a few main organic monomer chemical groupings, such as ethylene and propylene, from which various polymers are produced. A handful of these polymers form the inputs into manufactured intermediate and final plastic products. Although polymerization occurs via a variety of reaction mechanisms with different degrees of complexity, the industrial production of most polymers is more or less the same, from an operations management point of view. More specifically, it is common for polymerization plants to operate in a continuous manner in which several grades are produced using the same equipment. In this context, grades are understood as products made from the same polymer but with different end use properties, such as brightness, color, mechanical strength, etc. These end use properties of grades are dependent on molecular weight distribution and monomer conversion, which in turn are determined by operating conditions. Transition times in grade polymerization plants can be long, resulting in a considerable amount of off-specifications production. As such, the number of transitions to be made during a production sequence is an important aspect to consider when determining a production schedule for polymerization plants (Terrazas-Moreno et al. 2007).

One of the most important classes of polymers in use today is polyesters, which contain the ester functional group in their main chain. The widespread uses of polyesters range from bottles for carbonated soft drinks and water to fibers for shirts and other apparel. Polyesters also form the basis for photographic film and recording tape. Although there are many polyesters, the term “polyester” as a specific material most commonly refers to *Polyethylene Terephthalate* (PET), which is the workhorse polyester used for packaging, stretch-blown bottles and for the production of fiber of textile products. In this paper, we focus on the production scheduling of bottle-grade PET. The scheduling paradigm that we develop for PET, however, is representative of the entire polymer production industry, because it has similar characteristics from an operations management point of view, as was mentioned above.

PET is an inert plastic that does not leach harmful materials into its contents, when used as a container. For this reason, it has been the main solution for the production of packaging containers for over 20 years. The US *Food and Drug Administration* (FDA) has done rigorous testing to ensure that PET containers are safe and suitable for food and beverage storage and use. As a result, PET has been widely used for the production of food and beverage containers. An additional advantage of PET containers is that they are 100% recyclable and extremely light. Thus, they help diminish the formation of packaging waste and reduce the emission of contaminants during their transport. Furthermore, since they require less fuel during transportation, they also help saving energy.

According to McGehee et al. (2004), the key factors that increase the cost of production in a PET plant are: 1) insufficient equipment utilization, 2) unscheduled down-time and upsets, 3) variations in grade quality/waste and 4) transitions during grade changes. The first three factors can be dealt with by using good engineering and operational practices and by adopting process changes and revamps, such as implementing effective hardware modifications, carefully scheduling preventive maintenance, instituting rational quality management programs, and minimizing the effect of systematic sources of variability to the plant. The fourth factor can be dealt with by implementing careful and intelligent production scheduling. McGehee et al. (2004), expect that the practice of managing solid state polymerization plants by predictive scheduling will become more crucial in the upcoming years, since this is the most effective way to quickly respond to customer requirements with grade campaigns without large storage volumes or waste.

In this work, we present a discrete-time *Mixed Integer Linear Programming* (MILP) model for the production scheduling of a continuous-process plant that produces several grades of PET resin that is to be used for making beverage bottles. The present research was conducted as part of a project entitled “Optimization of production planning and grade distribution of a PET resin chemical plant,” which was funded by national (Greece’s) and European Union funds as well as by private funds coming from the largest PET plant in South-East Europe. Having been developed for a real *Operations Research* (OR) application, our model is tailor-made, because it includes several features that are specific to this application and can not be incorporated into any of the general-purpose, discrete-time or continuous-time model formulations that have been proposed in the literature. These special features will become apparent in the following paragraphs, where we describe in detail the operation of the PET plant that motivated this work. At the same time, however, our model is general enough to be suitable for use in other similar applications, particularly those in the polymer production industry, after performing the appropriate adjustments.

PET production is relatively simple in that yields are practically fixed and bygrade waste is minimal. The production process is non-stop and continuous, and consists of two stages in series: *Liquid State* (*or Melt*) *Polymerization* (POLY) and *Solid State Polymerization (*or *Polycondensation*) (SSP) which raises the molecular weight and hence the tensile properties of the fibers obtained by melt polymerization. Feed rate changes are possible but highly undesirable, because they cause variations in the production process and grade characteristics. A common industrial practice is to set the production rates of POLY and SSP equal to each other so that the material flow in the two stages is synchronized; if this were not the case, the storage area between them would eventually become either full (if POLY produced faster than SSP) or empty (if POLY produced at a lower rate than SSP), at which point one or both rates would have to change to avoid violating the buffer capacity constraint (typically, the two rates would be set equal to each other). Asynchronous material flow between consecutive production stages, which causes the material level in the storage space between the stages to change dynamically, has been studied quite extensively in the context of unreliable discrete-parts manufacturing (e.g., see the review paper by Dallery and Gershwin (1992)). In the continuous-flow setting that we consider in this paper, which is typical in the process industries, however, the material flow between the two processing stages is synchronized and the common production rate of the two stages may be tuned once in a while in the long run so as to match the total expected demand for all grades, in case the demand has seasonal or other long-run variations. For the purposes of short-term scheduling that we consider in this paper, however, the common production rate is assumed to be constant and equal to (or close to) the total expected demand for all grades. This assumption holds true in most real PET plants, including the one that inspired this study.

The final product or *grade* coming out of SSP is characterized by two key properties: *Color* and *Intrinsic Viscosity* (IV). IV is related to the length of the polymer chains; the higher the IV, the stiffer the material. The color is determined in the first production stage (POLY), while the IV is determined in the second stage (SSP). In the bottle-grade PET plant that inspired this work, there are four acceptable combinations of color and IV. These combinations lead to four final products, respectively, as shown in Table 1. A dash (-) denotes a color and IV combination that is not produced, because there is no demand for it. The abbreviations WG, SD, G and FH correspond to the grades *Water Grade*, *Soft Drink*, *Gray*, and *Fast Heat*, respectively.

**Table 1.** Grade of final product based on color and IV combination

| | Color | | |
|---|---|---|---|
| IV | Light (L) | Gray (G) | Dark (D) |
| Low ( < 0.8) | WG | - | - |
| High (> 0.8) | SD | G | FH |

WG is primarily used for water bottles. It is light-colored, because consumers are known to prefer clear and transparent water bottles. Moreover, it has low IV, because water bottles need not be as stiff as bottles for carbonated soft-drinks, which are under higher pressure. Carbonated soft drinks, on the other hand, are stored in high-IV bottles and can be either light-colored (SD), usually for light-colored soft drinks, or dark-colored (FH), usually for dark-colored soft drinks. From a production process viewpoint, dark-colored PET is preferable to light-colored PET, because it can produce bottles with more uniformly distributed mass density – hence, higher quality – faster, in the fast-heat and inflation molding stage of bottle making.

Grade changeovers are necessary in order to meet dynamic customer demand on time but are undesirable, because they last a significant amount of time and cause variations in base resin properties and processing conditions during the transition period. The only allowable grade changeovers are from WG to SD to G to FH and backwards (always in this order). G is an intermediate off-specification grade produced inevitably during the color changeover transition from SD to FH and vice versa. Typically, there is no regular demand for it in the primary market for PET, but it can be sold in a secondary market at a lower price. Another type of intermediate grade is produced during the IV changeover transition from WG to SD and backwards. A common industrial practice, which is also employed by the plant that inspired this work, is to divide this intermediate grade into two halves and classify the first half as WG and the second half as SD. The opposite is done in a changeover transition from SD to WG. Therefore, the entire quantity of the intermediate grade is mixed in with the pure WG and SD grades and is sold in the primary market. In effect, however, this mixing lowers the overall on-specification grade percentage, and is therefore highly undesirable.

The two production stages, POLY and SSP, are separated by an intermediate storage area, which we refer to as *Temporary Storage Stage* (TSS) and typically consists of 2-3 silos (see Figure 1). One possible way of using these silos would be to dedicate them to the different color grades coming out of POLY. For example, if there were three TSS silos, then the first silo would be used for storing *Light-colored* (L) PET, the second for storing gray (G) PET, and the third for storing *Dark-colored* (D) PET. This way, if production were to change over, say, from light- to dark-colored PET, the material coming out of POLY would have to be redirected from silo L to silo G, during the color changeover transition period, and then to silo D upon the end of the transition. Similarly, if the final grade production were to change over from SD to FH, then the silo feeding the SSP reactor would have to be switched from L to D.

In effect, however, redirecting the feeds in and out of the TSS is not instantaneous but takes a small transition time during which the grades before and after the changeover are mixed, because the pipes in and out of the TSS must be emptied from one grade before they can be filled with the next. To avoid this extra mixing, the plant that inspired this work actually uses only one of the silos in the TSS area, and reserves the other silos for special situations, such as for storing the product produced from POLY during an interruption of the SSP process caused by an unforeseen equipment failure or a scheduled maintenance. Thus, at any given time, the actively used silo in TSS has different layers of light-colored, gray, and dark-colored material stashed on top of each other.

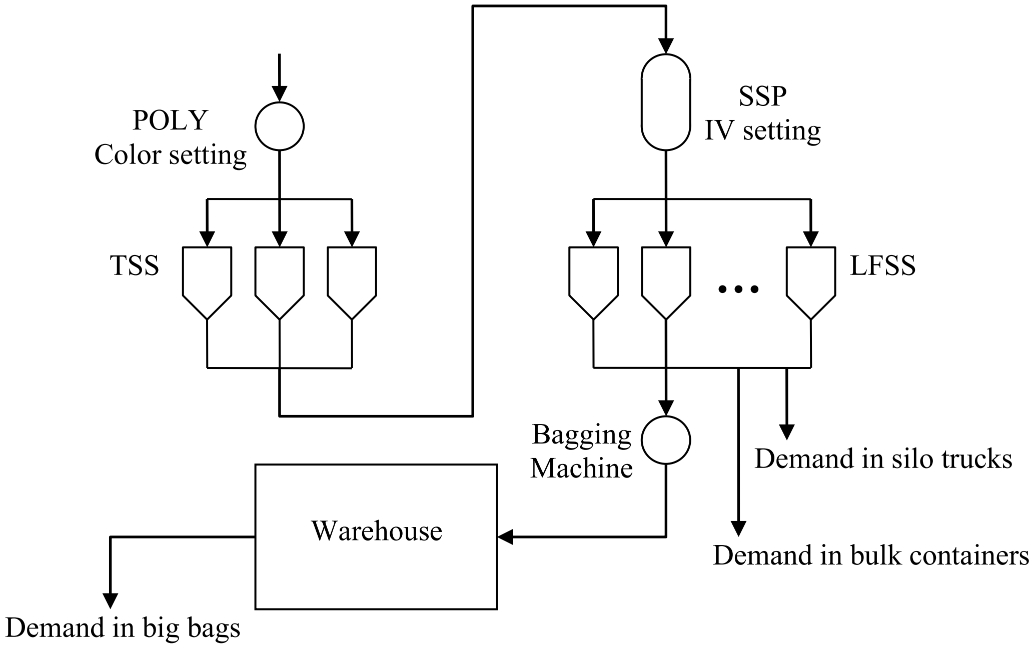


**Figure 1.** Material flow in a PET resin production plant

With this in mind, henceforth, we will assume that only one silo is actively used in TSS. This assumption eliminates the dilemma of which silo to feed POLY into, and which silo to feed SSP from; hence, it simplifies the scheduling problem. At the same time, however, it complicates the model, because one must keep track of the different layers of color present in the TSS silo. It is also worth mentioning that the SSP reactor is itself a silo with non-negligible space capacity, in which clean inert gas moves upward and chips downward. This means that material needs a significant time to travel through the reactor, and therefore what goes in SSP comes out from it with a time delay. This adds another factor of complication to the model.

The grade coming out of SSP is loaded into one of several silos at the so-called *Loading or Final Storage Stage* (LFSS). Unlike the silos in the TSS, which allow the cohabitation of different colors, the silos in the LFSS do not. Thus, each silo can only contain a single final grade at any given time. There is a degree of flexibility, however, in that it is possible to switch the grade that a silo contains. In order for this to happen, though, the silo must first be completely emptied from one grade, before it starts being filled with another.

The grade coming out of the silos in LFSS is either filled into big bags with the use of a bagging machine and stored in a finished-goods warehouse, or is directly loaded into silo trucks or bulk containers to be shipped to customers. A different unloading rate applies for each of these three distinct unloading modes of the LFSS silos. Additionally, customers may also demand PET in big bags directly from the warehouse. In this case, the big bags are loaded onto regular trucks.

The scheduling model that we develop in this paper minimizes the cost associated with the number of grade changeovers in a fixed time horizon, while also satisfying several constraints related to sequence-dependent changeovers, sequential processing with production and space capacity, mixed and flexible finite intermediate storage, and intermediate demand due-dates at both the LFSS and the warehouse. We adopt a discrete-time representation, which keeps the model relatively simple, enhances its flexibility and facilitates the introduction of additional constraints. Furthermore, our computational results demonstrate that our model can handle practical problem cases in quite reasonable times. Given the complexity of our model, which stems from the complexity of the real system that it represents, we doubt that a continuous-time representation would offer significant computational benefits.

The main input for the scheduling model is the initial setup state of POLY and SSP, the initial inventory level and grade-type in TSS, LFSS and the warehouse, and the demand forecast for each grade and transportation mode, in each period of the scheduling horizon. Given that the sales department of the plant that motivated the development of our model can forecast the demand quite accurately for a week ahead of time, a typical length of the scheduling horizon is one week. Within this horizon, several scheduling decisions must be addressed, such as which grade to produce and when to initiate a color or IV changeover transition, which LFSS silo to pour the grade coming out of SSP into, which LFSS silo to sack big bags from, if any, and which LFSS silo to load trucks or bulk containers from, to meet the demand.

As was mentioned earlier, there are several features of our model which we have not encountered in the literature on general-purpose MILP modeling in process scheduling. One such feature is that the changeover sequence in one stage depends on the setup state of the other stage. More specifically, according to Table 1, the changeover from low to high IV in SSP is not allowed, if the color setting of the material currently being processed in SSP is G or D. This complicates things considerably, since the color of the material being processed in SSP in a particular time period has been determined several periods earlier when this material was processed in POLY. Moreover, as was also mentioned earlier, even though the changeover transition time from low to high IV (and reversely) is significant, in practice, the transition itself is conventionally considered to take place instantaneously in the middle of the transition time, as far as the classification of the grade produced by SSP is concerned. What complicates the model even more is that the SSP reactor has itself a finite space capacity which introduces a delay between what goes in and out of SSP.

Another special feature of our model is that layers of different color grades are allowed to be stored on top of each other in the active silo in TSS, making it necessary to keep track of these layers. Consequently, the storage requirements of that silo do not fall in any of the usual types of intermediate storage requirements encountered in the literature on MILP modeling in process scheduling, namely, unlimited, finite dedicated or flexible (but with no mixing allowed), zero-wait, and no storage requirements (e.g., see Shaik and Floudas (2007)). For this reason, we refer to these requirements as *mixed* finite intermediate storage requirements.

Additionally, the demand for final products does not only occur at different intermediate dates, but also at two different storage stages, namely, at the LFSS and at the warehouse. This makes the LFSS both an intermediate and a final storage area, raising the question “to sack or not to sack big bags,” because sacking big bags serves to increase the service level of customers requesting big bags from the warehouse but at the same time lowers the service level of customers requesting bulk material from the silos at the LFSS.

The above features complicate the mathematical formulation of our model but also make it more interesting and challenging. The real motivation for developing our model, however, stems from the fact that it is built for a real OR application. We present a case study that illustrates the application of the model on a real problem scenario and provides insight into its behavior. The numerical experience that we provide demonstrates that the computational requirements of the model are quite reasonable for problem sizes that typically arise in practical applications.

The rest of this paper is organized as follows. In Section 2, we present a review of related works from the literature. In Section 3, we present the MILP formulation that we developed for the problem under consideration. Section 4 illustrates the application of the model on a real problem scenario, and Section 5 summarizes our work and provides suggestions for possible directions for future research.

## 2. Literature Review

The literature on chemical process scheduling is vast and rapidly growing, as indicated by the existence of numerous published reviews that bring to light a wealth of general-purpose modeling approaches and solution techniques. A common theme in many of these reviews (e.g., Kallrath, 2002 and Méndez et al., 2006) is the classification of process scheduling models and solution approaches in terms of plant topology, process representation, time representation, operation modes, demand pattern, changeover and storage characteristics, and other features that are involved in most process scheduling problems.

An important differentiation is made between batch processes and continuous processes, with most of the published works addressing batch processes. Reklaitis (1992) overviews the scheduling and planning of batch process operations, focusing on the basic elements of chemical process scheduling problems and the available solution methods, while Kondili et al. (1993) present a general framework for handling a wide range of scheduling problems arising in batch chemical plants. There are numerous other more recent works on batch process scheduling. Typical examples are the work of Grünow et al. (2002), who present a hierarchical modeling approach to coordinate various plant operations in a multi-stage batch process chemical industry, and the works of Janak et al. (2006a, 2006b), who present efficient MILP formulations for scheduling large-scale industrial batch plants. In the context of continuous processes, a very recent work by Shaik et al. (2009) presents a framework for short-term and medium-term scheduling of large-scale industrial continuous plants.

Another important differentiation in the process scheduling literature is between discrete-time and continuous-time models. Ierapetritou and Floudas (1998a,1998b) propose effective continuous-time formulations for both batch and continuous processes. Janak et al. (2004) extend these formulations to incorporate several additional features, such as different storage policies, resource constraints, variable batch sizes and processing times, batch mixing and splitting, and sequence-dependent changeover times, while Shaik and Floudas (2007) further extend them to rigorously treat storage requirements. Lin and Floudas

(2001) propose a continuous-time formulation for design, synthesis and scheduling of multipurpose batch plants, and test it on both linear and nonlinear cases, and Shaik et al. (2006) present a performance comparison and evaluation of several continuous-time models for short-term scheduling of multipurpose batch plants.

Mockus and Reklaitis (1999) address the problem of decision timing in the context of batch and continuous process scheduling, Neumann et al. (2002) develop a batch scheduling problem that is modeled as a resource-constrained problem and is solved by an efficient truncated branch-and-bound algorithm, and Giannelos and Georgiadis (2002) propose a formulation for short-term scheduling of multipurpose continuous processes. A relatively recent overview and comparison of discrete-time and continuous-time approaches for the scheduling of chemical processes can be found in Floudas and Lin (2004). The focus there is on a class of processes called sequential, which exhibit a linear structure in the production recipe, without material merging/splitting or recycle. The model that we study in this paper falls into that class. Finally, in a recent monograph, Suerie (2005) addresses the issue of time-continuity in discrete time models.

Chemical process scheduling models can be efficiently formulated using mixed integer optimization techniques. Grossmann et al. (1996) provide an overview of such techniques for the design and scheduling of batch processes, emphasizing on general-purpose methods for MILP and *Mixed Integer Non Linear Programming* (MINLP) problems. Pinto and Grossmann (1998) present an overview of assignment and sequencing models used in the scheduling of process operations with mathematical programming techniques. The authors identify two major categories of scheduling models, single-unit and multiple-unit assignment models, and discuss the critical modeling issues of time domain representation and network structure. Méndez and Cerdá (2002) propose a MILP mathematical formulation for scheduling resource-constrained multigrade continuous chemical plants that uses a continuous-time domain representation. Janak and Floudas (2008) suggest preprocessing techniques for closing the integrality gap of MILP continuous-time formulations for batch processing scheduling. Other MILP models for production scheduling of chemical processes have been proposed by Pinto and Grossmann (1995), Lee et al. (1996), Pinto (1997), Hui et al., (2000) and Castro and Grossmann (2006), to name a few. A recent review of several MILP based approaches for the scheduling of chemical process facilities which focuses on short-term scheduling of processes that can be represented as general networks can be found in Floudas and Lin (2005).

Besides the general-purpose modeling approaches for the scheduling of generic chemical process industries, there have also been several works that are specific to the scheduling of different types of polymerization processes. One such example is the work by Qiu and Burch (1997), who develop a hierarchical production planning and scheduling model to solve a real-world problem in fiber manufacturing scheduling. The model requires determining production sequences in the presence of variable setup costs in a multi-machine and multi-grade environment. The emphasis is on the integration of the different levels of the hierarchy and on the development of the concept of the expected setup cost to circumvent the difficulty that until the production sequences are known, the exact setup costs can not be determined. Another example is the work of Wang et al. (2000), who develop a MINLP model for the batch scheduling of a polymer plant producing expandable polystyrene. None of the different products can be produced separately and only their relative proportion can be influenced by the choice of the recipes of the polymerizations. An augmented genetic algorithm is used to solve the model.

Recently, there have also been some works on the joint optimization of scheduling and process control during changeover transitions in polymerization processes. Mahadevan, Doyle, and Allcock (2002) analyze the schedule of grade transitions for a polymerization reactor (isothermal free radical polymerization of methyl methacrylate (MMA) with azobis-isobutyronitrile as initiator and toluene as the solvent) that is controlled by a simple linear controller. The dominant factor determining the schedule of grade transitions is the transition cost related to the off-specification product. Nyström at al. (2005) present a method for solving the problem of grade transition sequencing and dynamic optimization in polymerization processes. The method is based on decomposing the problem into two separate sub-problems – dynamic optimization (called primal problem) and scheduling (called master problem) – and solving them in an iterative manner. Terrazas-Moreno et al. (2007) present a *Mixed Integer Dynamic Optimization* (MIDO) model for the simultaneous optimal scheduling and control during transitions of a multi-grade polymerization continuous stirred-tank reactor. The schedules sought are strictly cyclic (each grade is produced once in each cycle), and the storage requirements downstream of the reactor are treated simplistically. The emphasis is on the behavior of the process during transitions. In a somewhat related work, Prata et al. (2008) present a MIDO modeling and numerical solution method for an integrated grade transition and production scheduling problem for a continuous polymerization reactor typically used for the production of homo- and copolymers of olefins. The emphasis is on modeling the nonlinear dynamics of the polymerization process in the reactor during transitions, but the downstream process units following the reactor are neglected. All the above works focus on different aspects of polymerization process scheduling (e.g., on the integration of planning and scheduling, on the use of genetic algorithms to solve the scheduling problem, on the combination of optimal scheduling and process control during transitions), but none is directly related to our work, as none includes in detail aspects such as inventory management and market demand for different grades.

Finally, there are many production scheduling models for continuous chemical processes that are similar to the one that we address in this work. For example, Bok and Park (1998) present an efficient short-term scheduling mixed integer programming model for a multipurpose pipeless plant over a continuous-time domain. Doganis et al. (2005) develop a MILP model for determining the optimal production schedule in a lubricant production plant, and Tousain and Bosgra (2006) propose an approach for flexible production scheduling in continuous multi-grade chemical processes.

To the best of our knowledge, the development of an optimization model for production scheduling in a PET production facility has not been addressed in the past. Moreover, as was mentioned earlier, the PET plant that we consider in this paper has several features that make it unbefitting the general-purpose models discussed above. For this reason, in what follows, we develop a specific MILP model for it that is general enough, however, to be applicable to other similar applications, particularly in the polymer production industry.

# 3. MILP Model Development

For the needs of our model, we discretize time by dividing the scheduling horizon, typically one week, into a finite number of identical time periods. The length of each period must be no bigger than the length of the shortest nonstop event that takes place in the entire process. This could be the transition time of a grade changeover, the time of a shift, if different shifts have different characteristics, etc.

The production facility operates on a 24-hour basis, so in each period, POLY produces an amount of material which is equal to the constant production rate of the plant, denoted by $P$, multiplied by the length of the period; therefore, POLY is considered as a source of material (we assume that it is never starved of raw material), and the material that it produces in each period is referred to as a *lot*.

The next step is to discretize space at the TSS and SSP stages by dividing their capacities into an integer number of *slots*, where each slot accommodates exactly one lot. At the beginning of the scheduling horizon, the active silo in the TSS has some initial material in it that occupies several slots – say $N$ slots – and the SSP reactor is filled with material up to its capacity, which is equal to, say, $M$ slots. The SSP reactor has the same production rate as POLY, as was mentioned in Section 1; therefore, in each period, the TSS and the SSP stages consume from their upstream stage and release into their downstream stage exactly one lot. This implies that in every period of the scheduling horizon, the number of lots in TSS and SSP is constant and equal to $N$ and $M$, respectively.

Note that if the production rates of POLY and SSP were allowed to be different, then we would have to keep track of the dynamically changing level of material (number of non-empty slots) in the TSS, as well as the type of material in each slot. In fact, this is more or less what we do in the case of the LFSS, where the input rate is constant but the output rate is partly variable and uncontrollable, due to the varying demand, and partly controllable, as the rate of bagging bulk material from the LFSS into big bags is a decision variable.

The color (L, G or D) of the lot in the $n^{\text{th}}$ slot of the $N + M$ slots of the TSS and the SSP reactor taken together depends on the setup state (L, G or D) of POLY $n$ periods before the beginning of the time horizon. Therefore, in order to characterize the color in the $N + M$ slots of the TSS and the SSP reactor, we need to know the setup state of POLY during the last $N + M$ periods before the beginning of the scheduling horizon. With this in mind, we shift the time axis by $N + M$ periods so that the first period of the scheduling horizon is $N + M + 1$, and therefore periods 1 to $N + M$ refer to the past.

Next, we present the MILP formulation that we developed for the problem under consideration. The following notation is used:

**Sets:**

$I$ : set of colors produced by POLY, indexed by $i$, $I = \{1, 2, 3\} \equiv \{\text{L, G, D}\}$

$J$ : set of final grades, indexed by $j$, $J = \{1, 2, 3, 4\} \equiv \{\text{WG, SD, G, FH}\}$

$Q$ : set of silos in LFSS, indexed by $q$

**Parameters:**

$T$ : index of the last period of the scheduling horizon

$P$ : production quantity of the process in one period

$N$ : number of slots in TSS

$M$ : number of slots in SSP

$d$ : cost incurred per color changeover at POLY

$c$ : cost incurred per IV changeover at SSP

$B$ : duration of a color changeover transition at POLY (in number of periods)

$F$ : duration of an IV changeover transition at SSP (in number of periods)

$X0_{1t}$ : binary parameter that takes the value 1 if the lot produced by POLY in period $t$ has color L, and 0 otherwise, $t = 1,\ldots, N + M$

$X0_{2t}$ : binary parameter that takes the value 1 if the lot produced by POLY in period $t$ has color G, and 0 otherwise, $t = 1,\ldots, N + M$

$X0_{3t}$ : binary parameter that takes the value 1 if the lot produced by POLY in period $t$ has color D, and 0 otherwise, $t = 1,\ldots, N + M$

$A0_t$ : binary parameter that takes the value 1 if an IV change is initiated at the beginning of period $t$, and 0 otherwise, $t = N + M - F + 2,\ldots, N + M$

$Z0$: binary parameter that takes the value 1 if the IV of the lot stored in the last slot of SSP at the beginning of the scheduling horizon is high, and 0 otherwise

$W0_{qj}$ : binary parameter that takes the value 1 if grade $j$ is stored in silo $q$ of LFSS at the beginning of the scheduling horizon, and 0 otherwise

$S0_{qj}$ : quantity of grade $j$ contained in silo $q$ of LFSS at the beginning of the scheduling horizon

$S_{max}$ : capacity of a silo in LFSS

$S_{min}$ : minimum quantity of a nonempty silo in LFSS

$SS_{min\,j}$ : safety stock of grade $j$ in LFSS at the end of the scheduling horizon

$u_{ST}$ : maximum quantity of material that can be loaded from LFSS into a silo truck in one period

$u_{BC}$ : maximum quantity of material that can be loaded from LFSS into a bulk container in one period

$u_{BB}$ : maximum quantity of material that can be sacked from LFSS into big bags in one period

$R0_j$ : grade $j$ inventory in the warehouse at the beginning of the scheduling horizon

$R_{max}$ : warehouse capacity

$R_{min\,j}$ : safety stock of grade $j$ in the warehouse at the end of the scheduling horizon

$dST_{jt}$: silo trucks demand of grade $j$ in period $t$, $t = N + M + 1,\ldots, T$

$dBC_{jt}$: bulk containers demand of grade $j$ in period $t$, $t = N + M + 1,\ldots, T$

$dBB_{jt}$: big bags demand of grade $j$ in period $t$, $t = N + M + 1,\ldots, T$

**Decision Variables:**

$x_{it}$ : binary decision variable that takes the value 1 if the lot produced by POLY in period $t$ has color $i$, and 0 otherwise, $t = 1,\ldots, T$

$y_{jt}$: binary decision variable that takes the value 1 if final grade $j$ is produced by SSP in time period $t$, and 0 otherwise, $t = N + M + 1, \ldots, T + (F/2)$

$a_t$: binary decision variable that takes the value 1 if an IV changeover is initiated at the beginning of period $t$, and 0 otherwise, $t = N + M - F + 2, \ldots, T$

$z_t$: binary decision variable that takes the value 1 if the IV of the grade produced in period $t$ is high, and 0 otherwise, $t = N + M, \ldots, T + (F/2)$

$S_{qjt}$: quantity of grade $j$ in silo $q$ of LFSS at the end of period $t$, $t = N + M, \ldots, T$

$W_{qjt}$: binary decision variable that takes the value 1 if grade $j$ is contained in silo $q$ of LFSS in period $t$, and 0 otherwise, $t = N + M, \ldots, T$

$g_{qjt}$: binary decision variable that takes the value 1 if grade $j$ is loaded from SSP into silo $q$ of LFSS in period $t$, and 0 otherwise, $t = N + M + 1, \ldots, T$

$G_{qjt}$: quantity of grade $j$ that is unloaded from silo $q$ of LFSS in period $t$, $t = N + M + 1, \ldots, T$

$b_{qjt}$: quantity of grade $j$ that is loaded from silo $q$ of LFSS into big bags in period $t$, $t = N + M + 1, \ldots, T$

$f_{qjt}$: quantity of grade $j$ that is loaded from silo $q$ of LFSS into silo trucks in period $t$, $t = N + M + 1, \ldots, T$

$h_{qjt}$: quantity of grade $j$ that is loaded from silo $q$ of LFSS into bulk containers in period $t$, $t = N + M + 1, \ldots, T$

$R_{jt}$: quantity of grade $j$ in the warehouse at the end of period $t$, $t = N + M, \ldots, T$

The formulation that we develop next also assumes that the following inequalities hold: $F < N + M$, $B < N + M$, $N + M < T - (N + M)$. These restrictions hold in practice.

The objective function of our model is expressed as

$$\text{Minimize} \quad c\left(\sum_{t=N+M+1}^{T} a_t\right) + d\left(\frac{1}{B}\sum_{t=N+M+1}^{T} x_{2t}\right) \tag{1}$$

The above expression minimizes the weighted sum of the number of IV and color changeovers during the scheduling horizon, i.e., from period $N + M + 1$ to period $T$. The first summation in the objective function represents the number of IV changeovers. The second summation represents the total number of color changeover transition periods. It is divided by $B$, i.e., by the duration of a color changeover transition, to give the number of color changeovers.

Next, we present the constraints of our model. Constraints (2)-(11) are related to the processing part of the plant, which comprises POLY, TSS and SSP.

$$\sum_{i \in I} x_{it} = 1, \; t = 1, \ldots, T \tag{2}$$

$$\left.\begin{array}{l} x_{1t} + x_{3t+p} \le 1 \\ x_{3t} + x_{1t+p} \le 1 \end{array}\right\}, \; t = 1, \ldots, T - 1, \; p = 1, \ldots, \min(T - t, B) \tag{3}$$

$$\left.\begin{array}{l} y_{1t} + y_{3t+1} \le 1 \\ y_{3t} + y_{1t+1} \le 1 \end{array}\right\}, \; t = N + M, \ldots, T + (F/2) - 1 \tag{4}$$

Constraint set (2) states that POLY can only produce a single color in each period. Since the color of the final grade exiting SSP in any period was determined in POLY $N + M$ periods earlier, at the beginning of the scheduling horizon, the color in slots 1,…, $N + M$ has already been predetermined; therefore, in effect, constraint (2) must really be imposed from period $N + M + 1$ and on only. Its application to periods 1,…, $N + M$ is merely a routine check that serves to verify that the initial status of the system, as decided in the previous scheduling horizon, results in feasible production settings during the present horizon, too. This modeling technique is also adopted in several of the other model constraints which follow.

Constraint set (3) states that between two periods in which POLY produces colors L and D (in either order), $B$ periods in which POLY produces G must always intervene. Note that the actual number of constraints of this set depends not only on the length of the scheduling horizon but also on the value of $B$. More specifically, if $B = 1$, then POLY can not produce colors D and L in two adjacent periods. If $B > 1$, this restriction is imposed not only to adjacent periods, but also to periods that are spaced $i$ periods apart, for $i$ = 2,…, $B$.

Similarly, constraint set (4) states that final grades WG and G can not be produced in two adjacent periods, because at least one period in which grade SD is produced must always intervene. Since the color is determined in POLY and any IV change in SSP becomes effective $F/2$ periods after it is initiated, the final grade that will be produced in the first $F/2$ periods of the scheduling horizon, i.e., in periods $N + M + 1$,…, $N + M + (F/2)$, is predetermined by the initial state of the system. Therefore, constraint set (4) must really be imposed from period $N + M + (F/2)$ and on only. Its application to periods $N + M$,…, $N + M + (F/2) - 1$ serves to verify that the initial conditions are feasible. To ensure that the current production schedule will also remain feasible in the next scheduling horizon, this set of constraints also extends to periods $T + 1$,…, $T + (F/2) - 1$. Combined together, constraint sets (3) and (4) ensure that the only allowable grade changeovers are from WG to SD to G to FH and backwards, always in this exact sequence.

$$\sum_{s=t}^{t+F-1} a_s \le 1, \; t = N + M - F + 2, \dots, T - F + 1 \tag{5}$$

$$a_t \le x_{1t-N-M}, \; t = N + M + 1, \dots, T \tag{6}$$

$$\left.\begin{aligned} z_{t+(F/2)} - z_{t+(F/2)-1} &\le a_t \\ z_{t+(F/2)} - z_{t+(F/2)-1} &\ge -a_t \end{aligned}\right\}, \; t = N + M + 1 - (F/2), \dots, T \tag{7}$$

$$\left.\begin{aligned} z_{t+(F/2)} + z_{t+(F/2)-1} &\ge a_t \\ z_{t+(F/2)} + z_{t+(F/2)-1} &\le 2 - a_t \end{aligned}\right\}, \; t = N + M + 1 - (F/2), \dots, T \tag{8}$$

Constraint set (5) states that only one IV change can be initiated at SSP within $F$ consecutive periods. This constraint stems from the fact that an IV change in the SSP reactor lasts $F$ periods in total, and can not be interrupted before it is fully completed. The grade produced by SSP during the first $F/2$ periods after an IV changeover is initiated is considered to have the characteristics of the grade that was produced before the beginning of the changeover transition, while the grade being produced during the last $F/2$ periods is considered to have the characteristics of the grade that will be produced after the end of the transition. Therefore, $F$ is only limited to even integers.

Constraint set (6) states that an IV changeover can only be initiated if the color of the grade currently being produced is L, because, as can been seen from Table 1, no IV changeover is possible when the color setting is G or D. Constraint sets (7) and (8) ensure that if an IV changeover is initiated at the beginning of period $t$, then this change becomes effective in period $t + (F/2)$ and onward. If $a_t = 0$, constraint set (8) is redundant, and constraint set (7) reduces to $z_{t+(F/2)} = z_{t+(F/2)-1}$, ensuring that the IV remains unchanged. On the other hand, if $a_t = 1$, constraint set (7) is redundant, and constraint set (8) reduces to $z_{t+(F/2)} + z_{t+(F/2)-1} = 1$, ensuring that the IV changes at the beginning of period $t + (F/2)$.

To help clarify matters, a pictorial representation of the relationship between variables $x_{it}$, $y_{jt}$ and $z_t$ is shown in Figure 2. The top part of that figure is a snapshot of the contents of POLY, TSS and SSP at the end of the last period before the beginning of the scheduling horizon, i.e., at the end of period $N + M$. As shown in this snapshot, the color of the lots occupying slots 1 to $N + M$ has already been predetermined. For example, the color of the lot in slot $N + M$ was determined in period 1 and is given by vector $\mathbf{x}_1 \equiv (x_{11}, x_{21}, x_{31})$. The bottom part of Figure 2 shows the contents of POLY, TSS and SSP at the end of the first period of the scheduling horizon, i.e., period $N + M + 1$. As shown in this schematic representation, each lot has advanced by one slot. As a result, the lot that occupied the last slot of SSP has exited SSP. Its grade, which is given by vector $\mathbf{y}_{N+M+1} \equiv (y_{1N+M+1}, y_{2N+M+1}, y_{3N+M+1}, y_{4N+M+1})$, is a combination of its color, which was determined in period 1 by the value of $\mathbf{x}_1$, and its IV, which is determined in period $N + M + 1$ by the value of $z_{N+M+1}$.

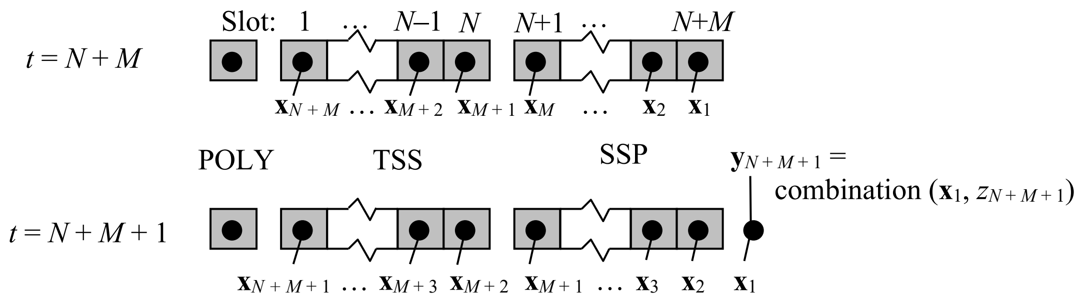


**Figure 2.** Time shift representation in the production process

$$\left.\begin{array}{l} x_{2\,t-N-M} \le z_t \\ x_{3\,t-N-M} \le z_t \end{array}\right\}, \; t = N + M + 1, \ldots, T + (F/2) \tag{9}$$

$$\left.\begin{array}{l} y_{1t} \ge x_{1\,t-N-M} - z_t \\ y_{2t} \ge z_t + x_{1\,t-N-M} - 1 \\ y_{3t} \ge z_t + x_{2\,t-N-M} - 1 \\ y_{4t} \ge z_t + x_{3\,t-N-M} - 1 \end{array}\right\}, \; t = N + M + 1, \ldots, T + (F/2) \tag{10}$$

$$\sum_{j \in J} y_{jt} = 1, \; t = N + M + 1, \ldots, T + (F/2) \tag{11}$$

Constraint set (9) is introduced to ensure that colors G and D can only be combined with high IV. Constraint set (10) determines the final grade based on the combination of color and IV, while constraints

(11) state that only a single grade can be produced in any period of the scheduling horizon. If status verification is not necessary, constraints (9)-(11) can be applied from period $N + M + (F/2) + 1$ and on.

Constraint sets (12)-(29) are related to the storage part of the plant, which comprises LFSS and the warehouse.

$$g_{qjt} \le W_{qjt}\, ,\, q \in Q, j \in J,\, t = N + M + 1,\ldots,\, T \tag{12}$$

$$\sum_{q} g_{qjt} \le y_{jt}\, ,\, j \in J,\, t = N + M + 1,\ldots,\, T \tag{13}$$

$$\sum_{q \in Q}\sum_{j \in J} g_{qjt} = 1\, ,\, t = N + M + 1,\ldots,\, T \tag{14}$$

$$\sum_{j \in J} W_{qjt} \le 1\, ,\, q \in Q,\, t = N + M + 1,\ldots,\, T \tag{15}$$

$$W_{qjt+1} - W_{qjt} \le 1 - \sum_{r \in J} W_{qrt}\, ,\, q \in Q, j \in J,\, t = N + M,\ldots,\, T - 1 \tag{16}$$

Constraint set (12) ensures that in each period, grade $j$ can not be loaded from SSP into silo $q$ of the LFSS, unless this silo already has grade $j$ in it at the beginning of this period. Constraint (13) ensures that in each period, the grade loaded into any silo of the LFSS is the same with the grade that is being produced by SSP in the same period. Constraint set (14) ensures that in each period, a single grade will be loaded from SSP into a single silo of LFSS. Constraint set (15) states that in each period, each silo of the LFSS can store at most one grade.

Constraint set (16) states that the grade stored in a silo of the LFSS can not change unless a period in which this silo is empty intervenes. The summation $\sum_{r \in J} W_{qrt}$ is equal to 1 when silo $q$ contains some final grade in period $t$, and 0 if it is empty. Thus, a difference equal to 0 in the right-hand side forces the difference in the left-hand side to be 0, ensuring that any grade $j$ which is different from the one that was contained in the silo in the previous period, can not be poured in this silo before it is completely emptied. Note that index $j$ is used in both terms of the left-hand side to disclose whether a *particular* grade $j$ can be poured into silo $q$ in period $t + 1$, while $r$ is used in the right-hand side to disclose whether silo $q$ contained *any* final grade $r$ in the previous period.

$$S_{qjt} \le S_{\max} W_{qjt}\, ,\, q \in Q, j \in J,\, t = N + M + 1,\ldots,\, T \tag{17}$$

$$S_{qjt} \ge S_{\min} W_{qjt}\, ,\, q \in Q, j \in J,\, t = N + M + 1,\ldots,\, T \tag{18}$$

$$G_{qjt} \le W_{qjt} \max(u_{ST}, u_{BC}, u_{BB})\, ,\, q \in Q, j \in J,\, t = N + M + 1,\ldots,\, T \tag{19}$$

$$S_{qjt} = S_{qjt-1} + g_{qjt} P - G_{qjt}\, ,\, q \in Q, j \in J,\, t = N + M + 1,\ldots,\, T \tag{20}$$

$$\sum_{q \in Q} S_{qjT} \ge SS_{min\, j}\, ,\, j \in J \tag{21}$$

Constraint set (17) states that the grade quantity stored in a silo can not exceed the silo’s capacity, and ensures that it will be zero whenever the corresponding variable $W$ determines that this silo is empty. Constraint set (18) imposes a lower bound on the quantity of a nonempty silo. It is introduced to eliminate the situation in which a silo stores a negligible but positive grade quantity. Constraint set (19) states that no grade can be unloaded from an empty silo and imposes the maximum rate in which a silo can be unloaded, based on the values of variables *u*. Constraint set (20) ensures flow continuity, by updating the quantity stored in each silo, based on the quantity that it contained in the previous period, and the quantities loaded into and out of it in the next period. Note that the quantity produced by POLY and SSP in one period and all the quantities that can be unloaded or sacked from the LFSS depend on the period length. Constraint set (21) ensures that the total inventory of each grade in the LFSS is at or above the specified safety stock for that grade at the end of the scheduling horizon.

$$G_{qjt} = f_{qjt} + h_{qjt} + b_{qjt} \, , q \in Q, j \in J, t = N + M + 1, \ldots, T \tag{22}$$

$$\frac{1}{u_{ST}} f_{qjt} + \frac{1}{u_{BC}} h_{qjt} + \frac{1}{u_{BB}} b_{qjt} \leq 1, \, q \in Q, j \in J, t = N + M + 1, \ldots, T \tag{23}$$

$$dST_{jt} = \sum_{q \in Q} f_{qjt} \, , j \in J, t = N + M + 1, \ldots, T \tag{24}$$

$$dBC_{jt} = \sum_{q \in Q} h_{qjt} \, , j \in J, t = N + M + 1, \ldots, T \tag{25}$$

$$\sum_{q \in Q} \sum_{j \in J} b_{qjt} \leq u_{BB} \, , t = N + M + 1, \ldots, T \tag{26}$$

$$R_{jt} = R_{jt-1} + \sum_{q \in Q} b_{qjt} - dBB_{jt} \, , j \in J, t = N + M + 1, \ldots, T \tag{27}$$

$$\sum_{j \in J} R_{jt} \leq R_{\max} \, , t = N + M + 1, \ldots, T \tag{28}$$

$$R_{jT} \geq R_{min\,j} \, , j \in J \tag{29}$$

Constraint set (22) states that, in each period, the total quantity of grade *j* unloaded from any silo of the LFSS is equal to the quantity that is loaded into silo trucks or bulk containers, or sacked into big bags and stored in the warehouse. Constraint set (23) defines the maximum unloading rate of any silo, based on the exact unloading mode. Constraint sets (24) and (25) ensure that the demand for silo trucks and bulk containers is satisfied for each period of the scheduling horizon. Constraint set (26) ensures that the maximum sacking rate is not exceeded. Note that, while several silos can be used simultaneously for loading silo trucks or bulk containers, bagging can only take place in one silo, because only one bagging machine is available. Constraint set (27) updates the inventory stored in the warehouse, and constraint set (28) ensures that the total grade quantity stored in the warehouse does not exceed its capacity. Finally, constraint set (29) ensures that the inventory of each grade in the warehouse is at or above the specified safety stock at the end of the scheduling horizon.

Constraints (30)-(35) initialize the state of the system at the beginning of the scheduling horizon.

$$x_{it} = X0_{it} \, , t = 1, \ldots, N + M \tag{30}$$

$$z_{N+M} = Z0 \tag{31}$$

$$a_t = A0_t \, , t = N + M - F + 2, \ldots, N + M \tag{32}$$

$$S_{qjt} = S0_{qj}\ , q \in Q, j \in J, t = N + M \tag{33}$$

$$W_{qjt} = W0_{qj}\ , q \in Q, j \in J, t = N + M \tag{34}$$

$$R_{jt} = R0_{j}\ , j \in J, t = N + M \tag{35}$$

More specifically, constraint sets (30)-(32) initialize the state of the production system at the beginning of the scheduling horizon. Note that, at the beginning of the scheduling horizon, the color has already been predetermined for all the in-process lots in TSS and SSP. Therefore, one needs to initialize the values of variables $x_{it}$, $i \in I$, for $t = 1$ to $N + M$. Also, the initialization of variables $a_t$ for the last $F - 1$ periods is required, since at most one IV change can be initiated within $F$ consecutive periods. Note, however, that at the beginning of the scheduling horizon, the IV has already been predetermined for the last $F/2$ slots of the SSP reactor only, since it takes $F/2$ periods for an IV changeover to take place. Yet, only the value of variable $z_t$, for $t = N + M$ needs to be initialized, since the remaining $(F/2) - 1$ values are determined through constraint sets (7)-(8) and variables $a_t$. As a consequence, the final grade that will be produced in the first $F/2$ periods of the scheduling horizon is already predetermined, too. Constraint sets (33)-(35) initialize the inventories in the LFSS silos and the warehouse at the beginning of the scheduling horizon.

$$x_{it} \text{ binary};\ i \in I, t = 1,\ldots, T \tag{36}$$

$$y_{jt} \text{ binary};\ j \in J, t = N + M + 1,\ldots, T + (F/2) \tag{37}$$

$$a_t \text{ binary};\ t = N + M\text{-}F + 2,\ldots, T \tag{38}$$

$$z_t \text{ binary};\ t = N + M,\ldots, T + (F/2) \tag{39}$$

$$W_{qjt} \text{ binary};\ q \in Q, j \in J, t = N + M,\ldots, T \tag{40}$$

$$g_{qjt} \text{ binary};\ q \in Q, j \in J, t = N + M + 1,\ldots, T \tag{41}$$

$$G_{qjt} \geq 0\ , q \in Q, j \in J, t = N + M + 1,\ldots, T \tag{42}$$

$$R_{jt} \geq 0\ , j \in J, t = N + M,\ \ldots, T \tag{43}$$

$$S_{qjt} \geq 0\ , q \in Q, j \in J, t = N + M,\ldots, T \tag{44}$$

$$b_{qjt} \geq 0\ , q \in Q, j \in J, t = N + M + 1,\ldots, T \tag{45}$$

$$f_{qjt} \geq 0\ , q \in Q, j \in J, t = N + M + 1,\ldots, T \tag{46}$$

$$h_{qjt} \geq 0\ , q \in Q, j \in J, t = N + M + 1,\ldots, T \tag{47}$$

Finally, constraint sets (36)-(41) and (42)-(47) impose the integrality and the nonnegativity of the decision variables, respectively. Note that the indexing of variables $y_{jt}$ begins from $t = N + M + 1$ instead of $t = N + M + (F/2) + 1$, in order to keep record of the final grade produced during the first $F/2$ periods, too, which was actually determined by the production schedule of the previous horizon.

Note that in the above formulation we have assumed that at the beginning of the scheduling horizon, the plant is in the state that it was left off at the end of the previous horizon, because this is the usual situation encountered in practice. There also exists the situation where the plant is just beginning its operations after a long shutdown, in which case, all the slots of TSS and SSP are empty and possibly the silos and the warehouse are at very low or even zero levels. This situation is very rare in practice and is typically encountered after a major breakdown or after the yearly maintenance of the plant. When the plant is starting up after a long shutdown, the main concern is to stabilize the process and get the production going, rather than solving the scheduling problem. In principle, however, our model can still address the scheduling problem during the startup (or warm up) period, by letting period 1 (instead of period $N + M + 1$) be the first period of the scheduling horizon and appropriately adjusting the sets of time indices for which the constraints hold.

Also note that constraint sets (24), (25) and (27) ensure that the demand for silo trucks, bulk containers and big bags is satisfied for each period of the scheduling horizon. The strict requirement for on-time satisfaction of the demand stems from the current practice of the plant that motivated this work. Specifically, the customers of the plant schedule to send their own (or third party) trucks or containers to pick up their orders on specific periods, and can not afford to wait. This requirement may seem restrictive, because it may lead to infeasibilities, but in practice, it does not pose a problem, because the capacities of the LFSS and the warehouse are big enough to absorb any reasonable variations in the demand. Moreover, the careful choice of safety stock levels for each grade and inventory stage (LFSS and warehouse) can help minimize the number of changeovers in the long run, while preventing stockouts and production process blocking due to the lack of storage space. In the following section, we present an application in which we set the scheduling horizon equal to one week that is discretized into 42 4-hour periods, and solved our model sequentially 24 times (weeks), i.e., for a total of 6 months, where at the beginning of each week, the state of the system was set equal to the state that it ended up in the previous week. We used real demand data for each week, and we did not encounter any infeasibility problems. The safety stock levels were carefully chosen by modeling and solving the continuous-process scheduling problem as a *Stochastic Economic Lot Scheduling Problem* (SELSP), as described in Liberopoulos et al. (2009).

Still, in applications where the on-time satisfaction of demand is not a strict requirement, we can easily modify our model, by including in the objective function the following penalty cost term for not satisfying the demand on time:

$$e \sum_{t=N+M+1}^{T} \sum_{j \in J-\{3\}} \sum_{\tau=N+M+1}^{t} (dST_{j\tau} - \sum_{q \in Q} f_{qj\tau}) + (dBC_{j\tau} - \sum_{q \in Q} h_{qj\tau}) + (dBB_{j\tau} - db_{j\tau}),$$

where $e$ denotes the stockout penalty cost coefficient, and $db_{jt}$ denotes the quantity of product $j$ that is used to satisfy the demand for big bags in period $t$. In this case, constraints (24), (25) and (27) need to be modified, as follows:

$$\sum_{\tau=N+M+1}^{t} dST_{j\tau} \geq \sum_{\tau=N+M+1}^{t} \sum_{q \in Q} f_{qj\tau}, j \in J, t = N + M + 1, \ldots, T$$

$$\sum_{\tau=N+M+1}^{t} dBC_{j\tau} \geq \sum_{\tau=N+M+1}^{t} \sum_{q \in Q} h_{qj\tau}, j \in J, t = N + M + 1, \ldots, T$$

$$R_{jt} = R_{jt-1} + \sum_{q \in Q} b_{qjt} - db_{jt} \text{ }, j \in J, t = N + M + 1, \ldots, T$$

and the following constraint must be added to the model:

$$\sum_{\tau=N+M+1}^{t} dBB_{j\tau} \geq \sum_{\tau=N+M+1}^{t} \sum_{q \in Q} db_{qj\tau} \text{ }, j \in J, t = N + M + 1, \ldots, T.$$

Finally, we may further modify our model in a similar manner, by replacing the hard constraints (21) and (29), which require that the inventory levels at the end of the horizon be no less than the safety stock levels, with an extra term in the objective function, that penalizes any negative deviations of the inventory levels at the end of the horizon from the safety stock levels.

# 4. Application of the Model

In this section, we illustrate the application of the MILP model that we developed in the previous section on a problem instance drawn from the operation of the plant that inspired this work. The production rate of the facility is 200 tons/day, which is what the plant uses most of the time, although in the long run it can vary between 180 and 220 tons/day. The color changeover transition time between L and D in POLY is 4 hours, while the IV changeover transition between low and high IV in SSP is 24 hours. Both transition times are divisible by 4; hence, for the purposes of time discretization, we use a 4-hour time period. This makes $B$ = 1, $F$ = 6, and the production rate equal to 33.3 tons/period. Note that a 4-hour period is also convenient because it is a divisor of a 24-hour day and of a typical 8-hour work-shift.

The active silo at the TSS has a capacity of 430 tons but is usually less than half full. With this in mind, we assume that at the beginning of the scheduling horizon it has 200 tons of material in it. This initial quantity can be divided into $N$ = 6 identical slots, each with a capacity of 33.33 tons (the amount produced in a period). Similarly, the SSP reactor, which has a capacity of 200 tons, can be divided into $M$ = 6 identical slots, each with a capacity of 33.33 tons.

In the actual operation of the plant, production is scheduled on a weekly basis, because at the end of each week, the demand during the following week is known with certainty. With this in mind, we use a scheduling horizon of one week, i.e., 42 time periods. Given that $N$ = $M$ = 6, the first period of the scheduling horizon is period 13 (= $N$ + $M$ + 1), and the last period, $T$, is period 54 (= $N$ + $M$ + 42). The values of the other problem parameters are $Z0$ = 1, $S_{max}$ = 430 tons, $S_{min}$ = 1 ton, $R_{max}$ = 3500 tons, $u_{ST}$ = 224 tons, $u_{BC}$ = 69.2 tons, $u_{BB}$ = 40 tons, $c$ = 1, $d$ = 1.

We solved the MILP model sequentially, for 24 weeks, i.e., 6 months, using real demand data. For space consideration, we do not show the demand values for each period; instead, in Table 2, we show the sample mean and standard deviation of the daily demand, for each grade and demand type. Note that the total mean daily demand for all grades and types is ~195 tons, which is slightly below the production rate of 200 tons per day. This small difference between production capacity and demand is due to the unavoidable production of grade 3 (G), which takes away some of the production capacity. As was mentioned earlier, there is no scheduled demand for grade G; in reality, however, the plant occasionally removes the accumulated inventory of grade G by selling it at a lower price to interested buyers. Also, note that grade 2 (SD) is only demanded in big bags.

**Table 2.** Sample mean and standard deviation of the daily demand for each grade and demand type

| Grade $j$ | 1 | | 2 | | 4 | | Sum of |
|---|---|---|---|---|---|---|---|
| | mean | std. dev. | mean | std. dev. | mean | std. dev. | means |
| Demand in silo trucks | 25.82 | 41.00 | 0 | 0 | 17.67 | 29.52 | 43.49 |
| Demand in bulk containers | 29.96 | 41.52 | 0 | 0 | 16.13 | 19.63 | 46.09 |
| Demand in big bags | 25.27 | 32.15 | 45.43 | 58.45 | 34.37 | 46.77 | 105.07 |
| Total | 81.05 | | 45.43 | | 68.17 | | 194.65 |

In each week (run), the state of the system at the beginning of the scheduling horizon was set equal to the state of the system at the end of the previous run. The system at the beginning of the scheduling horizon of the first run was set to some reasonable initial state, which we do not show here for space considerations.

To obtain reasonable values for the safety stock levels, we modeled the scheduling problem as an SELSP, as in Liberopoulos et al. (2009), and solved it numerically. We then used the results of the SELSP solution to compute the safety stock levels. The details of these computations are shown in the Appendix. The resulting values of the safety stock levels are shown in Table 3.

**Table 3.** Safety stocks at the LSSS and the warehouse, and initial quantities in the warehouse

| Grade $j$ | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| Safety stock $SS_{min\,j}$ | 450 | 0 | 0 | 450 |
| Safety stock $R_{min\,j}$ | 250 | 880 | 0 | 450 |

The results of all 24 runs are shown in Figures 3-6. More specifically, Figure 3 shows the trajectory of the final grade produced in each period. Throughout the entire 6-month period, there were 45 grade changeovers (20 color and 25 IV changeovers), which amounts to approximately 1.875 changeovers per week. As seen from Table 2, the mean demand for SD was relatively low, accounting for approximately 23 percent of the total mean demand. For this reason, most of the changeovers were between WG and FH, producing some SD and G along the way.

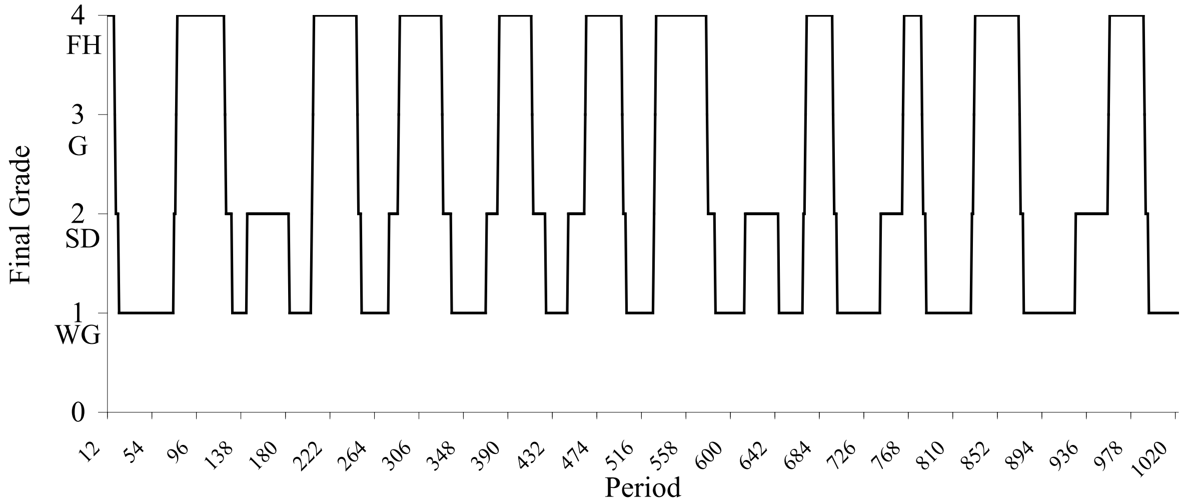


**Figure 3.** Evolution of the final grade produced in each period

Figures 4-6 show the evolution of the inventory levels in the LFSS silos and the warehouse at the end of each week. From Figures 4 and 5, it can be seen that the LFSS silos were used as dedicated storage buffers throughout the entire 6-month period. More specifically, three silos (1, 3 and 5) contained WG throughout the entire 6-month period, three silos (4, 6 and 7) contained FH, one silo (8) contained SD, and one silo (2) contained G. In all but one week (week 5), grade G was emptied from silo 2 and filled in big bags which were then stored in the warehouse. There, its inventory kept increasing, because we had assumed that there is no demand for it, as was mentioned above. In fact, the amount of grade G produced was close to 4 tons per day on average (= 20 color changeovers/24 weeks × 1 period/changeover × 33.33 tons/period ÷ 7 days/ week), which approximately covers the difference between average daily demand and production capacity.

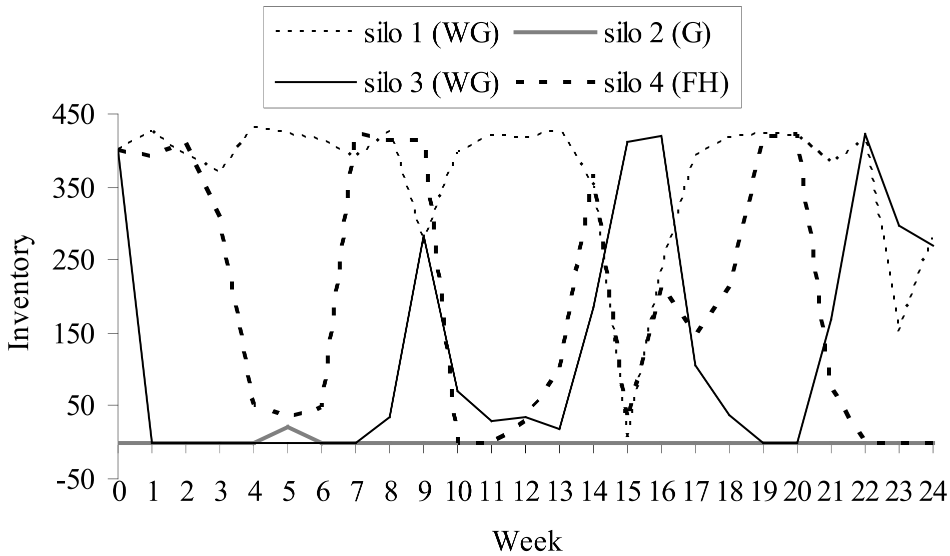


**Figure 4.** Evolution of inventory level in silos 1-4 of the LFSS at the end of each week

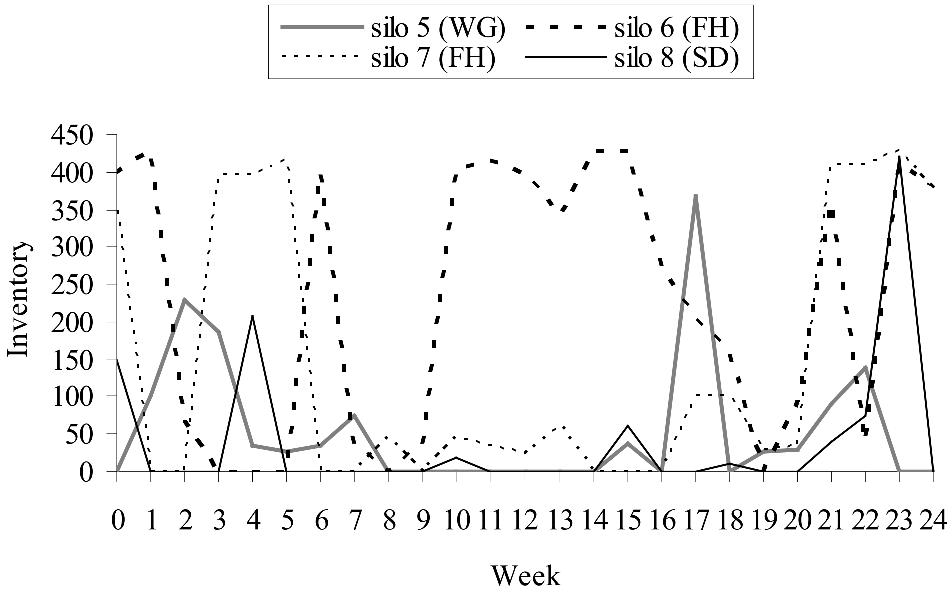


**Figure 5.** Evolution of inventory level in silos 5-8 of the LFSS at the end of each week

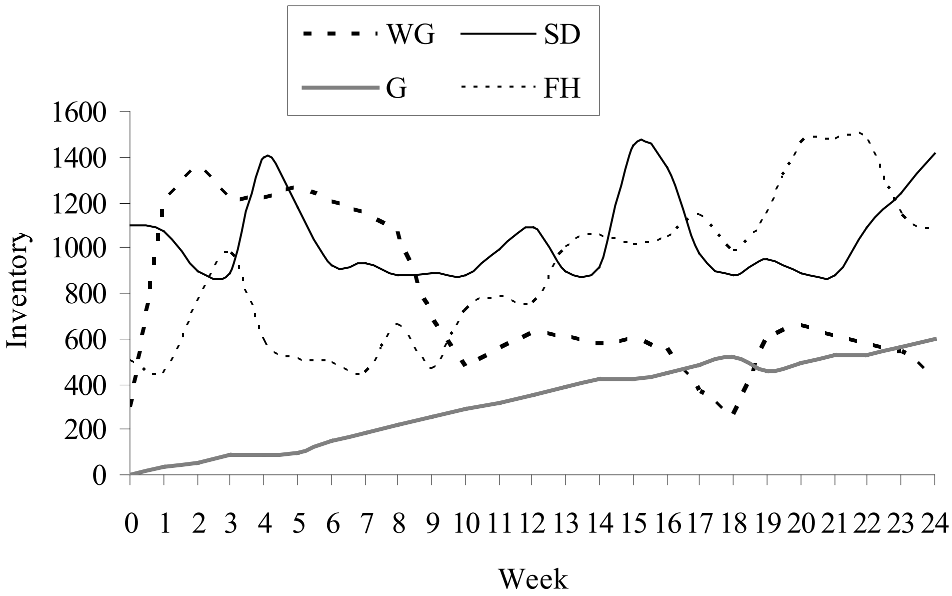


**Figure 6.** Evolution of inventory level in the warehouse at the end of each week

In Figures 4-6, the inventory levels at the end of each week are connected with a straight line to help visualize their weekly evolution. The variation of the inventory levels from period to period within each week, however, was far from linear, at least for the LFSS silos. Figures 7-9 show the evolution of inventory levels in the LFSS silos and the warehouse at the end of each period, during week 5 (periods 180-222). For example, from Figure 7 , it can be seen that the inventory level of WG in silo 3 started and ended at zero in week 5, but went up to approximately 240 tons in the middle of that week. The inventory levels in the warehouse, however, were kept more or less stable during that week, as seen from Figure 8.

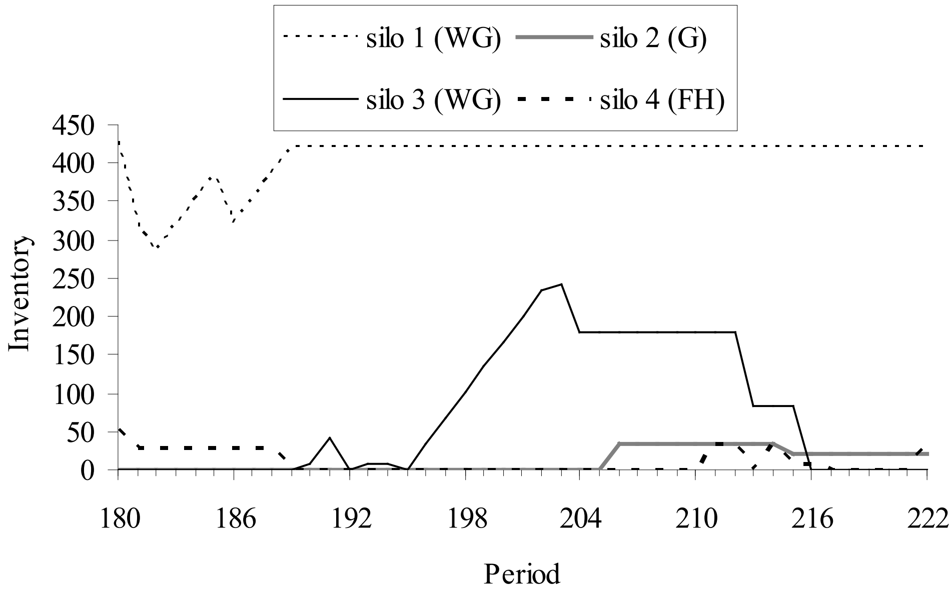


**Figure 7.** Evolution of inventory level in silos 1-4 of the LFSS at the end of each period in week 5

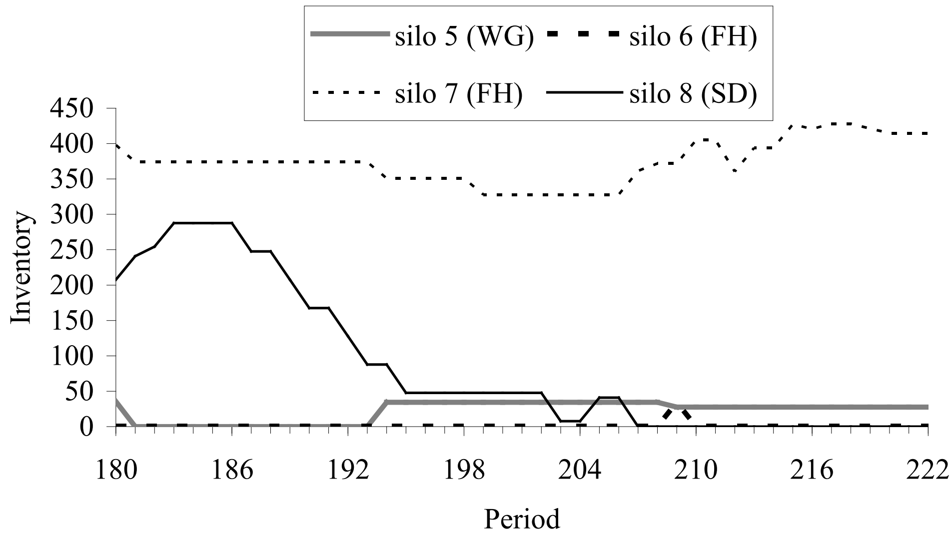


**Figure 8.** Evolution of inventory level in silos 5-8 of the LFSS at the end of each period in week 5

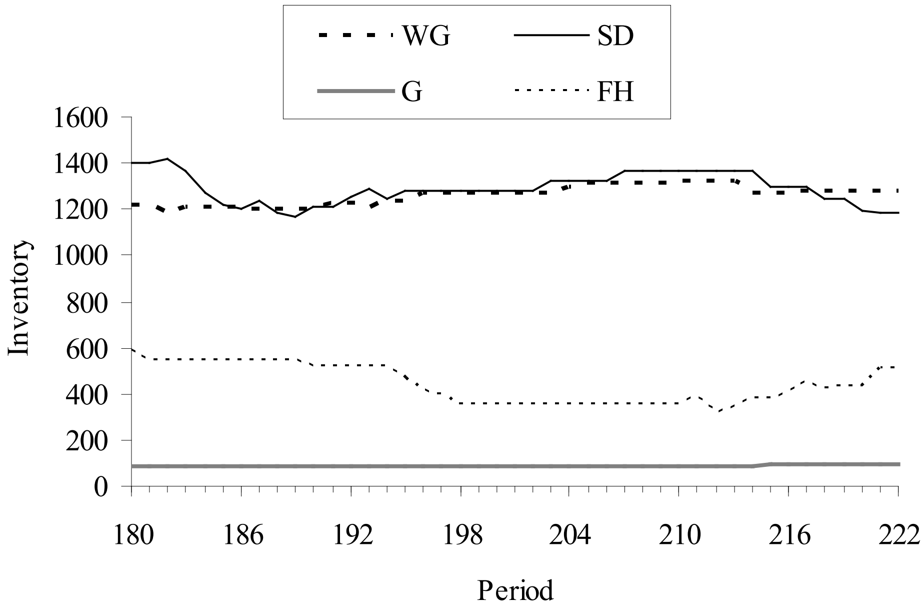


**Figure 9.** Evolution of inventory level in the warehouse at the end of each period in week 5

For the completeness of presentation, Figure 10 shows the demands per grade and type for each period of week 5. Also, Figure 11 shows in detail the optimal color setting at POLY, the optimal IV setting at SSP, and the final grade coming out of SSP, based on the optimal color and IV combination, in each period of week 5. From Figure 11, note that during the changeover transition from high to low IV, which was initiated at the beginning of period 181 and lasted through period 186, the intermediate grade produced was divided into two halves, where the first half (periods 181-183) was characterized as SD and the second half (periods 184-185) as WG. Also note that the color changeover that was initiated at the beginning of period 194 resulted in the production of grade G in period 206, i.e., 12 periods later.

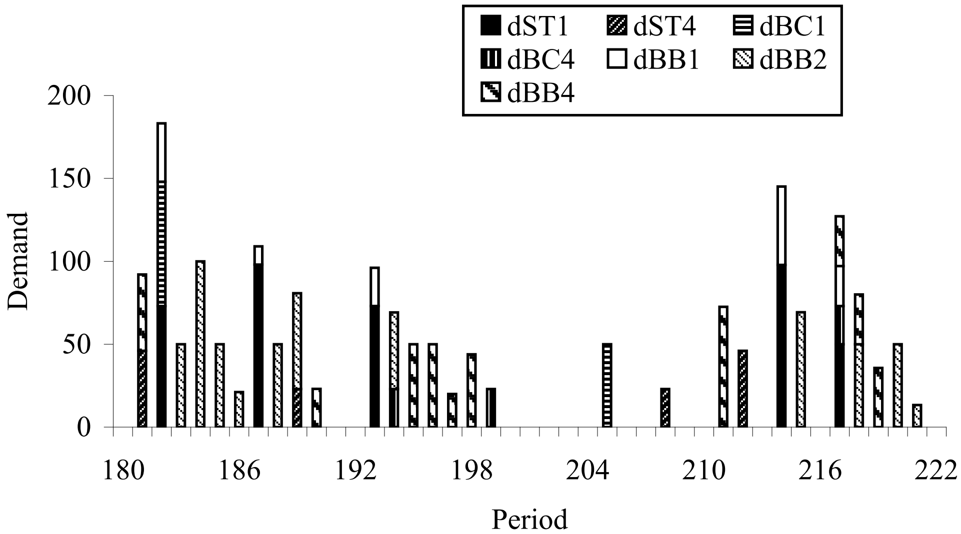


**Figure 10.** Scheduled demand per grade and type for each period in week 5

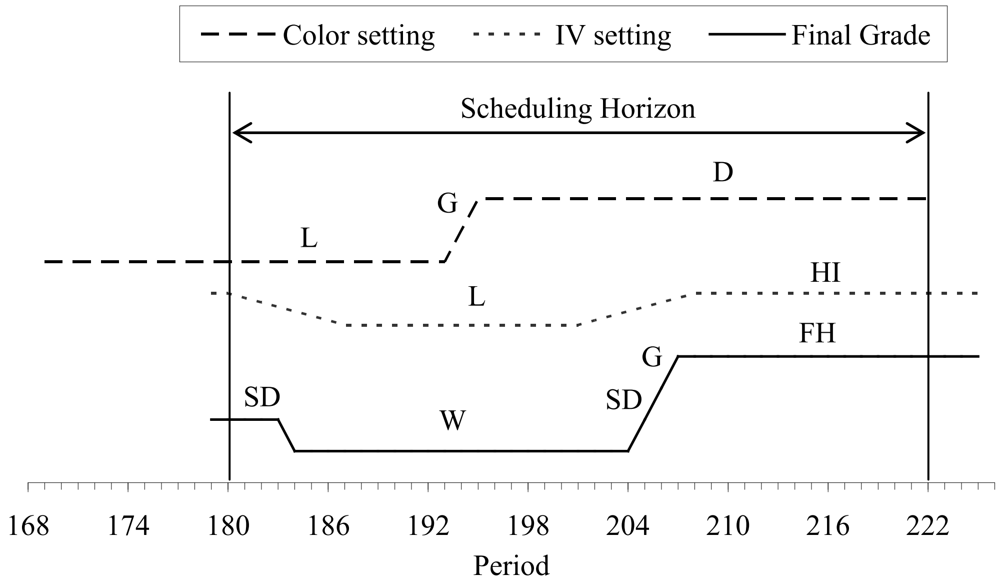


**Figure 11.** Color setting at POLY, IV setting at SSP and final grade produced in each period of week 5

Before closing this section, a few words about the computational effort to reach an optimal solution are in order. The results for the 24 runs presented above were obtained in 17.5 seconds per run on average, with a standard deviation of 10.4 seconds, on a Pentium IV/1.8 GHz dual core processor with 1 GB system memory, using AMPL/CPLEX (see Fourer et al., 2002) version 9.1, with default values as the optimization software. The variation of the run times was quite significant, and the minimum and maximum computation times were 4.1 and 40.1 seconds, respectively, implying that the actual values of the problem parameters have a strong influence on the total computational effort.

An increase in the problem size is generally expected to increase the total computational effort. To explore the effect of problem size on the computational time, we solved several instances of the model, where in each instance we set the initial state of the system equal to the state of the system at the end of week 4, and gradually increased the scheduling horizon by one day (6 periods), starting with a horizon of 7 days (42 periods) and ending with a horizon of 14 days (84 periods). In other words, we solved the scheduling problem of week 5, then week 5 plus the first day of week 6, then week 5 plus the first two days of week 6, and so on. The scheduling horizon of the last problem instance was exactly two weeks, corresponding to weeks 5 and 6.

The results are shown in Table 4. As can be seen from that table, the computational time increases significantly with the size of the problem, although not in all cases, which reveals that the size of the problem alone is not indicative of the computational effort needed to reach an optimal solution; the actual values of the problem parameters have a strong influence on the total computational effort too, as was mentioned above. An interesting observation from Table 4 is that the objective function (number of changeovers) remains at 3 for all instances. This means that 3 changeovers are optimal, whether we schedule production for week 5 alone or for weeks 5 and 6 together, assuming that we know the demands for both weeks. Note that in the original solution shown in Figure 3, where we sequentially solved the MILP problem for each week, the optimal number of changeovers for weeks 5 and 6 (periods 180-221 and 222-263) was 3 and 2, respectively, yielding a total of 5 changeovers. This example reveals the potential benefits from extending the scheduling horizon for which demand information is available.

**Table 4.** Effect of increasing the length of the scheduling horizon

| Scheduling Horizon (periods) | Time (secs) | Objective Function |
|---|---|---|
| 42 | 17.74 | 3 |
| 48 | 50.62 | 3 |
| 54 | 55.14 | 3 |
| 60 | 41.37 | 3 |
| 66 | 81.13 | 3 |
| 72 | 62.49 | 3 |
| 78 | 154.23 | 3 |
| 84 | 161.55 | 3 |

# 5. Conclusions

We developed an MILP model for the production scheduling of a multi-grade PET processing chemical plant. We also presented an application of the model on a real case study, along with some discussion that provides insight into its behavior. The model minimizes the cost associated with the number of grade changeovers, while also ensuring that the capacity constraints of the problem are not violated and that the demand for final products is satisfied on time. The model incorporates all aspects of the problem under consideration and can be easily extended to address additional ones that may arise in different situations, because of the large number of decision variables that enhances its flexibility. We believe that the main contribution of this work is that it addresses efficiently an important practical application, whose solution exhibits high complexity.

A number of possible directions for future research arise from this work. Firstly, one could try to develop a continuous-time model formulation for this problem and compare its results to those of the discrete-time model that we present here. Our guess is that the development of such a model would be demanding and would not necessarily be computationally more efficient than the present discrete-time model. It would, however, represent more accurately the real production and storage process, which is continuous in nature. A second possible direction would be to relax some of the hard constraints, e.g. the on-time delivery of demand constraints (24), (25) and (27) and the safety stock constraints (21) and (29), as was discussed at the end of Section 3, and see if this leads to significant benefits. Another possible direction would be to develop a more accurate SELSP formulation than the one presented in Liberopoulos et al. (2009) to better design the safety stock levels, or resort to some stochastic integer programming technique to solve the scheduling problem under uncertainties. A recent work relevant to this subject is due to Sand and Engell (2004), who utilize two-stage stochastic integer programming techniques to solve scheduling problems of flexible chemical batch processes that exhibit uncertainties. Finally, one could try to fit the scheduling model developed in this paper within a broader planning and supply chain framework, e.g., as discussed in Kallrath (2002).

## Acknowledgements

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## Appendix

In this section, we present a methodology for computing the safety stock levels for the LFSS silos and the warehouse. This methodology is based on the solution of an SELSP formulation of a simplified version of a continuous-process scheduling problem, such as the one presented in this paper, introduced in Liberopoulos et al. (2009).

More specifically Liberopoulos et al. (2009) study a variant of the SELSP in which a single production facility must produce several grades to meet random stationary demand for each grade from a common FG inventory buffer with limited storage capacity. Demand that can not be satisfied directly from inventory is lost. Raw material is always available, and the production facility produces at a constant rate. When the facility is set up to produce a particular grade, the only allowable changeovers are from that grade to the next lower or higher grade. All changeover times are deterministic and equal to each other. There is a changeover cost per changeover occasion, a spill-over cost per unit of product in excess, whenever there is not enough space in the FG buffer to store the produced grade, and a lost-sales cost per unit short, whenever there is not enough FG inventory to satisfy demand. They model the SELSP as a discrete-time *Markov Decision Process* (MDP), where in each time period it must be decided whether to initiate a changeover to a neighboring grade or keep the setup of the production facility unchanged, based on the current state of the system, which is determined by the current setup of the facility and the FG inventory levels of all the grades. The goal is to minimize the infinite-horizon expected average cost. For 2-grade and 3-grade problems they numerically solve the resulting MDP problem using successive approximations. The solution includes the optimal state-dependent policy and the optimal differential cost (value function) for each state of the system. The optimal policy partitions the state space into different regions, each characterized by a different optimal changeover action. The FG inventory levels at which the value function is minimized for a given setup state are the "ideal" target inventory levels for that setup state and in that sense can be thought of as the optimal safety stock levels for that state. In other words, the optimal safety stock levels really depend on the setup state of the facility.

We used the above methodology to find the optimal safety stock levels for a 3-grade system, where the three grades are WG, SD, and FH. To this end, we discretized the inventory space and time, and we used a demand distribution for each grade based on the real demand data for 6 months that we had available, without differentiating between the individual types of demand (silo trucks, bulk containers and big bags). The optimal safety stock level of grade $j$, when the facility is set up to produce grade $i$, denoted by $I_{\min,i,j}$, is shown in Table 5. Note that the safety stock levels strongly depend on the setup of the facility. For example, the safety stock level for WG is only 60 tons, if the facility is setup to produce WG, but goes up all the way to 1410 tons, if the facility is setup to produce FH.

**Table 5.** Optimal safety stock level of grade $j$, when the facility is set up to produce grade $i$, $I_{\min,i,j}$

| Grade $j$ | WG | SD | FH |
|---|---|---|---|
| $I_{\min,\mathrm{WG},j}$ | 60 | 660 | 1410 |
| $I_{\min,\mathrm{SD},j}$ | 660 | 90 | 930 |
| $I_{\min,\mathrm{FH},j}$ | 1410 | 1680 | 90 |

In the MILP formulation that we developed in this paper, we assumed that the safety stock levels do not depend on the setup state of the system. With this in mind, we used the results of Table 5 to compute a weighted average safety stock level for each grade $j$ over all setup states, denoted by $I_{\min,j}$, where as weight for each setup state we used the percentage of time that the facility is set up in that state, given by its market share. Thus, if we let $E[d_j]$ denote the mean daily demand (see Table 2) and $p_j$ denote the market share of grade $j$, we have

$$I_{\min,j} = \sum_{i\in\{\mathrm{WG,SD,FH}\}} p_j I_{\min,i,j} \text{ }, j \in \{\mathrm{WG, SD, FH}\}$$

where

$$p_j = E[d_j] \Big/ \sum_{k\in\{\mathrm{WG,SD,FH}\}} E[d_k] \text{ }, j \in \{\mathrm{WG, SD, FH}\}$$

$$E[d_j] = E_t[dST_{jt}] + E_t[dBC_{jt}] + E_t[dBB_{jt}], j \in \{\mathrm{WG, SD, FH}\}$$

The results of the above computations are shown in Table 6.

**Table 6.** Mean daily demand, $E[d_j]$, market share, $p_j$, and safety stock level, $I_{\min,j}$, for each grade $j$

| Grade $j$ | WG | SD | FH |
|---|---|---|---|
| $E[d_j]$ | 81.05 | 45.43 | 68.17 |
| $p_j$ | 0.4164 | 0.2334 | 0.3502 |
| $I_{\min,j}$ | 672.83 | 884.17 | 835.69 |

Finally, in the MILP formulation that we developed in this paper, we assumed that the safety stock levels depend on the FH inventory stage (LFSS or warehouse) of the system, whereas in the SELSP formulation and solution it was assumed that there is a single FG inventory stage. With this in mind, we allocated the safety stock level, $I_{\min,j}$, shown in Table 6, to the LFSS silos and to the warehouse in proportion to their demand share. Thus, if we let $p_{\mathrm{LFSS},j}$ and $p_{\mathrm{W},j}$ denote the fraction of the demand for grade $j$ requested from the LFSS silos and the warehouse, respectively, we have

$SS_{\min j} = p_{\mathrm{LFSS},j}\, I_{\min,j},\ j \in \{\mathrm{WG, SD, FH}\}$

$R_{\min j} = p_{\mathrm{W},j}\, I_{\min,j},\ j \in \{\mathrm{WG, SD, FH}\}$

where

$p_{\mathrm{LFSS},j} = (E_t[dST_{jt}] + E_t[dBC_{jt}])/E[d_j],\ j \in \{\mathrm{WG, SD, FH}\}$

$p_{\mathrm{W},j} = E_t[dBB_{jt}]/E[d_j],\ j \in \{\mathrm{WG, SD, FH}\}$

The results of the above computations are shown in Table 7.

**Table 7.** Fraction of the demand requested from the LFSS silos and the warehouse, and safety stock level in the LFSS silos and the warehouse, for each grade $j$

| Grade $j$ | WG | SD | FH |
|---|---|---|---|
| $p_{\mathrm{LFSS},j}$ | 0.6882 | 0 | 0.4958 |
| $p_{\mathrm{W},j}$ | 0.3118 | 1 | 0.5042 |
| $SS_{\min j}$ | 463.05 | 0 | 414.35 |
| $R_{\min j}$ | 209.78 | 884.17 | 421.34 |

The safety stock levels that we used in the numerical example in Section 4, shown in Table 3, were set approximately equal (with some rounding) to the values shown in Table 7.

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